NASA TECHNICAL MEMORANDUM

NASA TM-78890

(NASA-TM-78890) ADHESION OF A BIMETALLIC INTERFACE Ph.D. Thesis - Case Western Reserve Univ. (NASA) 332 p HC A15/MF A01 CSCL 11A

N78-29214

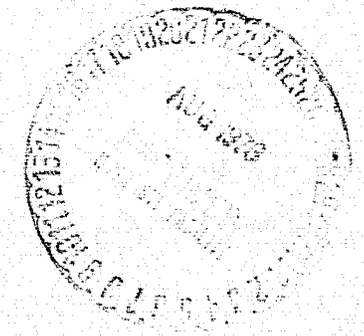
Unclas
G3/26 27213

NASA TM-78890

ADHESION OF A BIMETALLIC INTERFACE

by John Ferrante
Lewis Research Center
Cleveland, Ohio 44135

June 1978



ADHESION AT A BIMETALLIC INTERFACE

by

JOHN FERRANTE

Submitted in partial fulfillment of the requirements

for the Degree of Doctor of Philosophy

Thesis Advisor: Phillip L. Taylor

Department of Physics

CASE WESTERN RESERVE UNIVERSITY

August 1978

ADHESION OF A BIMETALLIC INTERFACE

Abstract

by

John Ferrante

The Hohenberg-Kohn and Kohn-Sham formalisms are used to examine adhesive binding (binding energy as a function of separation) between combinations of simple metals in contact. The metals examined are Al (111), Zn (0001), Mg (0001), and Na (110). The adhesion of dissimilar metal contacts of Al, Zn, Mg are examined using a simple overlap model with the Hohenberg-Kohn formalism along with Smith's parameterized density. The adhesion of similar metal contacts between Al, Zn, Mg, and Na are examined completely self-consistently in an entirely ab initio calculation using the Kohn-Sham formalism. Crystallinity is included using the Ashcroft pseudopotential via first order perturbation theory for the electron-ion interaction; and the ion-ion interaction is included exactly via a lattice sum. The adhesive binding energy was determined both in the local-density approximation and including gradient corrections to the exchange and correlation energy using the gradient corrections of Rasolt and Geldart. Binding was found in all cases, In dissimilar metal contacts the interfacial bonding energy was greater than that in the weaker material predicting the experimentally observed possibility

of metallic transfer. The nonzero position of the binding energy minimum in like metal contacts is explained in terms of consistency between the Ashcroft pseudopotential and the bulk charge density. Good agreement with experimental surface energies is obtained in the self-consistent calculation when nonlocal terms in the exchange and correlation energies are included. Good agreement is also obtained with experimental elastic stiffness constants as compared with values obtained from the curvature of the binding energy curves near the minimum. The range of the strong chemical bonding force was found to be of the order of 0.2 nanometers. Strong similarities with molecular binding are found when examining the kinetic and potential energy contributions to the binding energy as compared with the Ruedenberg and Feinberg examination of molecular binding in hydrogen. Excellent agreement is obtained with the Budd-Vannemenus sum rule as compared with the jellium force at zero separation indicating a high degree of self-consistency.

DEDICATION

I would like to dedicate this work to my dear wife, Patrica, for her support and confidence.

ACKNOWLEDGEMENTS

I would like to thank Prof. P. L. Taylor for his support and his patience which would make Job seem hyperactive, Dr. John R. Smith for years of collaboration and friendship, Dr. Steven V. Pepper for many helpful discussions, friendship, and encouragement, and Dr. Donald H. Buckley for creating a working atmosphere where venturing into untried areas is supported.

CONTENTS

LIST OF TABLES

LIST OF FIGURES

BACKGROUND

Friction and wear are of great technological importance. Adhesion, the mutual attractive force between similar or dissimilar materials when brought into contact is of fundamental importance to friction and wear [1,2,3]. In spite of the importance of metallic adhesion, little work has been done to describe the nature of the strong attractive force between metals in contact or at small separations. This has been due in part to the lack of theoretical techniques for modeling metal surfaces, the lack of experimental data on clean metals and the complexities involved in friction, wear, and adhesion experiments. The experimental data available in the literature is at best only statistically repeatable, i.e., a sufficient number of experiments will give a most probable value. The eruption of surface oxides during rubbing which results in strong adhesion and thus the generation of wear particles is at best a random process. A number of difficulties exist even in adhesion experiments carefully performed in ultrahigh vacuum systems with characterized clean metal surfaces [4,5]. The first difficulty is the fact that real surfaces are not ideally flat, there is a hill and valley structure which makes the true contact area unknown. Second, there are mechanical effects such as recovery of elastically stored energy or bulk defect structures [4] which affect the breaking strength of the bond. Consequently, in order to tackle the complicated problems involved in

metallic adhesion it is necessary to separate its various parts, i.e., binding force, mechanical effects, true surface area, etc. The hope is therefore that an understanding of these isolated phenomena will result in the ability to put the results together and gain a general understanding. In this spirit the present work attempts to understand one phase of the problem, the nature of the clean metal-metal binding force.

Another aspect of the present work is that in previous surface energy calculations only energies at zero and infinite separation were computed. There is a further check which must be performed to verify these results and that is that the binding energy curve must have the correct behavior at zero separation, i.e., zero slope. Therefore, the present work is also a necessary check upon surface energy calculations [6,7]. In addition, a further comparison with experiment can be made in that elastic constants can be estimated from the curvature of the binding energy at the minimum. This study therefore consists of several parts. The adhesive energy (binding energy for two metals versus separation) is calculated for a simple overlap model where the electron gas is held fixed at its bare surface distribution for all combinations of Al, Zn, and Mg. The adhesive energy is then calculated for the more difficult situation allowing relaxation of the electron gas with separation for the like metal pairs Al, Zn, Mg, and Na. Crystallinity is included in both cases. Finally, the constituents of the binding energy are examined for analogies between adhesive and molecular binding.

I - SELF-CONSISTENT CALCULATIONS OF THE ELECTRON NUMBER DENSITY

A. Hohenberg-Kohn-Sham Formalism

The present calculation relies on recent advances in surface theory based on the work of Hohenberg, Kohn, and Sham [8,9] who extended the Thomas-Fermi-Dirac Theory. The Hohenberg-Kohn-Sham Theory is an exact formal variational principle for the total energy of an interacting inhomogeneous electron gas in which the total electron density is the functional variable. A number of excellent reviews of this theory are available in the literature [10,11,12]. In this section we will summarize the highlights of the Hohenberg-Kohn-Sham Formalism.

Hohenberg and Kohn (HK), [8] formulate the total energy of a system of interacting particles as a functional of the electron number density $n(\underline{r})$ for an external potential $v(\underline{r})$. They write

$$E_v[n(\underline{r})] = \int d\underline{r}\, v(\underline{r})\, n(\underline{r}) + F[n(\underline{r})] \tag{1}$$

where

$$F[n(\underline{r})] = T_s[n(\underline{r})] + \tfrac{1}{2}\iint d\underline{r}\, d\underline{r}' \frac{n(\underline{r})\, n(\underline{r}')}{|\underline{r}-\underline{r}'|} + E_{xc}[n(\underline{r})] \tag{2}$$

The functional $T_s[n(\underline{r})]$ is the kinetic energy of the noninteracting electron gas, the second term is the classical Coulomb energy and $E_{xc}[n(\underline{r})]$ is the exchange and correlation energy which accounts for the remainder.

HK then proceed to argue that for a given external potential

$v(\underline{r})$ the energy functional $E_v[n]$ acquires its minimum value for the correct density $n(\underline{r})$ subject to the constraint $\int n(\underline{r})\,d\underline{r} = N$ that states the conservation of the total number of particles. HK then define a new functional $G[n]$ which omits the classical coulomb energy and for a slow variation (though possibly large) in the density $n(\underline{r})$, $G[n]$ is expanded in terms of the gradient of n.

$$G[n(\underline{r})] = \int d\underline{r}\,[g_0(n(\underline{r})) + g_2(n(\underline{r}))\,|\nabla n(\underline{r})|^2 + \cdots] \qquad (3)$$

Where $G[n] = T_s[n] + E_{xc}[n]$. The term $g_0(n)$ represents the energy density of a gas of uniform density, n_+, and is referred to as the local density approximation (LDA). The LDA has been to date the approximation most frequently used in surface energy calculations [12]. More recent surface energy calculations [13,14,15] have been extended beyond the LDA to include the gradient terms represented by $g_2(n(\underline{r}))$. Once an approximation is selected for the exchange and correlation energies, nonlocal energy, and a potential is specified, then the variational principle

$$\delta\left(E_v[n(\underline{r})] - \mu\int d\underline{r}\,n(\underline{r})\right) = 0 \qquad (4)$$

is applied where μ is a Lagrange multiplier. A differential equation for $n(\underline{r})$ can then be derived and solved self-consistently with Poisson's equation enabling the calculation of the electron number density, the electrostatic potential, and the total energy of the system.

Kohn and Sham (KS), [9] have extended the principles in the HK Formalism by considering the variational equations

$$\int \delta n(\underline{r}) \left\{ \phi(\underline{r}) + \frac{\delta T_s[n]}{\delta n} + \mu_{xc}[n] \right\} d\underline{r} = 0 \tag{5a}$$

$$\int \delta n(\underline{r})\, d\underline{r} = 0 \tag{5b}$$

where

$$\phi(\underline{r}) = v(\underline{r}) + \int d\underline{r}' \; \frac{n(\underline{r}')}{|\underline{r} - \underline{r}'|} \tag{6}$$

and

$$\mu_{xc} = \frac{d}{dn} \left(n \epsilon_{xc}(n(\underline{r})) \right) \tag{7}$$

where ϵ_{xc} is the exchange and correlation energy/particle of the uniform electron-gas of density n. Therefore for a given $\phi(\underline{r})$ one obtains a result that is identical to the HK formalism for a system of noninteracting electrons moving in a potential $\phi(\underline{r}) + \mu_{xc}(n(\underline{r}))$. As a consequence they establish a set of one-particle Schroedinger equations (atomic units used throughout $\hbar$ = m = e = c = 1)

$$\left\{ -\frac{1}{2} \nabla^2 + \left[\phi(\underline{r}) + \mu_{xc}(n(\underline{r})) \right] \right\} \psi_i = \epsilon_i \psi_i \tag{8}$$

with a self-consistent potential $\phi(\underline{r}) + \mu_{xc}(n(\underline{r}))$ where

$$n(\underline{r}) = \sum_i |\psi_i(\underline{r})|^2 \tag{9}$$

$\psi_i(\underline{r})$ are the N-lowest lying orthonormal solutions of equation (8). The only approximation in the procedure is that $\varepsilon_{xc}(n)$ is an adequate representation of exchange and correlation effects. Inclusion of nonlocal terms will be considered later.

B. Lang-Kohn Surface Energy Calculations [7]

1. Formulation of the Kohn-Sham Equations

The papers most relevant to the present results are the surface energy calculations of Lang and Kohn (LK) ([7] and references cited therein) and Smith [6]. The LK approach work will be summarized here. The application of Smith's results is discussed in the theory section. LK used the Kohn-Sham Formalism to calculate the surface energy of metals ranging from $r_s = 2$ to $r_s = 6$ where r_s is the radius of the Wigner-Seitz sphere. The surface energy is the energy per unit area required to form a free surface. Alternatively it may be thought of as the energy per unit area required to separate a slab of metal into two pieces along a plane to infinite separation.

LK solved the Kohn-Sham equations for a bare metal surface using the jellium model. In this model the external potential $v(\underline{r})$ is that obtained from the jellium positive charge density $n_+(\underline{r})$. Where

$$n_+(\underline{r}) = \begin{cases} 0 & x > 0 \\ n_+ & x \leq 0 \end{cases} \qquad (10)$$

where x is the dimension perpendicular to the surface and n_+ is the magnitude of the bulk electron density. For this model the electrostatic potential is given by Eq. (6) and is modified to the form

$$\phi(\underline{r}) = \int d\underline{r}' \frac{n(\underline{r}') - n_+(\underline{r}')}{|\underline{r} - \underline{r}'|} \tag{11}$$

therefore $\phi(\underline{r})$ can be determined by Poisson's equation

$$\nabla^2 \phi = -4\pi (n(\underline{r}) - n_+(\underline{r})) \tag{12}$$

The constraint on the total number of particles can be incorporated into the expression via a Lagrange multiplier

$$\delta \left[E_v[n] - \mu \int n(\underline{r})\, d\underline{r} \right] = 0 \tag{13}$$

therefore for the correct density

$$\mu = \frac{\delta E_v[n]}{\delta n(\underline{r})} = \phi(\underline{r}) + \frac{\delta G[n]}{\delta n(\underline{r})} \tag{14}$$

for large N, μ is equal to the chemical potential. Performing a volume average over the metal gives

$$\mu = \bar{\phi} + \bar{\mu} \tag{15}$$

where $\bar{\mu}$ is the bulk chemical potential relative to the mean interior electrostatic potential (in an infinite metal jellium model $\bar{\phi} = 0$). From Eqs. (3) and (13)

$$\bar{\mu} = +\frac{1}{2} k_F^2 + \left. \frac{\delta E_{xc}[n]}{\delta n} \right|_{n = n_+} \tag{16}$$

LK defined

$$V_{eff}(\underline{r}) = \phi(\underline{r}) + \mu_{xc}(n(\underline{r})) \tag{17}$$

in Eq. (8) and labeled the states by the quantum numbers k, k_y, k_z with the following meaning

$$\psi_{k,k_y,k_z}(\mathbf{r}) = \psi_k(x)\, \exp(ik_y y + ik_z z) \tag{18}$$

where for $x \to -\infty$

$$\psi_k(x) = \sin(kx - \gamma(k)) \tag{19}$$

where $\gamma(k)$ is the phase shift introduced by the presence of the surface. The choice of $\mu = 0$ to define the zero of energy gives finally $v_{eff}(x) \xrightarrow[x\to-\infty]{} -1/2\, k_F^2$ from Eqs. (15), (16), and (17) and

$$-\frac{1}{2}\left(\frac{d^2}{dx^2} + v_{eff}(n,x)\right)\psi_k(x) = \frac{1}{2}(k^2 - k_F^2)\,\psi_k(x) \tag{20}$$

Picking the Kohn-Sham form for the exchange energy per particle and the Wigner interpolation formula for the correlation energy per particle of the uniform gas they have

$$\epsilon_{xc} = -\frac{0.458}{r_s} - \frac{0.44}{r_s + 7.8} \tag{21}$$

where

$$n_+^{-1} = \left(\frac{4\pi}{3}\right) r_s^3 \tag{22}$$

Finally converting the sum in Eq. (9) to an integral, they find

$$n(x) = \frac{1}{\pi^2} \int_0^{k_F} dk\, (k_F^2 - k^2)\, |\psi_k(x)|^2 \tag{23}$$

to order L^{-1} where L is the slab length in the x direction normal to the surface. Equations (12), (17), (22), and (23) establish

a self-consistent set of equations that could be used to obtain a solution within the LDA. These equations form the bases for part of the present paper.

2. Surface Energy Calculation

LK used the calculation of the bare surface electron density within the jellium model to calculate the surface energy of the solid. The surface energy was defined as

$$\sigma = \frac{1}{2A}\left[2\left(G[n]+E_{es}[n]\right)-\left(G[n']-E_{es}[n']\right)\right] \tag{24}$$

where $n(\underline{r})$ is the distribution for the bare surface and $n'(\underline{r})$ is the distribution for the uncleaved solid, A is the cross-sectional area of the sample, and E_{es} is the electrostatic contribution to the total energy. The surface energy in the jellium model is

$$\sigma_U = \sigma_S + \sigma_{xc} + \sigma_{es} \tag{25}$$

where

$$\sigma_S = \frac{1}{2\pi^2}\int_0^{k_F} dk\,k\left(\frac{\pi}{4}-\gamma(k)\right) - \int_{-\infty}^{\infty} dx\, n(x)\left[v_{eff}(n,x)-v_{eff}(n,-\infty)\right] \tag{26}$$

This is the equation for the kinetic energy from an expression derived by Huntington [16].

$$\sigma_{xc} = \int_{-\infty}^{\infty} dx\, n(x)\left(\epsilon_{xc}(n(x)-\epsilon_{xc}(n_+)\right) \tag{27}$$

is the exchange and correlation contribution to the surface energy and

$$\sigma_{es} = \int_{-\infty}^{\infty} dx\, \phi(n,x)(n(x) - n_+(x)) \tag{28}$$

is the total electron-jellium contribution to the electrostatic energy.

The result of this calculation was that the system was unbound in the jellium model for $r_s < 4.0$. Consequently, LK introduced two corrections to the jellium energy which include crystallinity. The first which will be discussed in greater detail later was to include the effects of the ion-ion interaction exactly by performing a lattice sum. In this sum the jellium-jellium interaction is subtracted and consequently acts like a background electron gas for the lattice of point positive ions. LK refer to this term as $\delta\sigma_{c\ell}$. The second correction includes the electron-ion interaction via first order perturbation theory. In this the Ashcroft pseudopotential

$$V_{ps}(\underline{r}) = \begin{cases} 0 & r \le r_c \\ -\frac{z}{r} & r > r_c \end{cases} \tag{29}$$

which has been used successfully to calculate bulk properties of simple metals is used to model the electron-ion interaction. The contribution due to the electron-ion interaction for split minus unsplit crystal is given by

$$\delta\sigma_{ps} = \int_{-\infty}^{\infty} dx \, [n(x) - n_+(x)] \, \delta v(x) \tag{30}$$

where $\delta v(x)$ is the average over the y-z plane of the sum of the ionic pseudopotentials of the half lattice minus the potential due to the semi-infinite charge background. Details and criticisms of this result will be presented later. The general approach in the Lang-Kohn calculation is similar to that used in the present study for determining the binding energy versus separation.

II. OTHER SURFACE ENERGY CALCULATIONS

After the initial calculations of Lang and Kohn, an alternate model to explain surface energies was proposed by Schmit and Lucas [17] and Craig [18]. The result of the model was that the dependence of the surface energy on r_s could be explained by the assumption that correlation was dominant. An excellent summary of this model and its implications is presented by Brown and March [12] and references cited therein. The theory expresses the surface energy in terms of the change in the zero point energy of the plasmons and points out that this could be a large contribution. The surface plasmon model has been criticized from a number of standpoints and now has become passé as a criticism of the Lang and Kohn Calculations. The criticisms involved the cutoff wave number selected for surface plasmons, inclusion of dispersion, effects of particle-hole excitations and changes in bulk-plasmon energy. Griffin and Kranz [19] have recently performed a model calculation determining the bulk and surface changes in the plasmons using an infinite-barrier, random-

phase approximation which they argue reflects the situation of a real metal. They conclude that the surface plasmon contribution to the surface energy and the bulk plasmon contribution to the surface energy are of comparable magnitude but of opposite sign thus giving a small net contribution and supporting the work of Lang and Kohn. The Lang-Kohn calculations and related calculations such as the present work are applicable for simple bulk metals where the s-p character of the conduction band is well separated from d-states. Cyrot-Lackmann [20] has successfully predicted trends in surface energies using a tight-binding approximation and an expansion of the density of states in terms of moments for transition metals. Brown and March [12] also give an excellent summary of these calculations.

III. NONLOCAL TERMS IN THE GRADIENT EXPANSION

As indicated in Eq. (3), Kohn and Sham suggested a form for the gradient expansion.

$$E_{xc}[n] = \int \underline{dr}\ \left(A_{xc}[n] + B_{xc}[n]\,|\nabla n|^2\right) \tag{31}$$

Smith and others [21] have pointed out the importance of the gradient terms to surface theory. Until recently an expression for B_{xc} was not available in the range of metallic densities. Because of the importance of these terms there have been a number of recent attempts to include them in surface calculations. Rasolt and Geldart have determined B_{xc} numerically within the random phase approximation [22]. Lau and Kohn [13] have obtained an approximate expression for B_{xc} by requiring that the surface energy for two adjacent

metal films of nearly equal density be the same as that obtained from the electronic polarizability of Vashista and Singwi, [23]. Rasolt, Wang, and Kahn [24] have examined the convergence of the exchange energy by calculating the exchange energy exactly for a Yukawa potential with a finite barrier potential with a barrier height chosen to reproduce the LK density profile. The model potential approach was used since a calculation for real systems would be prohibitively difficult, if not impossible. The results indicate that the gradient term models the exact energy very closely over the entire range of Yukawa screening length λ, whereas the local term is ~15% too high for $\lambda < 0.4\ \lambda_{TF}$ (λ_{TF} = Thomas-Fermi screening length). The agreement is excellent for $r_s = 3$ and is slightly worse for $r_s = 4$. An argument is given for the correlation energy which would be difficult to calculate having the same behavior. Therefore, they conclude that the gradient expansion is an adequate representation of the exact energy.

Rose, et al. [14] have included the gradient expansion self-consistently into the surface energy calculation. Lau and Kohn [13] have included it through perturbation theory. Both found an approximately 50% increase in the energy for aluminum. Rose found only a small change in the electron density by including this term and a small change in the work function. This discrepancy was attributed to the perturbation approach and the fact that small changes in the density can produce large changes in the dipole layer.

Rose, et al. and Lau and Kohn disagree about this correction with regard to how well they represent experimental surface energies.

This results from a conflict in the experimental literature. This will be discussed later in the paper.

Gupta and Singwi [25] have also estimated this term using the gradient expansion and the work of Bvashista and Singwi, and obtained results which are somewhat smaller but agree to within 30%. Perdew, Langreth, and Sahni [26] have used a wave vector analysis rather than a gradient expansion to extend the results beyond the LDA. They again obtain a result which is ~50% smaller using a wave vector analysis. In general, the calculation of this term is quite difficult. The degree of agreement ~50% and that all calculations are in the direction of increasing the surface energy can be taken as confirming the general magnitude and direction of this term. (The Rasolt-Geldert gradient term is included in the present calculation.)

IV. METALLIC INTERFACE CALCULATIONS

The first attempt to calculate interfacial densities and potentials using the Kohn-Sham Formalism was performed by Bennet and Duke [27]. They used a parameterized form for the number density and potential and solved the Kohn-Sham Equations self-consistently by varying parameters. The first attempt to calculate the adhesive energy for a metallic interface was performed by Ferrante and Smith [28,29]. They used the HK Formalism and Smith's [6] parameterization of the electron number density but did not allow relaxation of the electron gas. This work was the first to calculate binding energy versus separation for Al, Zn, Mg, and all possible combinations. Details of this calculation are presented herein. Ferrante and Smith

[30] were the first to obtain a completely self-consistent numerical solution of the Kohn-Sham equations for the case of similar metals in contact versus separation and to include higher order terms in the gradient-expansion self-consistently [31] for the like metal combinations Al, Zn, Mg, and Na. No detailed account of this work is in the literature and will be presented herein. Nieminen [32] solved the Kohn-Sham Equations for the force versus separation for metals ranging from $r_s = 2$ to 6 self-consistently. Vannemenus and Budd [33] solved the HK Equations self-consistently for two jelliums in contact. Rouhani and Schuttler [34] and Mehrotra, Pant and Das [35] and references cited therein calculated the adhesive energy for alkali-metals in contact comparing zero and infinite separation using the HK Formalism and Smith's parameterized density. Finally, Allan, Lannoo, and Dobrzynski [37] estimated the adhesive energy for zero and infinite separation for dissimilar metals in contact using the techniques of Cyrot-Lackmann.

A more detailed discussion of these papers will be presented later in comparison with the present results. The paper will now proceed by application of the Kohn-Sham Formalism to the calculation of binding energy as a function of separation for bimetallic contacts.

THEORY

I - SIMPLE OVERLAP MODEL

A. Model

In this section are described the procedures of Ferrante and Smith [28] for calculating binding energy as a function of separation for similar and dissimilar metal combinations of Al, Zn, and Mg. In this calculation the contribution of electron overlap to the binding energy is presented. The electron density distribution is held fixed for each metal at the distribution for the bare metal case and therefore relaxation of the electron gas is not permitted. It will be shown that this simple approach has some appealing features and gives some surprisingly accurate results. The model is shown schematically in Figure 1 where

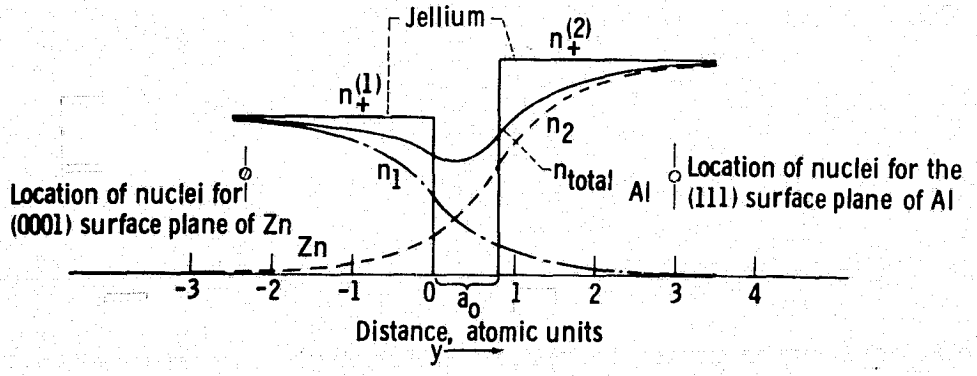


Fig. 1. - Jellium charge density to scale for Al-Zn, n_1 and n_2 denote the metal vacuum electron number densities for Al and Zn, respectively.

where

$$n_1(x) = \left[n_+^{(1)} - \tfrac{1}{2} n_+^{(1)} \exp(\beta_1 x)\right]\theta(-x) + \tfrac{1}{2} n_+^{(1)} \exp(-\beta_1 x)\,\theta(x)$$

$$n_2(x) = \left[n_+^{(2)} - \tfrac{1}{2} n_+^{(2)} \exp(-\beta_2 (x-a)\right]\theta(x-a) + \tfrac{1}{2} n_+^{(2)} \exp(\beta_2 (x-a))\,\theta(a-x) \tag{32}$$

$n(x) = n_1(x) + n_2(x)$ and $\theta(x) = \begin{cases} \theta(x) = 1, & x > 0 \\ \theta(x) = 0, & x < 0 \end{cases}$ is the Heaviside function [37]. The electron density $n(x)$ is the parameterized form used by Smith and β is the exponential decay constant determined by Smith for the bare metal surface. The most densely packed planes are assumed in modeling the density. This assumption is used to minimize the effect of density variations in the y-z plane which are assumed to be uniform.

B. Definition of the Energy

Following the Hohenberg-Kohn Formalism we first define the adhesive binding energy by

$$E_{AD} = \frac{E(\infty) - E(a)}{2A} \tag{33}$$

where

$$E(n) = \int d\underline{r}\, V(\underline{r})\, n(\underline{r}) + \frac{1}{2} \sum_{i,j} \frac{Z_i Z_j}{R_{ij}} + F(n) \tag{34}$$

and $$F(n) = \frac{3}{10}(3\pi^2)^{2/3} \int d\underline{r}\, n^{5/3}(\underline{r}) - \frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} \int d\underline{r}\, n^{4/3}(\underline{r})$$

$$-0.056 \int d\underline{r}\, \frac{n^{4/3}(\underline{r})}{0.079 + n(\underline{r})} + \frac{1}{72} \int d\underline{r}\, \frac{|\nabla n|^2}{n(\underline{r})} + \frac{1}{2} \iint d\underline{r}\, d\underline{r}'\, \frac{n(\underline{r})\, n(\underline{r}')}{|\underline{r} - \underline{r}'|}$$

The first two terms in E[n] are the electron-ion and ion-ion interaction energies and R_{ij} is the distance between ion cores. The first three terms in F[n] are the kinetic and exchange energies and Wigner's interpolation formula for the correlation energy, each for the uniform electron gas. The next term is the next order term in the gradient expansion for the kinetic energy, which is large compared to the correlation energy, and the last term is the classical electrostatic electron-electron interaction energy.

C. Calculation Procedures

The calculation proceeds by first evaluating the energy for jellium and then introducing crystallinity exactly for the ion-ion interaction, and approximately for the electron-ion interaction via perturbation theory following Lang and Kohn. In evaluating the jellium part of the electrostatic energy it is convenient to combine a part of the first term in Eq. (34) with the last term, the classical electron electrostatic energy giving

$$E_{es} = -\tfrac{1}{2}\int dx\, \rho(x,a)\,\phi(x,a) \tag{35}$$

where $\phi(x,a)$ is given by

$$\frac{d^2\phi}{dx^2} = 4\pi\rho(x,a) = 4\pi\left[n_+^{(1)}\theta(-x) + n_+^{(2)}\theta(x-a) - n(x,a)\right]. \tag{36}$$

Once the jellium adhesive binding energies were obtained these energies were modified to correct the jellium electron binding energy to include the effects of the actual ion core potentials via first

order perturbation theory. The Ashcroft pseudopotential is used to give the energy

$$E_{PS} = A\int dx\, \delta v(x,a)\, n(x,a) \tag{37}$$

where $\delta v(x,a)$ is an average over planes parallel to the surface of the difference in potential between an array of pseudopotentials and the jellium and thus is treated as a perturbation in the jellium potential. Details of this calculation are given in Appendix I. In addition, the ion-ion contribution to the total energy is included exactly by a lattice sum.

D. Classical Interaction Energy

The ion-ion interaction energy is then included exactly via a lattice sum using a technique developed by Rao and Kohn [38]. In this sum the interaction energy between the two half spaces for arrays of positive ions having the correct geometrical positions for the planes chosen minus the jellium-jellium interaction energy is calculated. The subtracted jellium-jellium term serves the role of a negative background, thus gives a convergent result.

Formally, the interaction energy is written as

$$W_{int}(a) = \iint \underline{dr}\, \underline{dr}'\, \frac{\rho_1(\underline{r})\,\rho_2(\underline{r}')}{|\underline{r}-\underline{r}'|} \tag{38}$$

where

$$\rho(\underline{r}) = Z\sum_m \delta(x-x_m)\sum_\ell\sum_h \delta(y-y_\ell)\,\delta(z-z_h) - \sigma\sum_m \delta(x-x_m)$$

the subscripts 1 and 2 refer to the two half spaces, z is the

ionic valence, σ is the ionic charge per unit area representing the jellium background. The net density $\rho(\underline{r})$ can then be expanded in a Fourier series in the y-z plane, so that

$$\rho(\underline{r}) = \sigma \sum_{m=1}^{\infty} \delta(x-x_m) \sum_{\ell=-\infty}^{\infty\prime} \sum_{h=-\infty}^{\infty\prime} C_{m\ell h} \exp(i g_\ell y) \exp(i g_h z) \tag{39}$$

the primes in the ℓ and h summations indicate that the term $g_\ell = g_h = 0$ which cancels the jellium background has been omitted from the summation. W_{int} is evaluated for the fcc[111] direction, the hcp[0001] direction and the bcc[110] direction. A sample calculation for the fcc[111] direction, the most difficult of the three, is presented in Appendix II. W_{int}/A is given by:

fcc[111]

$$\frac{W_{int}(a)}{A} = \frac{2\sqrt{6}}{3} Z M_+ \sum_{m=1}^{\infty} \sum_{h=1}^{\infty} \frac{(1+\cos\pi h)}{h} (m-1) X^{-3\alpha m} X^{-\frac{a\alpha h}{d}} \left\{ \cos\frac{\pi h}{3} X^{5\alpha h} \right.$$
$$+ \left(\cos\frac{2\pi h}{3} + \cos\frac{\pi h}{3}\right) X^{4\alpha h} + 3X^{\alpha h} + \left(\cos\frac{\pi h}{3} + \cos\frac{2\pi h}{3}\right) X^{2\alpha h} + \cos\frac{\pi h}{3} X^{\alpha h} \Big\}$$
$$+ \frac{2\sqrt{2}}{3} Z M_+ \sum_{m=1}^{\infty} \sum_{\ell=1}^{\infty} (m-1) \frac{(1+\cos\pi\ell)}{\ell} X^{-3m\ell} X^{-\frac{a\ell}{d}} \left\{ \cos\pi\ell X^{5\ell} \right.$$
$$\left. + (1+\cos\pi\ell) X^{4\ell} + 3X^{\ell} + (1+\cos\pi\ell) X^{2\ell} + \cos\pi\ell X^{\ell} \right\}$$
$$+ \frac{4\sqrt{2}}{3} Z M_+ \sum_{m=1}^{\infty} \sum_{\ell=1}^{\infty} \sum_{h=1}^{\infty} (m-1) \frac{(1+\cos\pi(h+\ell))}{D} X^{-3Dm} X^{-\frac{aD}{d}} \left\{ \cos\frac{\pi h}{3} \right.$$
$$\cdot \cos\pi\ell X^{5D} + \left[\cos\frac{2\pi h}{3} + \cos\frac{\pi h}{3} \cos\pi\ell\right] X^{4D} + 3X^{3D}$$
$$\left. + \left[\cos\frac{\pi h}{3} \cos\pi\ell + \cos\frac{2\pi h}{3}\right] X^{2D} + \cos\pi\ell X^{D} \right\}$$

(40a)

where d is the interplanar spacing, c is the nearest neighbor distance

$x = \exp(-2\pi d/c)$, $D = \sqrt{\ell^2 + h^2/3}$, $\alpha = \sqrt{3}/3$;

hcp[0001]

$$\frac{W_{int}(a)}{A} = 4\beta\sqrt{3}\,Z M_+ \sum_{m=1}^{\infty}\sum_{h=1}^{\infty}(m-1)\,X^{-2\alpha m h}\,X^{-\frac{a\alpha h}{d}}$$
$$\cdot\left\{\cos\frac{2\pi h}{3} + 2X^{2\alpha h} + \cos\frac{2\pi h}{3}\,X^{\alpha h}\right\}$$
$$+ 4\beta Z M_+ \sum_{m=1}^{\infty}\sum_{\ell=1}^{\infty}(m-1)\,\frac{(1+\cos\pi\ell)}{\ell}\,X^{-2m\ell}\,X^{-\frac{a}{d}\ell}\left\{X^{3\ell} + 2X^{\ell} + X^{\ell}\right\}$$
$$+ 8\beta Z M_+ \sum_{m=1}^{\infty}\sum_{\ell=1}^{\infty}\sum_{h=1}^{\infty}(m-1)\,\frac{(1+\cos\pi(h+\ell))}{D}\,X^{-2mD}\,X^{-\left(\frac{a}{d}\right)D}$$
$$\cdot\left\{\cos\frac{2\pi h}{3}\,X^{3D} + 2X^{2D} + \cos\frac{2\pi h}{3}\,X^{D}\right\}$$

(40b)

where $\beta = (\sqrt{3}d)/(45c)$;

bcc[110]

$$\frac{W_{int}(a)}{A} = \frac{\sqrt{2}}{2} Z M_+ \sum_{m=1}^{\infty}\sum_{h=1}^{\infty}(m-1)\,\frac{(1+\cos\pi h)}{h}\cos\pi h\,X^{-2m\alpha h}\,X^{-\frac{\alpha h a}{d}}$$
$$\cdot\left\{X^{3\alpha h} + 2\cos\pi h\,X^{2\alpha h} + X^{\alpha h}\right\} + \frac{Z M_+}{2}\sum_{m=1}^{\infty}\sum_{\ell=1}^{\infty}(m-1)\,\frac{(1+\cos\pi\ell)}{\ell}$$
$$\cdot X^{-2m\ell}\,X^{-\frac{a}{d}\ell}\left\{X^{3\ell} + 2X^{2\ell} + X^{\ell}\right\} + Z M_+ \sum_{m=1}^{\infty}\sum_{\ell=1}^{\infty}\sum_{h=1}^{\infty}(m-1)\,\frac{(1+\cos\pi(h+\ell))}{D}$$
$$\cdot X^{-2mD}\,X^{-\left(\frac{a}{d}\right)D}\cos\pi h\left\{X^{3D} + 2\cos\pi h\,X^{2D} + X^{D}\right\}$$

(40c)

where $D = \sqrt{\ell^2 + h^2/2}$, $\alpha = \sqrt{2}/2$. For the hcp and fcc cases a simplifying approximation which agrees to the exact value (summed to six significant figures) to 1.0 percent is now presented as

$$\frac{W_{int}(a)}{A} = -\frac{2\sqrt{3}Z^2}{c^3}\exp\left(-\frac{4\pi\sqrt{3}}{3c}(d+a)\right) \tag{41}$$

The exact values for the sums are tabulated in Appendix II along with a comparison of the exact values with Eq. (41).

E. The Order of the Error

This simple overlap model might be expected to give reasonably accurate results for $\left[n_+^{(2)}\right]\Big/\left[n_+^{(1)}\right] \approx 1$. It is exact for $a = 0$ and $n_+^{(1)} = n_+^{(2)}$ since expanding $E[n(\underline{r})]$ we have

$$E[M(\underline{r},a)] = E[n] + \int \underline{dr}\,\delta n(\underline{r})\left(\delta E[n]/\delta n(\underline{r})\right)$$
$$+ \frac{1}{2}\iint \underline{dr}\,\underline{dr}'\,\delta n(\underline{r})\delta n(\underline{r}')\left(\delta^2 E[n]/\delta n(\underline{r})\delta n(\underline{r}')\right) + \cdots \tag{42}$$

where δn is the variation of the electron number density. Since $\int \underline{dr}\,\delta n(\underline{r})(\delta E[n]/\delta n) = 0$ by the variational principle, $E[n(x,a)]$ is accurate to second order in δn. As will be seen for the case of like metal pairs, the simple overlap model predicts all of the principle physical features of the binding energy.

II - SELF-CONSISTENT CALCULATION

A. Background

In establishing the theory for the like metal calculation, the presentation will proceed with a more general discussion of dissimilar metals in contact. Then these results will be applied to the

specific case of like metal couples. The case of two dissimilar metals in contact can be represented schematically in an energy diagram as in Figure 2.

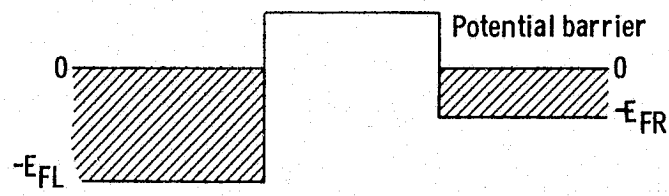


Fig. 2. - Schematic energy diagram for dissimilar metals in contact.

where the shaded areas are the conduction bands, the zero of energy (after equilibration) is taken at the Fermi Level and E_{FL} and E_{FR} are the Fermi energies of the left and right hand metals. We would have for the Schroedinger equation $(-1/2)\,\nabla^2\psi + v_{eff}\psi = E\psi$. The details of v_{eff} will be discussed later but at present we can see that it has a general form that can be represented by Figure 3.

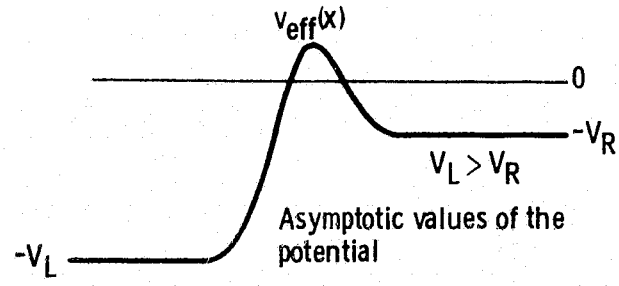


Fig. 3. - General bimetallic potential.

$v_{eff}(x) = \begin{cases} -V_L & x \to -\infty \\ -V_R & x \to \infty \end{cases}$ which is the condition we would have for two dissimilar metals in contact, taking V_R and V_L to be positive.

In the asymptotic regions there are two types of degenerate solutions

$$\begin{aligned} \omega_L &\sim e^{ik_L x} + R_L e^{-ik_L x} && x \to -\infty \qquad 0 > -E > -V_R \\ &\sim T_L e^{ik_R x} && x \to \infty \end{aligned} \tag{43}$$

$$\begin{aligned} \omega_R &\sim T_R e^{-ik_L x} && x \to -\infty \\ &\sim e^{-ik_R x} + R_R e^{-ik_L x} && x \to \infty \end{aligned} \tag{44}$$

where $k_R^L = \sqrt{2\left(V_R^L - E\right)}$, taking E to be positive, and R and T are complex constants. For $-V_R > -E > -V_L$

$$\begin{aligned} \omega_L &\sim e^{ik_L x} + R_L e^{-ik_L x} && x \to -\infty \\ &\sim T_L e^{-\beta_R x} && x \to \infty \end{aligned} \tag{45}$$

where now $|R_L| = 1$ since there can be no net flux into the classically forbidden region and $q_R = \sqrt{2(E - V_R)}$ for $-E < -V_R$ and using the property of the Wronskian that if two solutions correspond to the same energy then the Wronskian of those solutions is independent of X [39]. It can easily be shown that using the asymptotic solutions will give

$$k_L(1-|R_L|^2) = k_R|T_L|^2 \tag{46a}$$

$$k_L|T_R|^2 = k_R(1-|R_R|^2) \tag{46b}$$

$$k_R T_L = k_L T_R \tag{46c}$$

With this frame work we can now examine the asymptotic form of the electron number density in each solid. Starting with Eq. (9) we have $n(\underline{r}) = \sum_{i=1}^{N} |\psi_i(\underline{r})|^2$. Converting the sum to an integral we have $n(\underline{r}) = \frac{2}{(2\pi)^3}\sum_{j=1}^{2}\int d^3\underline{k}|\psi_k^j|^2$ where the summation index j is over the two degenerate solutions. Using cylindrical coordinates we have

$$n(\underline{r}) = \frac{2}{(2\pi)^3}\sum_{j=1}^{2}\int_0^{2\pi}\int_0^{k_F}\int_0^{\sqrt{k_F^2-k^2}} d\phi\, k_\parallel\, dk_\parallel\, dk\, |\psi_k^j|^2. \tag{47}$$

Integrating gives

$$n(\underline{r}) = \frac{1}{4\pi^2}\sum_{j=1}^{2}\int_0^{k_F} dk\,(k_F^2-k^2)|\psi_k^j|^2.$$

Taking the left hand metal, using the asymptotic form for the wave function, Eq. (46) and the definition of the bulk density in terms of k_F we get

$$n(X) = \frac{1}{2\pi^2} \int_0^{k_{FL}} dk_L (k_{FL}^2 - k_L)^2 \, Re\left(R_L(k_L) e^{2ik_L X}\right) \tag{48}$$

Adawi [40] has shown that the integral has a leading term

$$\Delta n \sim \frac{k_{FL}^2}{2\pi^2 X^2} \, Re\left(R_L(k_{FL}) e^{2ik_{FL}X}\right); \qquad \Delta n = n(X) - n_{+L} \tag{49}$$

The result for the right hand metal is similar. Therefore the electron number density in the bulk of either metal is represented by the bulk density plus terms with decaying oscillations whose wavelength is half the Fermi wavelength and whose amplitude depends on the reflection coefficient evaluated at the Fermi momentum. This result is similar to that obtained by Lang and Kohn [7] as would be expected. The result shows that the wave function normalization consistent with Eq. (47) is an incident wave of unit amplitude. Obviously, for the same metal couples the problem simplifies greatly since we have symmetry about the midpoint between the two metals. It is interesting to note that this formulation can be viewed as a scattering problem in terms of Jost functions [41] where the eigenfunctions can be represented as a linear combination of the two linearly independent solutions $\phi(\underline{k},\underline{r})$ and $\phi(-\underline{k},\underline{r})$ whose asymptotic limits are $\phi(k,X) \sim e^{ikX}$ $\phi(-k,X) \sim e^{-ikX}$.

B. Working Equations

The next step in the present work is to establish the working equations for the calculation. A model for the jellium and electron density for Al is shown in Figure 4. As presented previously the effective potential can be expressed in general as

$$V_{eff}(\underline{r}) = V(\underline{r}) + \int d\underline{r}' \frac{n(\underline{r}')}{|\underline{r} - \underline{r}'|} + V_{xc}(n, \underline{r})$$

where $v(\underline{r})$ is an external potential, e.g., from the jellium background $\int \underline{dr}' \frac{n(\underline{r}')}{|\underline{r} - \underline{r}'|}$ is the classical electrostatic potential and v_{xc} is the exchange and correlation potential (Eq. (6), (7), and (11)). For the jellium model the first two terms can be lumped together to give the total electrostatic potential. We now want to develop explicit expressions for these terms in order to determine the self consistent potential and electron number density.

Since we are dealing with a variational problem we use a standard calculus of variations approached in order to obtain the working equations. Thus the symbolic notation $\delta E[n]/\delta n$ becomes the operational equation $\frac{\partial E}{\partial n} - \frac{d}{dx}\frac{\partial E}{\partial n'}$ where $n' = dn/dx$.

1. Electrostatic Potential

Starting with the electrostatic terms in the total energy with the jellium giving the external potential, we get the same result as Lang and Kohn for the total electrostatic potential previously given in Eq. (11) as

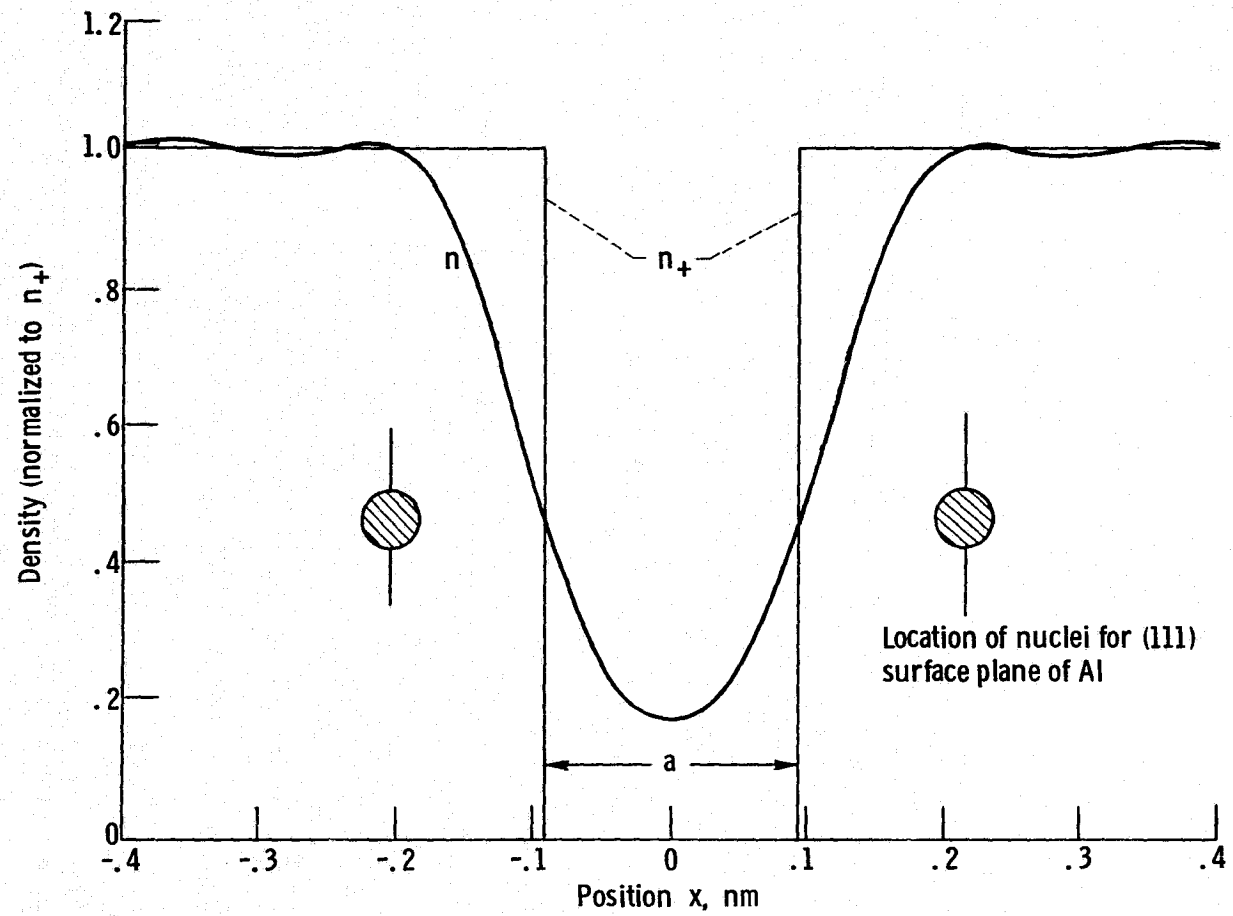


Fig. 4. - Electron number density n and jellium ion charge density, n_+, for an Al-Al contact normalized to unit density.

$$\phi(\underline{r}) = \int d\underline{r}' \; \frac{n(\underline{r}) - n_+(\underline{r})}{|\underline{r} - \underline{r}'|}$$

This equation can be simply restated in terms of Poisson's equation which for one dimension is $d^2\phi/dx^2 = -4\pi(n(x) - n_+(x))$. Boundary conditions will be discussed later in this section and numerical methods will be discussed in the calculations procedures section.

2. Exchange and Correlation Potential

a. Local density approximation

The total exchange and correlation energy is given by the expression $E_{xc}[n(\underline{r})] = \int d\underline{r}\; n(\underline{r})\varepsilon_{xc}(n(\underline{r}))$ where ε_{xc} is the exchange and correlation energy per particle. Therefore, the exchange and correlation contribution to the potential is $\mu_{xc} = (d/dn)(n\varepsilon_{xc})$. Using the Kohn-Sham exchange and the Wigner interpolation formula for the correlation energy (Eq. (21)) as did Lang and Kohn [7], we get

$$\mu_{xc}(n(x)) = -0.458\left(\frac{4}{3}\right)\left(\frac{4\pi}{3}\right)^{1/3} n^{1/3} - \frac{0.44\left(\frac{4}{3}\right)\left(\frac{4\pi}{3}\right)^{1/3} n^{1/3}}{\left(1 + 7.8\left(\frac{4\pi}{3}\right)^{1/3} n^{1/3}\right)} + \frac{0.44\left(\frac{1}{3}\right)\left(\frac{4\pi}{3}\right)^{2/3}(7.8)\, n^{\frac{2}{3}}}{\left(1 + 7.8\left(\frac{4\pi}{3}\right)^{1/3} n^{1/3}\right)^2} \tag{50}$$

b. Nonlocal Terms (Higher Order in the Gradient Expansion)

As pointed out in the background section, inclusion of the next higher order terms in the gradient expansion should be considered in surface energy calculations since there is a substantial change in the electron number density and thus the gradient of the density is large near the jellium surface. The difficulty with including these

terms from the recent work of Geldart and Rasolt [22] arises from the fact that an analytic expression for the coefficient in the gradient expansion is not available. Therefore, in order to interpolate and extrapolate the numerical values, the coefficient as a function of r_s (kindly provided by Dr. Rasolt) was curve fit to an expression which was found to fit the values well.

The expression for the energy per particle is given by

$$f = \frac{C_{xc}(n)}{n^{4/3}} |\nabla n|^2 \tag{51}$$

where C_{xc} has been approximated by

$$C_{xc}(n) = A\, n^{C}\, e^{-B n^{-2/3}} \tag{52}$$

where
$$A = 2.69413 \times 10^{-3}$$
$$B = 2.61294 \times 10^{-3}$$
$$C = 3.44333 \times 10^{-2}$$

The term chosen for C_{xc} prevents a divergence [41] in the potential which would otherwise occur for small number density. The limitations of this procedure will be discussed later. A plot of the curve fit along with the values of Rasolt and Geldart are presented in Figure 5. Applying the variational principle to Eq. (51) gives

$$\mu'_{xc}(n) = -\frac{C_{xc}(n)}{n^{4/3}} \left(2\frac{d^2 n}{dx^2} + S(n)\left(\frac{dn}{dx}\right)^2\right) \tag{53}$$

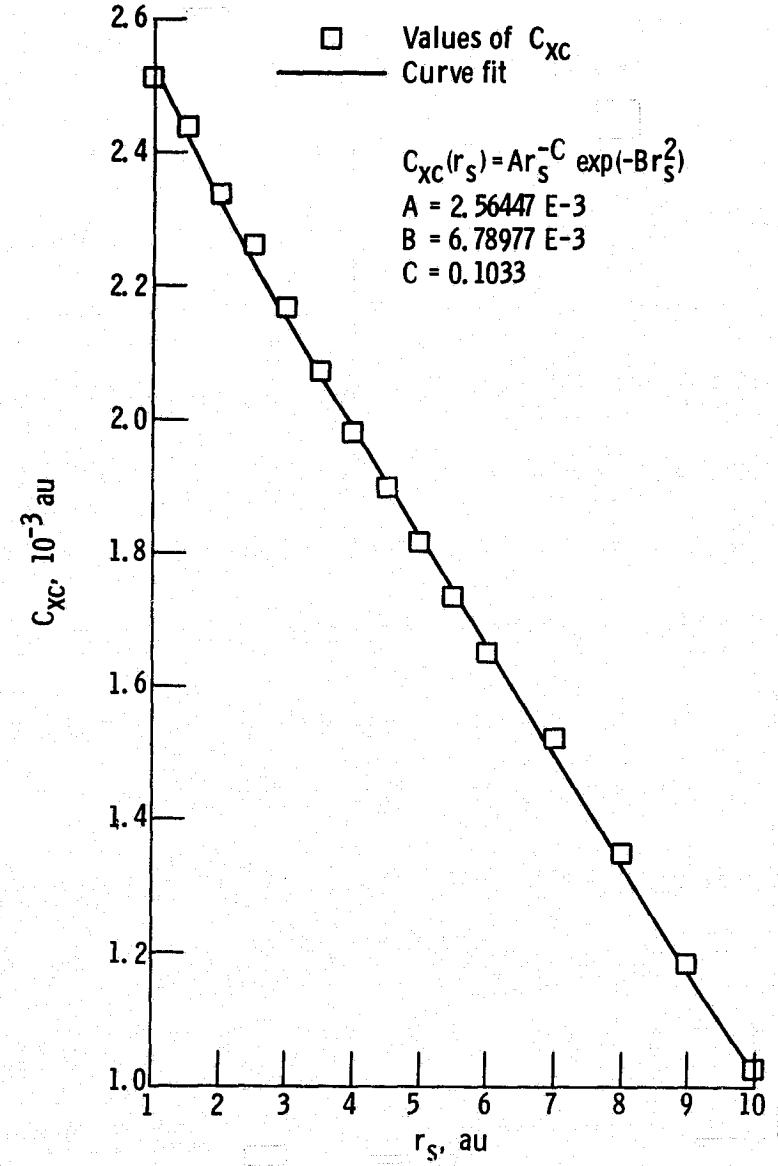


Fig. 5. - Curve fit to the Rasolt and Geldart [22] gradient coefficient, C_{xc} as a function of r_s.

where

$$S(n) = \frac{1}{3n}\left(3C - 4 + 2B n^{-2/3}\right) \tag{54}$$

3. Boundary Conditions

a. Potential

The jellium potential is of the form

$$V_{eff}(x) = \phi(n(x)) - \mu_{xc}(n(x)) + D \tag{55}$$

where D is a constant and where we now are considering the LDA. We must take the numerically derived ϕ and μ and include the correct asymptotic values for v_{eff}. As stated previously

$v_{eff}(x) = \begin{cases} -1/2\ k_{FL}^2 & x \to -\infty \\ -1/2\ k_{FR}^2 & x \to \infty \end{cases}$ for the zero of energy chosen. Therefore,

$$-\tfrac{1}{2}k_{FL}^2 = \phi(-\infty) + \mu_{xc}(n_{+L}) + D$$

$$V_{eff}(x) = \phi(x) + \mu_{xc}(x) - \phi(-\infty) - \mu_{xc}(n_{+L}) - \tfrac{1}{2}k_{FL}^2 \tag{56}$$

At the right limit we have

$$-\tfrac{1}{2}k_{FR}^2 = \phi(\infty) + \mu_{xc}(n_{+R}) - \phi(-\infty) - \mu_{xc}(n_{+L}) - \tfrac{1}{2}k_{FL}^2$$

Therefore

$$\Delta\phi = \phi(\infty) - \phi(-\infty) = \tfrac{1}{2}(k_{FL}^2 - k_{FR}^2) + \mu_{xc}(n_{+L}) - \mu_{xc}(n_{+R}) \tag{57}$$

and we have a restriction on the electrostatic potential. In

addition the electrostatic potential must satisfy the conditions

$$\frac{d\phi}{dx} \xrightarrow[x\to\pm\infty]{} 0 \quad ; \quad \frac{dV_{eff}}{dx} \xrightarrow[x\to\pm\infty]{} 0 \tag{58}$$

in order to satisfy charge neutrality in the bulk of the materials. A similar result applies to the nonlocal case. However, we note that $\mu'_{xc} \xrightarrow[x\to\pm\infty]{} 0$ since $\nabla n = 0$ in the bulk. The situation for the symmetric like metal problem is obviously simpler and we can in this case use the condition that $d\phi/dx = 0$ at the symmetry point thus requiring less computational effort. This condition on the electrostatic potential is used to solve Poisson's equation.

In the present and other numerical calculations, the boundary conditions as $x\to\pm\infty$ cannot be satisfied directly because of the finite computational space. This problem has been approached from a number of different standpoints [7,32]. In general, in this work the numerical solutions were forced to match the bulk conditions at the computational space (slab) boundaries selecting them so that they are large enough not to cause serious perturbations in the solutions. The charge neutrality condition was handled differently in that initially charge neutrality was imposed in the computational space to promote convergence. Then this restriction was removed when the solution was sufficiently convergent and allowed to relax to the final solution. The assumption was that since the self-consistent solution for the semi-infinite film is charge neutral, the final solution would be driven towards this condition. An evaluation and comparison with other results of the success of these

calculations will be presented later. They will be presented in the DISCUSSION section.

b. Wave functions

The form of the wave functions in the asymptotic region is given in Eqs. (43) to (45). In this calculation the potential at the slab (computational space boundaries) is assumed to be sufficiently flat that the asymptotic forms of the wave functions apply and therefore the numerical solutions are matched to these values at the slab boundary. The details of this matching are given in the section devoted to describing the calculational procedures.

C. Self-Consistent Equations

In summary, we have the following self-consistent equations

$$-\frac{1}{2}\frac{d^2\psi_k^i}{dx^2} + V_{eff}(x)\psi_k^i = \frac{1}{2}(k^2 - k_F^2)\psi_k^i \tag{58a}$$

$$n(x) = \frac{1}{4\pi^2}\sum_{i=1}^{2}\int_0^{k_F} dk\,(k_F^2 - k^2)\,|\psi_k^i|^2 \tag{58b}$$

$$\frac{d^2\phi}{dx^2} = 4\pi(n(x) - n_+(x)) \tag{58c}$$

$$\mu_{xc}' = \frac{C_{xc}}{n^{4/3}}\left(2\frac{d^2n}{dx^2} + S(n)\left(\frac{dn}{dx}\right)^2\right) \tag{58d}$$

and/or

$$\mu_{xc} = -0.984390\,n^{1/3} - \frac{0.945702\,n^{1/3}}{(1+12.5735\,n^{1/3})} + \frac{2.97271\,n^{2/3}}{(1+12.5735\,n^{1/3})^2} \tag{58e}$$

The procedure then is (a) to solve for the wave functions; (b) calculate the number density from the wave functions; (c) solve Poisson's Equation for the electrostatic potential; (d) calculate the second order contribution to the potential evaluated locally (first order = 0) for the gradient expansion for the nonlocal case and/or (e) calculate the 0th order exchange and correlation contribution to the potential evaluated locally (for the LDA only this term is included). Equations (58c), (58d), and (58e) give a new potential, $V_{eff(x)}$, which can be used to repeat the process.

D. Calculation of the Binding Energy

The adhesive energy is defined in this calculation as $E_{Ad} = \frac{E(a) - E(\infty)}{2A}$ where a is the separation between materials and A is the sectional area. The reason for this particular form for the definition of the energy is that it emphasizes the similarity to molecular binding. The difference in energy is given by

$$E(n(x,a)) = \frac{A}{2}\int dx\, \phi(x,a)\,(n(x,a) - n_+(x,a)) + V_{int}(a)$$
$$+ T_S(n(x,a)) + E_{xc}(n(x,a)) + E'_{xc}(n(x,a)) + A\int dx\, \delta v(x,a)\, n(x,a) \tag{59}$$

where $n_+(x,a)$ represents the total jellium density for both materials. The kinetic energy difference is given by

$$T_S = (2S+1)\int_{-X_0}^{X_0} dx \left\{ \sum_{occ,i} \psi_k^{i*}(-\tfrac{1}{2}\nabla^2)\psi_k^i - \frac{3}{10}(3\pi^2)^{2/3}\left(n_{+L}^{5/3}\theta(-(x+\tfrac{a}{2})) + n_{+R}^{5/3}\theta(x-\tfrac{a}{2})\right)\right\} \tag{60}$$

where n_{+L} and n_{+R} are the bulk densities in each material, θ is the Heaviside function, and s is the spin.

The energy in Eqs. (59) and (60) is referenced to zero separation for each bulk material for computational convenience. Infinite separation is chosen for the referencing when the results are plotted because it emphasizes the similarity to molecular binding. The finite limits on the integral indicates that the slab is sufficiently large that the deviation from bulk conditions past the slab boundaries is not significant. This can be tested by the form in which the integral is written by increasing the slab length in a test case and then estimating convergence on the basis of the form of the density in the bulk. Equation (10) is modified by use of the Schroedinger equation to the form

$$T_S = (2S+1)A\int_{-X_0}^{X_0} dx \left\{ \sum_{occ,i} |\psi_k^i|^2 \frac{(k^2+k_{\parallel}^2)}{2} - \frac{3}{10}(3\pi^2)^{2/3}\left(n_{+L}^{5/3}\theta(-(x+\tfrac{a}{2})) + n_{+R}^{5/3}\theta(x-\tfrac{a}{2})\right)\right\} + A\int_{-X_0}^{X_0} dx \left\{V_{eff}(n_{L,R}, \pm\infty) - V_{eff}(x,a)\right\} n(x,a) \tag{61}$$

where the $\pm$ and L,R are chosen to suit the proper half-space. The first term can be evaluated to order L^{-1} (appendix IV) in a

manner similar to that used in calculating the electron number density. Changing the sum to an integral and using cylindrical coordinates we get for the integration over k-space

$$\frac{1}{8\pi^2}\sum_{i=1}^{2}\int_0^{k_F} dk\,|\psi_k^i|^2 k^2(k_F^2-k^2) + \frac{1}{16\pi^2}\sum_{i=1}^{2}\int_0^{k_F} dk\,|\psi_k^i|^2(k_F^2-k^2)^2 \tag{62}$$

Substituting these expressions for the first term in expression (61) gives the Kinetic Energy Contribution to the total energy. The difference in electrostatic energy difference is given by

$$E_{es} = \frac{A}{2}\int_{-X_0}^{X_0} dx\,\phi(x,a)\left(n(x,a)-n_+(x,a)\right) + W_{int+}(a). \tag{63}$$

Expressions for W_{int} (a) are given in the previous section.

$$n_+(x,a) = n_{+L}\,\theta(-(x+a/2)) + n_{+R}\,\theta(x-a/2) \tag{64}$$

The exchange and correlation energy (LDA) difference is given by

$$E_X = \frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} A\int_{-X_0}^{X_0} dx\left\{n^{4/3}(x,a) - n_{+L}^{4/3}\theta(-(x+a/2)) + n_{+R}\,\theta(x-\tfrac{a}{2})\right\} \tag{65}$$

$$E_C = 0.056A\int_{-X_0}^{X_0} dx\left\{\frac{n^{4/3}(x,a)}{0.079+n^{1/3}(x,a)} - \frac{n_{+L}^{4/3}\theta(-(x+a/2))}{0.079+n_{+R}^{1/3}} - \frac{n_{+R}^{4/3}\theta(x-a/2)}{0.079+n_{+R}^{1/3}}\right\}. \tag{66}$$

For the nonlocal contributions

$$E_{xc}' = A\int_{-x_0}^{x_0} dx \quad \frac{C_{xc}(n(x,a))}{n^{4/3}(x,a)} \left(\frac{dn(x,a)}{dx}\right)^2 . \tag{67}$$

The pseudopotential contribution to the energy requires a somewhat more detailed discussion. These details taken from Lang and Kohn [7] are repeated here for completeness. In addition, some derivations not given by Lang and Kohn are presented in Appendix I. The general expression for the pseudopotential contribution to the energy is

$$E_{ps} = A\int_{-x_0}^{x_0} dx\, \delta v(x,a)\, n(x,a) \tag{68}$$

(The presentation here will be for one half-space since the extension to both is simple.) Where

$$\delta v(x,a) = \left\langle \sum_{\delta(x<0)} v_{ps}^{(\nu)} \right\rangle - \phi_+(x) \tag{69}$$

and where the brackets indicate an average over the y-z directions and the summation is over planes passing through the centers of the lattice planes perpendicular to the x-direction. The second term is the potential due to the semi-infinite jellium. The general purpose of expression (68) therefore is to add in the proper electron-ion interaction and subtract off the electron-jellium interaction which is already included in expression (63). As can be seen, the additional term is introduced through first order perturbation theory on the assumption that this term is small compared to the total

potential. This point has been in contention but recent work which will be presented in the DISCUSSION section will show that this is a good approximation for the simple metals. LK now break up this term into two terms

$$\delta V(x) = \delta V_1(x) + \delta V_2(x) \tag{70}$$

where

$$\delta V_1(x) = \left\langle \sum_{\nu(x<0)} -Z/|\underline{r}-\underline{r}_\nu|^{-1} \right\rangle - \phi_+(x) \tag{70a}$$

$$\delta V_2(x) = \sum_{\nu(x<0)} \left\langle V_{PS}^{(\nu)} + Z/|\underline{r}-\underline{r}_\nu|^{-1} \right\rangle \tag{70b}$$

The average in (70a) treats the charges as though they are smeared out over a lattice plane. From the previous definition (Eq. (29)) of the Ashcroft pseudopotential we see that the term (70b) is zero outside the ion core and has a $1/r$ dependence inside the core which is averaged over the y-z planes. Working through the electrostatics for these terms (details of which are presented in Appendix I) gives

$$\delta V_1(x) = -2\pi n_+ \left[x + \ell d\, \theta\left(-x-(2\ell-1)d/2\right)\right]^2 \tag{71a}$$

and

$$\delta V_2(x) = 2\pi d n_+ \left(r_c - |x+(2\ell-1)d/2|\right)\theta\left(r_c - |x+(2\ell-1)\tfrac{d}{2}|\right) \tag{71b}$$

where ℓ is an integer designating the lattice plane and these results apply if there is no core overlap, as is obvious from the method used to do the averaging.

E. Checks on Self-Consistency

Fortunately there is now a method to examine the degree of self-consistency for the jellium part of the calculation. Budd and Vannemenus [42] have derived an expression for the force at zero separation using the Hellman-Feynman Theorem. The force per unit area is given by

$$F/A = -n_+ \Delta\phi(a) \tag{72}$$

where a is the separation between the two jellium slabs and $\Delta\phi$ is the difference in electron electrostatic potential energy between the jellium surface at a separation a and the jellium surface at infinite separation. F/A is also given by $\partial E/\partial\Omega$ where E is the total energy and Ω is the total volume.

$$\frac{\partial E_0}{\partial \Omega} = n^2 \frac{\partial f}{\partial n} \tag{73}$$

where f is the energy per electron for the uniform electron gas and where the subscript 0 indicates $a = 0$. Since we have an expression for the energy per particle for the uniform electron gas a comparison of Eqs. (72) and (73) gives a check on the degree of self-consistency for the numerical calculations. Heinrichs and Kumar [43] derive a similar expression for dissimilar metal contacts and this

result will be used to evaluate the validity of the simple-overlap model. Equation (72) also enables evaluation of the force versus separation for the jellium and thus the total force when the lattice sum and pseudopotential contributions are included in the total energy by taking the derivative of these terms. Equation (73) expressed in terms of r_s the Wigner-Seitz radius is

$$\frac{\partial E_0}{\partial \Omega} = 0.439646\, r_s^{-5}\left(0.4 - .0829 r_s - \frac{0.796\, r_s^3}{(r_s+7.8)^2}\right) \tag{74}$$

The Heinrichs-Kumar expression for the jellium force between dissimilar metals is

$$F_{12}(0) = P_i' + P_i\, \Delta V(0) \quad i = 1,2 \tag{75}$$

where

$$P_i = \frac{0.175858}{r_s^5} - \frac{0.0364466}{r_s^4} - \frac{0.0350142}{(r_s^2+7.8 r_s)^2} \tag{75a}$$

$$\Delta V_2(0) = \frac{1}{M_+^{(1)} - M_+^{(2)}}\left[M_+^{(1)}(\mu_1-\mu_2) - (P_1-P_2)\right] \tag{75b}$$

$$\mu_i = \frac{1.84158}{r_s^2} - \frac{0.610667}{r_s} - \frac{0.44}{(r_s+7.8)} - \frac{0.146667 r_s}{(r_s+7.8)^2} \tag{75c}$$

$\Delta V_1(0)$ is obtained from $\Delta V_2(0)$ by interchanging subscripts 1 and 2. In evaluating the simple overlap model the results of Eq. (75) will be compared with $(\text{dE jellium/da})_{a=0}$ the derivative of the jellium portion of the binding energy evaluated at $a = 0$.

F. Other Checks on Results

There are a number of checks that the results of these calculations must meet. The first is that the binding energy and its component energies must agree with the bare metal results at large separation. Another comparison of practical importance would be to predict experimental surface energies. These two conditions essentially only examine one point on the binding energy curves. An additional comparison which can be made with experiment is to obtain the elastic constants for a given direction from the curvature of the binding energy curve at equilibrium. This comparison has the additional feature of not simply depending on the energy at a single point but on the behavior of the binding energy curves at small separations. Since for small separations from equilibrium Hooke's Law will apply (Fig. 6)

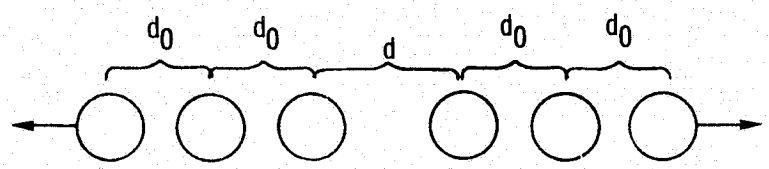


Fig. 6. - Change in interplanar spacing upon forming a surface.

$$F = C\epsilon = ka \tag{76}$$

where F is the force unit area, C is the elastic constant, ϵ is the strain, k is the spring constant and a is the change in distance between lattice planes from pulling the metals apart, however, $\epsilon = \frac{d - d_0}{d_0}$ and $a = d - d_0$, therefore,

$$C = kd_0 \tag{77}$$

In this we assume a nonuniform strain between the two planes forming the surfaces with the other planes undisturbed [44,45]. In addition, we assume no distortion in the y or z directions.

CALCULATIONAL PROCEDURES

Obtaining a numerical self-consistent solution to the surface problem has proven to be quite difficult. L-K [7] found that they couldn't get a solution using convergence factor techniques, therefore, they resorted to a functional equivalent of the Newton-Raphson method [46]. Rose and Shore [47] took a different approach in which a parameterized trial potential was used as input in which the parameters were varied by a simplex method [48] in order to minimize the total energy. The trial potential obtained in this manner reproduced the LK number densities and surface energies. Alldrege and Kleinman [49] and Appelbaum and Hamman [50] were able to obtain self-consistent solutions to three-dimensional problems by using convergent factor methods. Both found that the zeroth order ($k_{||} = 0$) term was the most unstable part of the calculation and the higher order terms in the Fourier expansion converged rapidly. It is this unstable term that is evaluated in the present study.

In this section the techniques used to obtain a solution for the like-metal bimetallic Kohn-Sham equations with varying separation between the half-spaces are described. An IBM 360-67 time sharing system was used for the computations.

I - SOLUTION OF SCHROEDINGER EQUATION AND POISSON's EQUATION

The Numerov method [46] is used to obtain a solution for the Schroedinger Equation (Eq. (58a)). The Numerov method is a predictor corrector technique for second order differential equations in which the first derivative does not appear and has a remainder of the order of $y^{(6)}h^5/240$ where $y^{(6)}$ is the sixth derivative of the function and h is the mesh size in configuration space.

Quadrature is used for the solution of Poisson's equation (Eq. (58d)). Therefore, the potential is found by integrating the net charge twice. The Adams' method [51] with error of order h^6 is used to perform the integrations since Simpson's rule [49] with an interpolation proved to be unstable. The instability arose from the fact that the integral of the net charge density was a decreasing rather than increasing function of position in the bulk of the solid; therefore, in the asymptotic region errors of the order of the charge density fluctuations arose from the need to interpolate to obtain alternate mesh points with Simpson's rule curve fit to the number density. A spline fit (Appendix V) followed by integration was also adequate but required substantially greater computer time and storage. The jellium net charge and potential were determined analytically and then combined with the numerical integration of the electron density. The solution of Poisson's Equation was checked by constructing a trial density similar to Smith's [6] with a small sinusoidal form in the bulk to simulate Friedel oscillations. The results agreed to 1-2 parts in 10^6. In the calculation of the electrostatic potential the integration proceeded from the symmetry point

where the slope or the field was taken to be equal to zero. The integration proceeded into the bulk to the end of the slab where the entire potential, electrostatic plus exchange and correlation was required to equal the bulk potential.

A different test was applied to the solution of Schroedinger's equation. The solution was checked by comparing the wave function and number densities obtained from the solution of the Schroedinger equation for a triangular potential, the details of which are presented in Appendix III. It was found that the slope discontinuities for a square barrier created large errors in the solution obtained from the Numerov method.

Once the wave functions were determined both analytically and numerically the electron number density was calculated using Eq. (58b) by performing the k-space integrations. The results for the calculated and analytic densities are shown in Figure 7. The agreement was again good. The final self-consistent solution was probably superior to even these since small errors were introduced into the wave functions at the discontinuities in the slope of the triangular potential. The k-space integrations for the number density were performed by Simpson's rule since it required keeping only three wave functions in computer storage. The configuration space and k-space mesh sizes were selected by determining the maximum values that were necessary for accurate solutions. These were found to be 0.25 au and 0.02 k_F.

The solution of Schroedinger's equation for a given potential proceeded by assuming the form of the wave function for the trans-

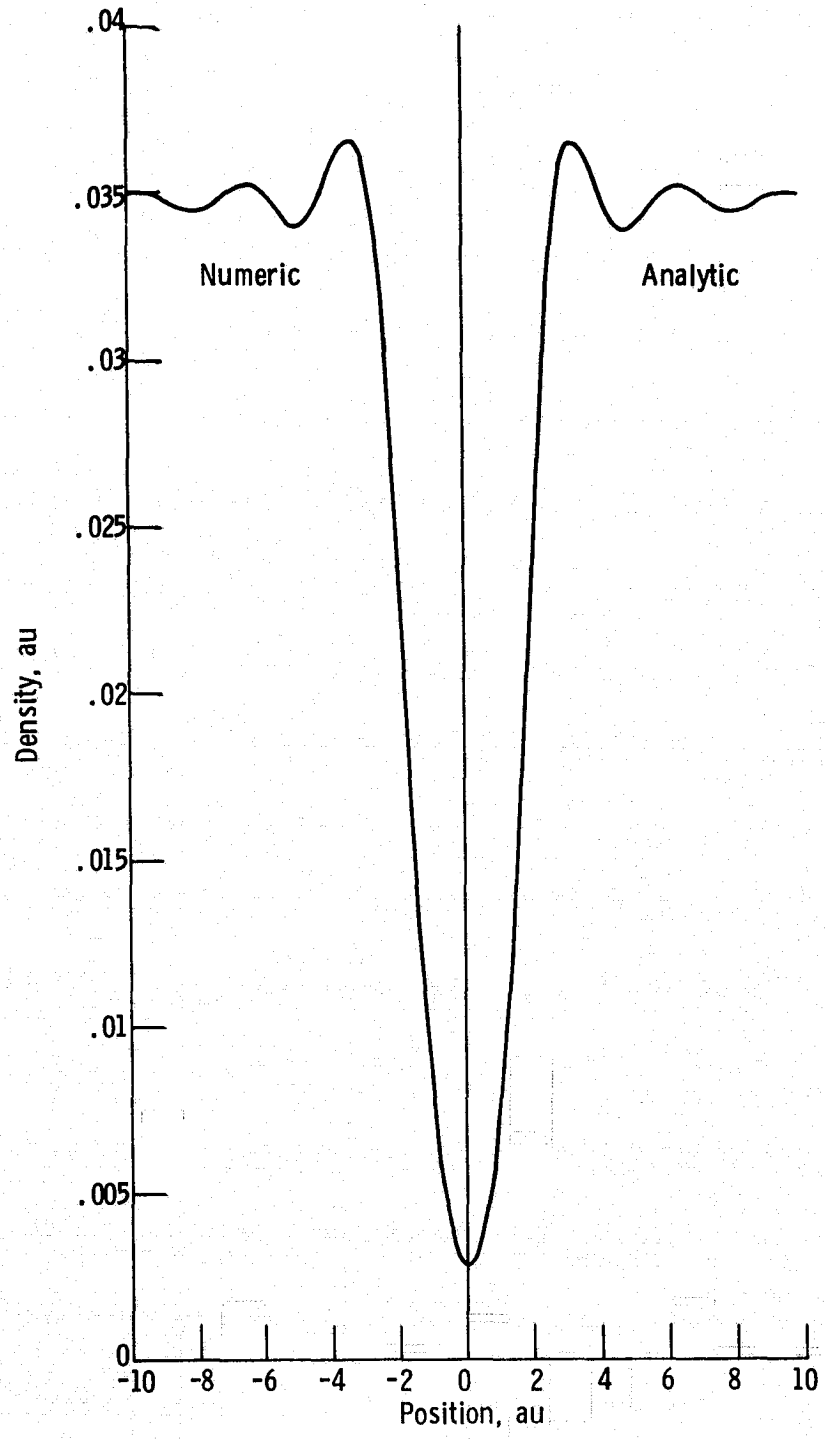


Fig. 7. - Electron density for a triangular potential for a barrier height k_F^2 with a Fermi wave number, $k_F = 1$ au and barrier width of 2 au.

mitted wave for an electron incident from the left half space to be $e^{ik_R L_R}$ deep in the bulk of the second half space where $k_R = \{2[\varepsilon(k) - V(L_R)]\}^{1/2}$ where $V(L_R)$ is the value of the total potential at the right hand boundary L_R. The Numerov Method uses two points to start the calculation rather than the slope and function, therefore, the same value of k was used for the second point which has an x value one mesh point from the right hand extreme which is equivalent to assuming the potential is constant at this point. The integration proceeded into the bulk of the second material where the numerical solutions were matched to

$$\psi_k(x) = A\left(e^{ik_L L_L} + R_L e^{-ik_L L_L}\right) \tag{78}$$

where the coefficients were chosen as described in the THEORY section. The same assumption holds in this form of the wave function as for the starting values, i.e., the potential is essentially flat. The matching was performed by requiring the slope and function to be equal at $X = L_L$. Numerical derivatives were obtained with an I.B.M. computer routine called DET5 (Appendix VI). The wave functions were then renormalized by division by the constant A as outlined in the THEORY section. These wave functions are then used to calculate the electron number density (Eq. (58b)).

II - TRIAL SOLUTIONS AND SELF-CONSISTENCY PROCEDURE

A. Trial Solutions

The calculation proceeded by first constructing a trial

potential at the smallest separation between half-spaces used, 0.25 au, on the assumption that the system would deviate least from the uniform density at zero separation. A trial density of the Smith type as discussed in Chapter 2 was used in constructing a trial potential, but this proved to be unstable. The criterion used for judging the sufficiency of the trial potential was that the differences between input and output potential between the second and third iterative loops should decrease. The potential derived from the simple exponential density was insufficient to satisfy this criterion, by varying the exponential decay constant β. A successful trial potential was obtained by using the previous trial potential with a Gaussian well which simulated the first Friedel oscillation in the potential and whose position and strength could be varied along with β. This potential proved to be an adequate starting point to obtain a self-consistent solution at a separation of 0.25 au. For the subsequent separations a trial potential was obtained from the potential at the previous separation. First the potential at the previous separation was fixed relative to the jellium surface, then the points needed to complete the potential between the two metals were obtained by a linear extrapolation. At larger separations it was necessary also to increase the jellium slab length because of the increase in amplitude and range of the Friedel Oscillations near the jellium surface. In these cases the potential for large x was extrapolated by using the bulk value of the potential. It was later found that trial solutions for intermediate separations could be obtained starting from a solution at a larger separation by fixing the

potential relative to the jellium and reflecting those values through the symmetry point, thus omitting the need for extrapolation. Trial solutions could also be obtained at intermediate separations by interpolation of the potential between to previously obtained solutions, e.g., a solution at a separation of 2.5 au could be obtained from the solutions at 2 and 3 au.

This procedure was used to obtain a complete set of solutions for $r_s = 2$. Trial potentials were then generated for other values of r_s by multiplying the previously obtained self-consistent potential of the r_s value nearest to the desired value by k_{F2}^2/k_{F1}^2, the ratio of the bulk potentials squared. Trial potentials were also needed for the calculations including nonlocal terms in the exchange and correlation energies. The self-consistent solutions for the local density approximation were sufficient trial solutions.

B. Self-Consistency

1. Procedure

Before commenting on the procedure used to obtain self-consistency it should be mentioned that in order to obtain convergence it was initially necessary to require charge neutrality in the slab. The technique used to obtain neutrality was simply to renormalize the electron density by multiplying it by the appropriate constant to make the net charge in the slab equal to zero. This technique was also used by Applebaum and Hamman [48] and proved to be adequate. Lang and Kohn [7] obtained neutrality by adding a Gaussian which was centered at the jellium surface to the electronic

charge. The amplitude of the gaussian was adjusted to insure that $\frac{dv_{eff}}{dx} \xrightarrow[x\to-\infty]{} 0$. The converged number density obtained from requiring neutrality was in general nonneutral. Requiring neutrality in the slab was needed for the comparisons of input and output potentials. Once convergence was obtained with the charge neutrality restriction, it was removed and the self-consistency procedure was continued. These converged solutions proved to give adequate trial potentials for other values of r_s by the simple ratio technique without first requiring charge neutrality.

As stated earlier a convergence factor method was used to obtain self-consistency rather than the Lang-Kohn method which would have been cumbersome for this calculation. The convergence factor involves using a linear combination of the output and input potentials as the trial potential for the next loop of the iteration

$$(V_{in})_{i+1} = (V_{in})_i + \alpha((V_{out})_i - (V_{in})_i) \tag{79}$$

In the early stages of the calculation starting from the invented trial potential it was necessary to use a very small convergence factor $\alpha = 0.002$, to promote convergence due to the extreme instability of the system. This could be increased to 0.025 as convergence occurred. Larger convergence factors resulted in divergence. However, even with $\alpha = 0.025$ the rate of convergence proved to be quite slow. At this stage it was found that more rapid convergence could be promoted by using a large convergence factor, typ-

ically 0.25 to 0.5 depending on the separation between slabs in order to promote the establishment of features present in the final solution followed by a small convergence factor for a number of iterations in order to damp out instabilities introduced by the large convergence factor. The same procedure could be used for the solutions where the charge neutrality constraint was removed, but a much smaller convergence factor typically, 0.005, was necessary for convergence in subsequent loops since the lack of requiring charge neutrality in the slab during the iterations caused a much more severe instability. It was found that this procedure could be repeated to obtain any degree of self-consistency. The criterion for stopping the calculation will be discussed later.

The calculation of the wave functions and thus the number density consumed the greatest amount of computer time. In order to minimize computer time it was found that k-space intervals of $0.05\ k_F$ were sufficient to obtain convergence in the initial stages of iteration. In the final stages the k-space intervals were reduced to $0.02\ k_F$. This procedure was only used when the nonlocal terms were included in the potential but very likely would have been adequate in all cases.

2. Condition for Self-Consistency

In similar previous calculations the condition for self-consistency was based simply upon the difference between input and output potential presented as a fraction of the bulk value. However, in the present calculation a more reasonable criterion is to

base the maximum fractional difference as a percentage of the barrier height. This is comparable to previous bare surface calculations for large separations and a much more stringent condition for small separations. It should be mentioned that using the potential rather than the density to judge self-consistency is also much more stringent since the potential depends very strongly on the density. The highest deviation (3.5%) between input and output potentials was for sodium at a separation of 0.25 au. The deviations were as low as a fraction of a percent. The largest deviations were for the smallest separations since considerably more iterations were needed to obtain convergence at these separations. It was found that the binding energy which is the result of this study was not a strong function of the degree of self-consistency for deviations of less than 100 meV. For example, for aluminum a difference between 60 and 2 meV only made a difference of 2% in the binding energy for aluminum, nonlocal, at a separation of 15 au. An additional test was used to determine convergence. The final output potential was used as an input with a convergence factor of 1.0 to determine whether deviations between input and output would remain of the same order. However, continued iterations at large convergence factors would cause a divergence because of small deviations from neutrality.

It is possible to attain a higher degree of self-consistency for any separation. The potentials and densities are available on punched cards, if a higher degree of self-consistency is required.

III - BINDING ENERGIES

The binding energy were evaluated by performing quadrature with the exception of Wint as outlined in the THEORY section. These integrations were performed using QSF (Appendix VII). Since all of the functions were well behaved no problem arose in using this procedure.

IV - ELASTIC CONSTANTS

The procedure for transforming the elastic constants for a given crystal direction from experimental data are given in reference [52]. The calculated elastic constants were obtained by taking the second derivative of the binding energy curves by fitting them with a spline curve fit (Appendix V). This procedure allows a nonuniform spacing for the separations when fitting a function.

RESULTS

Presentation of the results will be in a form that reflects the order in which they are produced in the self-consistent calculations. Since the binding energy versus separation is the principle result of the calculation it will be presented last. Also included will be checks of the results, tables of self-consistent densities and potentials, force curves, tables of components of the binding energies, a comparison of experimentally and theoretically determined elastic constants, and a listing of the computer program. The tables of number densities and potential energies (Appendix X), energy breakdowns (Appendix IX) include a complete listing of all results obtained at each separation in the hope that this will serve as a comprehensive document. For results obtained from the simple overlap model only the binding energy curves will be presented for purposes of comparison. The number densities can be obtained simply by use of Smith's [6] bare-metal calculations, and the potential energy and components of the binding energy can be obtained using quadrature of the expressions presented in Section I of the THEORY section. The tabular results will be organized by presenting them in increasing order of r_s for the materials considered. A listing of the computer program is presented in Appendix VIII.

I - NUMBER DENSITIES AND POTENTIAL ENERGY

Figures 8 and 9 show some typical plots of the electron number

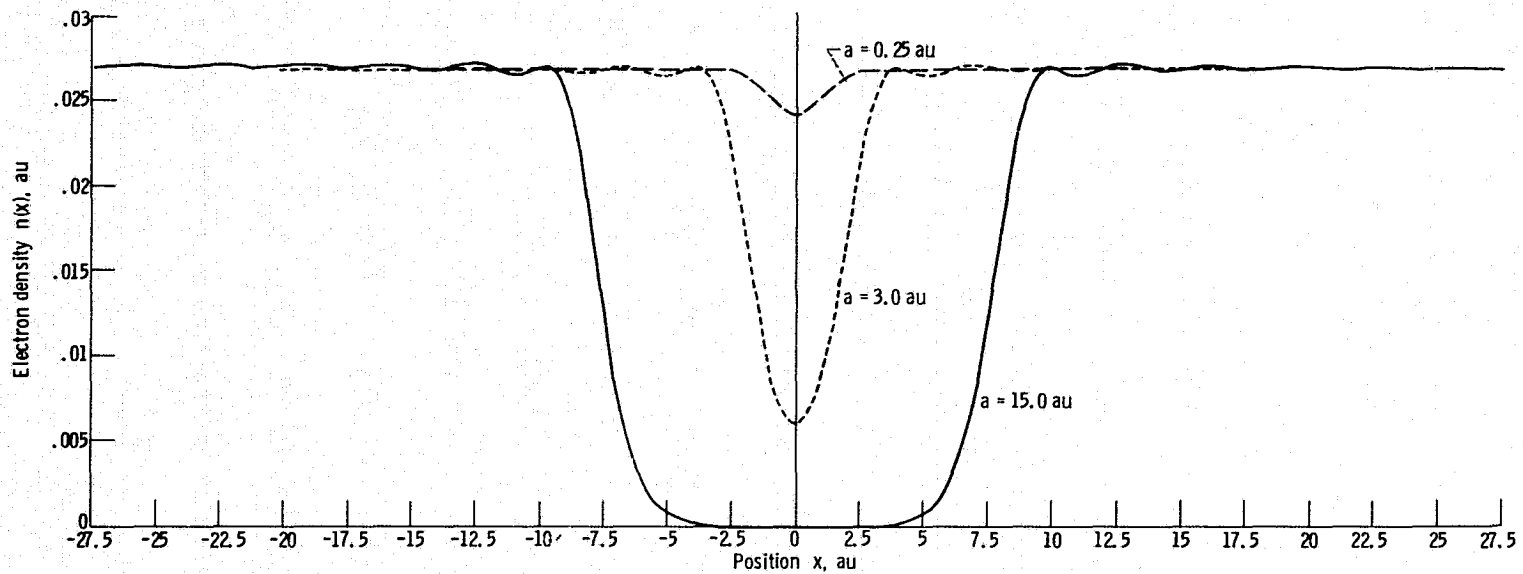


Fig. 8. - Electron density versus position for an Al(111)-Al(111) contact for separations of 0.25, 3.0, and 15 au.

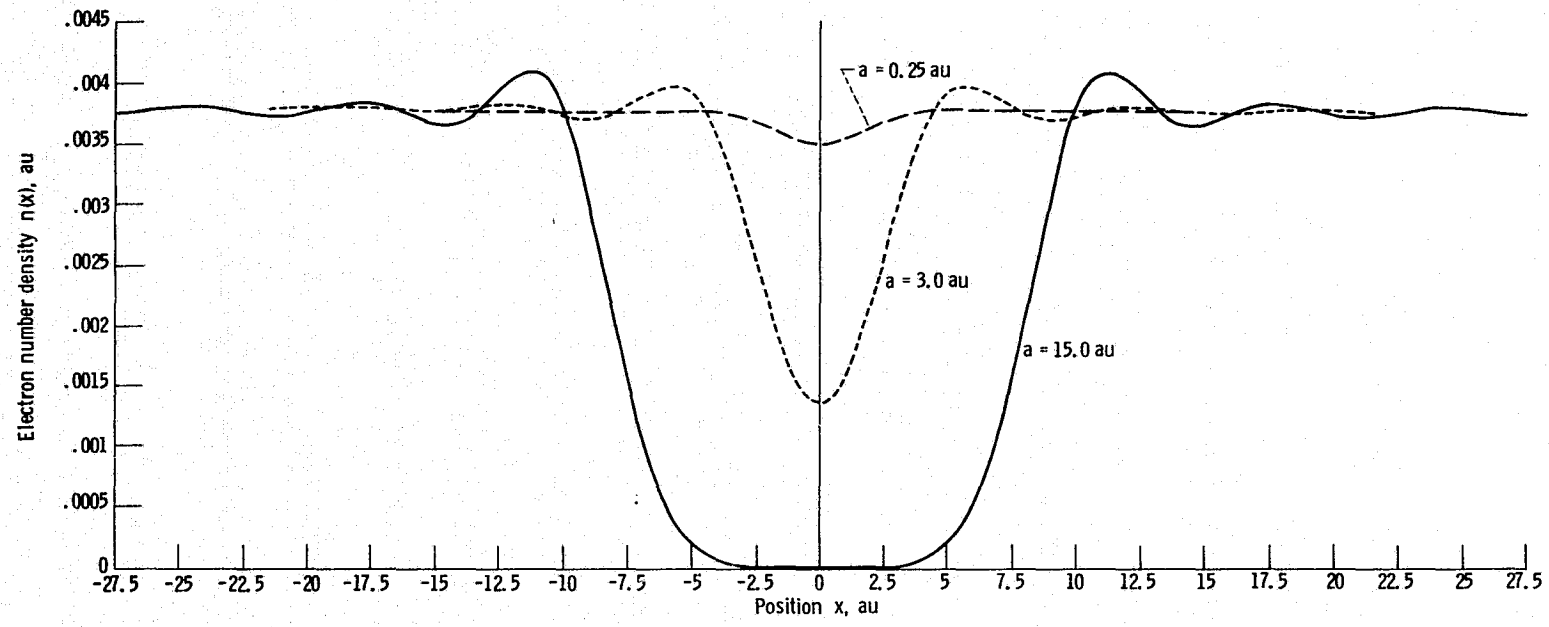


Fig. 9. - Electron density versus position for a Na(011)-Na(011) contact for separations of 0.25, 3.0, and 15.0 au.

density for Na and Al at 0.25, 3.0, and 15 atomic units. We can see two main features; the electron number density falls off rapidly as the separation increases, the oscillations in the density increase as the separation increases and the magnitude of the oscillations are larger for sodium than aluminum. Figures 10 and 11 shows similar plots for the potential energy $V_{eff(x)}$, as a function of separation for Al and Na. Here we see the barrier height increasing with separation and in addition again the oscillations are increasing with separation and likewise increase from Al to Na. Figure 12 is a plot showing the increase in barrier height versus separation for aluminum for both the local and nonlocal approximation. It can be seen that the barrier height versus separation differs for small separations which is typical of each element examined but the difference disappears at larger separations. In addition, at separations of 15 au the "work function," the difference between the barrier height and the top of the conduction band has not as yet saturated to the bare-metal value. The barrier height varies much more slowly than the number density with separation which changed little between a separation of 10 and a separation of 15 au.

Figure 13 shows a plot of the potential energy for Al at a separation of 15 au including the nonlocal terms in the potential. It is apparent that some anomaly has appeared at this separation. There is a dip in the potential energy on either side of the symmetry point. The question arises concerning whether this is an actual physical effect or a breakdown in the numerical techniques used. This point will be addressed in the DISCUSSION section. A listing

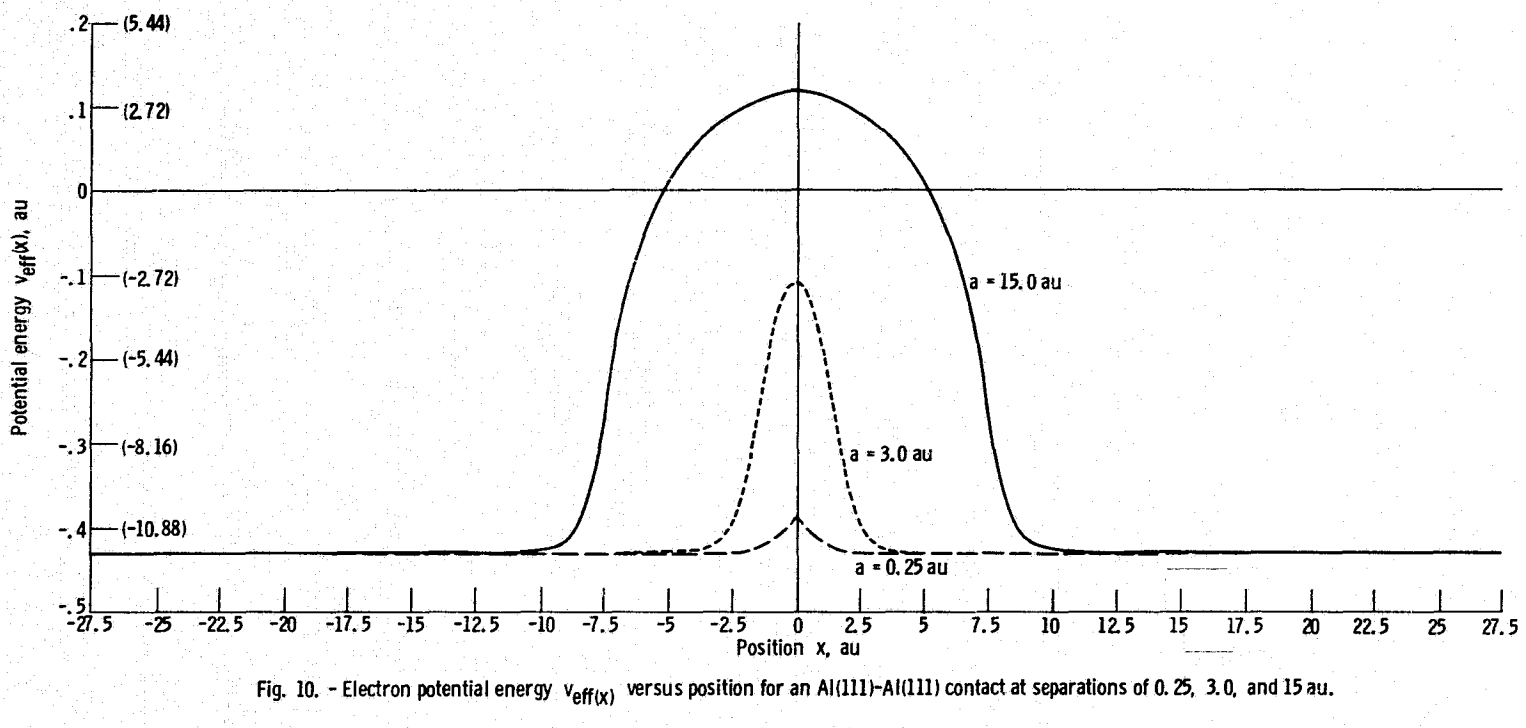


Fig. 10. - Electron potential energy $v_{eff(x)}$ versus position for an Al(111)-Al(111) contact at separations of 0.25, 3.0, and 15 au.

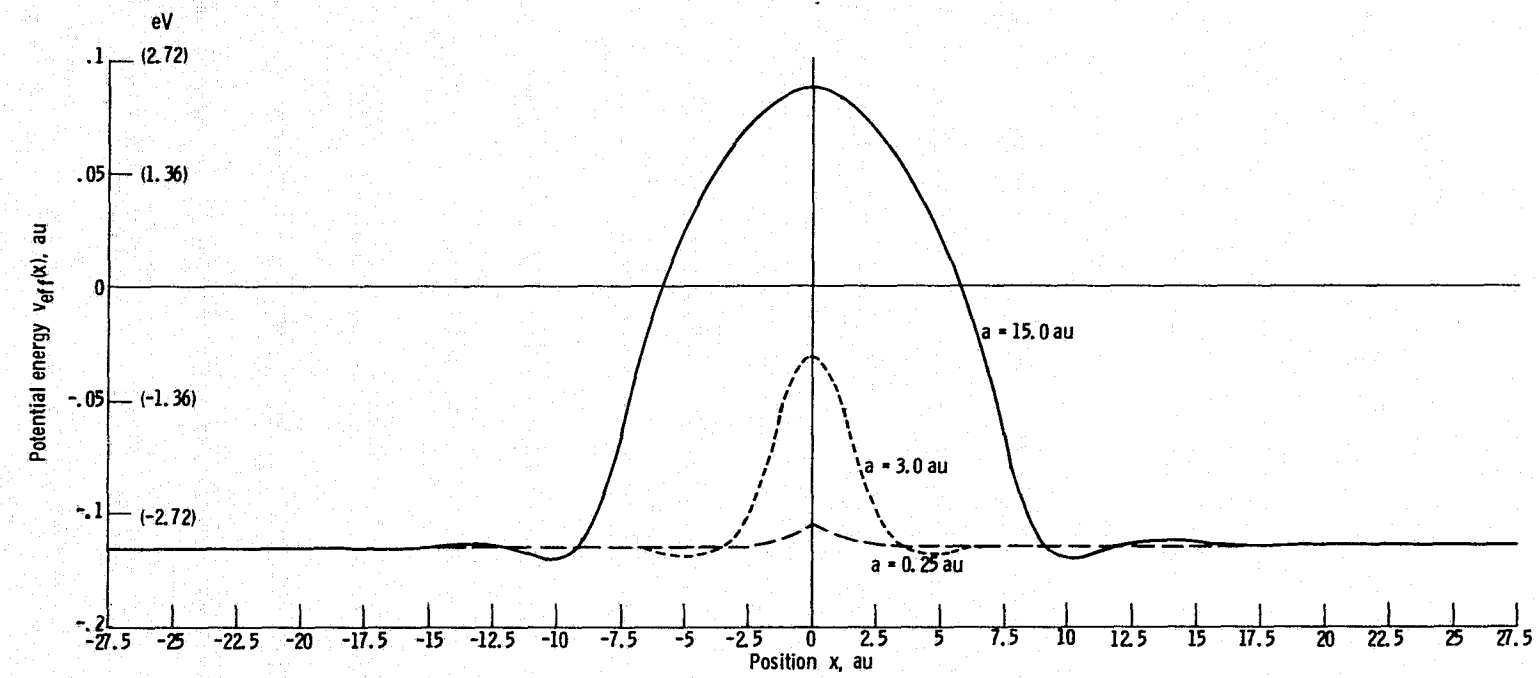


Fig. 11. - Electron potential energy $v_{eff(x)}$ versus position for a Na(011)-Na(011) contact at separations of 0.25.

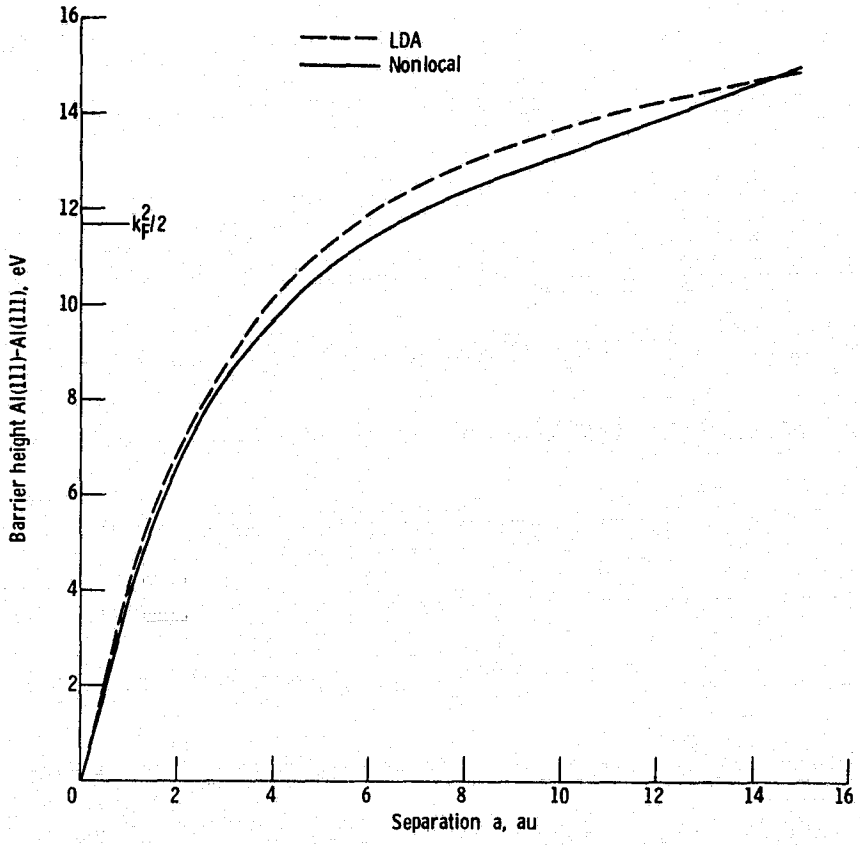


Fig. 12. - Electronic barrier height versus separation a for an Al(111)-Al(111) contact for the LDA and including nonlocal terms in the exchange and correlation energy.

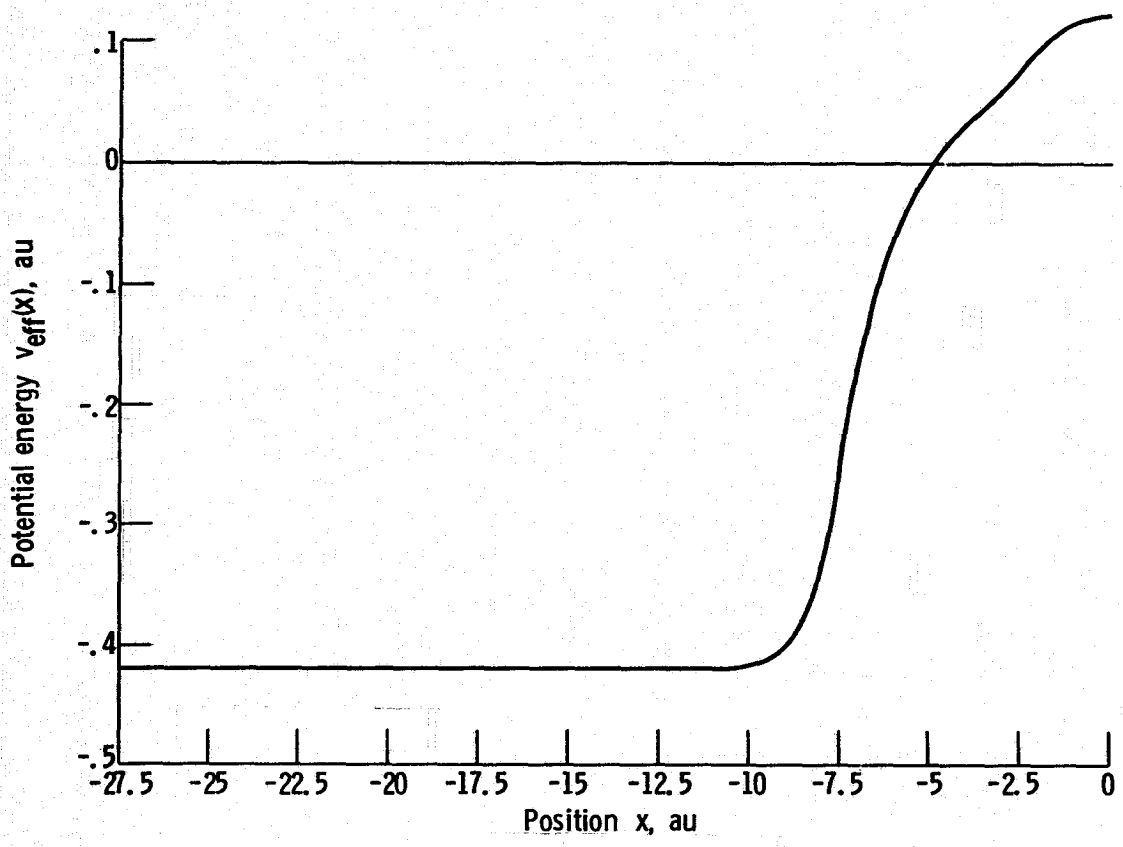


Fig. 13. - Potential energy $v_{eff(x)}$ versus position for Al (nonlocal) at a separation of 15 au.

of the computer program for the self-consistent calculation is in Appendix VII. The complete self-consistent densities and potential energy tables for the local and nonlocal gradient expansion are presented in Appendix X.

II - SIMPLE OVERLAP BINDING ENERGIES

Figure 14 shows a plot of binding energy as a function of separation for the densest packed planes of Al, Zn, and Mg for each possible combination of contacts between any pair of these elements. They also include the possibility of having the lattices in registry or lack of registry for the like-metal contacts which means that Wint is included or omitted from the total binding energy. The primary features of these curves are that the minimum was at a nonzero separation, the range of the strong binding force is 4.0 atomic units and that the dissimilar metal contacts had stronger binding than the weaker of the two similar metal contacts for nonregistry (Wint = 0) which would be the situation which has been observed in bimetallic contacts [4]. A list of the binding energies are presented in Table I. A check of the Budd-Vanemenus Sum Rule [42] for

Table I

Binding Energies Simple Overlap Model

	$W_{int} = 0$	Perfect Registry ($W_{int} \neq 0$)
Al-Al	405 ergs/cm^2	525 ergs/cm^2
Al-Zn	360	
Al-Mg	320	
Zn-Zn	320	345
Zn-Mg	285	
Mg-Mg	255	315

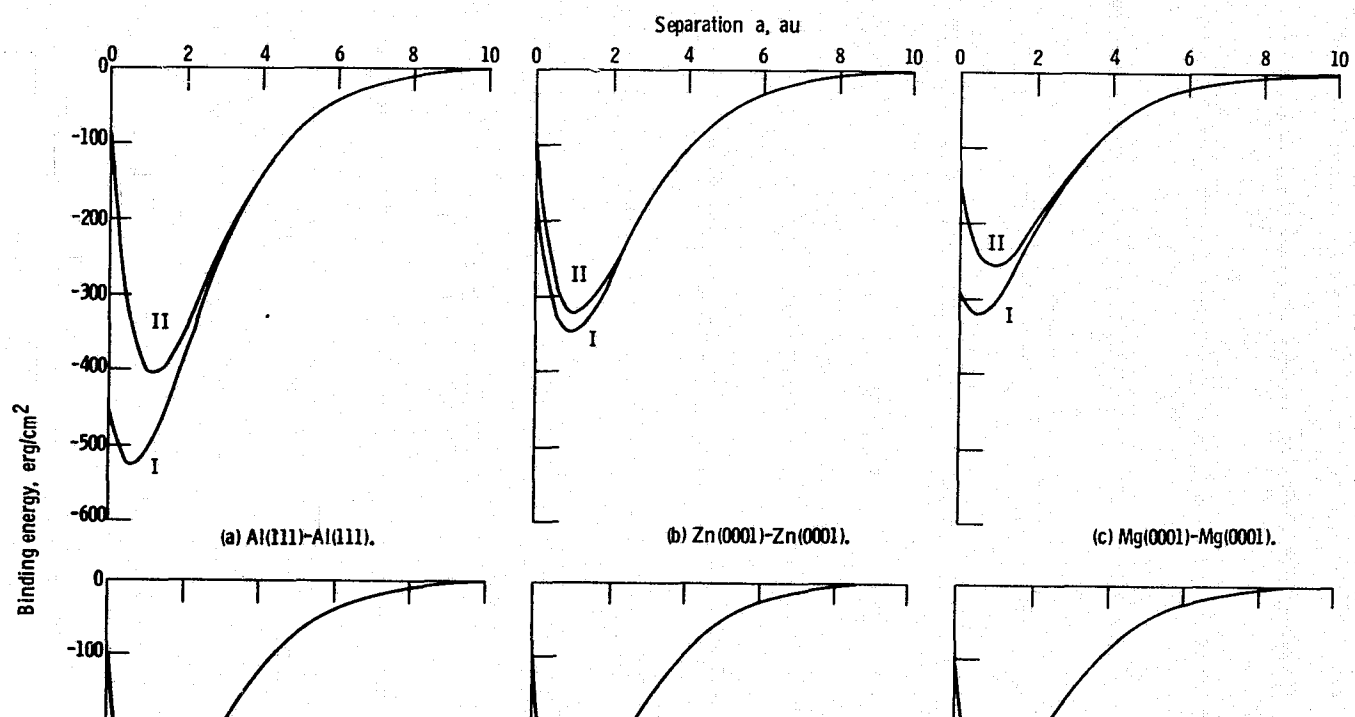


Fig. 14. - Binding energy versus separation simple overlap model for combinations as noted on the graphs. (II denotes $W_{int} = 0$.)

Table II

Jellium Force at Zero Separation
Simple Overlap Model

	Heinrich-Kumar [43]	Present Study
Al-Al	2.56×10^{-3} au	2.56×10^{-3} au
Zn-Zn	1.36×10^{-3}	1.36×10^{-3}
Mg-Mg	5.61×10^{-4}	5.60×10^{-4}
Al-Zn	1.87×10^{-3}	1.88×10^{-3}
Al-Mg	1.22×10^{-3}	1.22×10^{-3}
Zn-Mg	8.81×10^{-4}	8.78×10^{-4}

the jellium as altered by Heinrichs and Kumar [43] is presented in Table II.

III - SELF-CONSISTENT BINDING ENERGIES

The binding energy versus separation for the self-consistent like-metal contacts in registry are given in Figure 15. The two curves give the binding energies for the LDA and nonlocal approximation for the densest packed planes of Al, Mn, Mg, and Na. Infinite separation was taken at 15 au since the binding energy saturated at this value as can be seen by comparing to its value at 10 au. Figure 16 presents the binding energy for the metals obtained from finding the bulk density which minimizes the cohesive energy to first order holding the Ashcroft ion-core radius fixed. The self-consistent binding energies are qualitatively quite similar to the simple overlap results. There is a nonzero minimum and the attractive forces are quite short range as can be seen by comparing Figures 14 and 15. Quantitatively the binding energies are larger in magnitude and are slightly shorter in range than for simple overlap. A comparison of analytical (taken at the minimum in

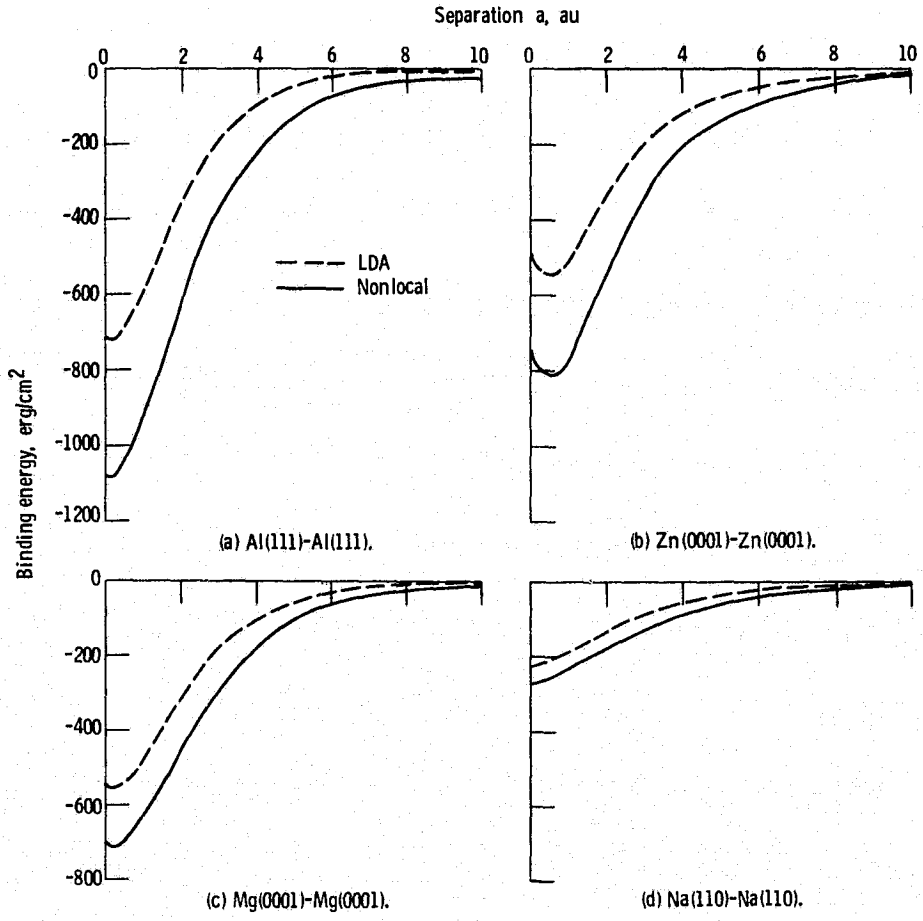


Fig. 15. - Self consistent binding energies versus separation for the LDA and nonlocal contributions to the exchange and correlation energy.

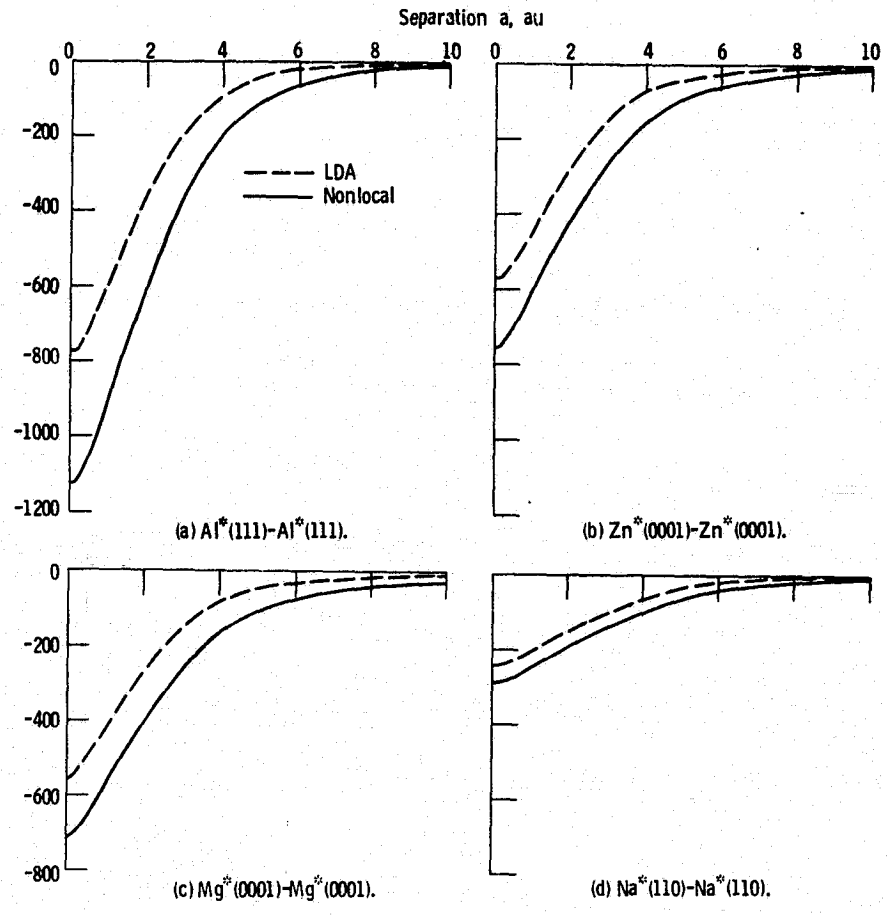


Fig. 16. - Self consistent adhesive binding energies versus separation using bulk densities obtained from minimizing the cohesive energy LDA and including nonlocal terms in the exchange and correlation energies.

the binding energy curve) and experimental surface energies are presented in Table III. The binding energies presented in Figs. 14 and 15

Table III

Comparison of Binding Energies with Surface Energy

	Simple Overlap	LDA	NLCL	Exp	Ref.
Al	525 ergs/cm^2	720	1090	1169	[53]
				(1140±200)	[54]
Zn	345	545	810	1040	[58]
Mg	315	550	710	730	[55]
				688	[56]
Na	---	240	275	273	[58]

differ from those using the experimental bulk density by the fact that the minima are at zero separation thus identifying the reason for the nonphysical, nonzero minima. Actually, the bulk density could have been held fixed and the ion-core radius could have been varied but since the primary objective was to identify the reason for the nonzero minimum and both n_+ and r_c are experimentally determined quantities the choice is somewhat arbitrary. This approach can be easily taken for those who are interested. Checks on the degree of self-consistency by calculating the jellium force at zero separation using the Budd-Vannemenus theorem [42] are presented in Table IV. A typical total force versus separation curve for magnesium including local and nonlocal effects is shown in Figure 17. These were obtained by numerical differentiation of the total energy curves using a spline fit.

The constituents of the binding energy at each separation and for all cases considered are presented in Appendix IX. Figure 18

Table IV

Jellium Force at Zero Separation
Self-Consistent Calculation

	B-V Theoreum [42]	LDA	NLCL
Al	2.558×10^{-3} au	2.558×10^{-3} au	2.580×10^{-3} au
Zn	1.365×10^{-3}	1.368×10^{-3}	1.363×10^{-3}
Mg	5.612×10^{-4}	5.615×10^{-4}	5.628×10^{-4}
Na	1.437×10^{-5}	1.452×10^{-5}	1.447×10^{-5}

presents a typical plot of these energies for the specific case of a Mg(0001)-Mg(0001) contact. There are two interesting features in these curves; the kinetic energy is negative and the potential energy is positive at intermediate separations relative to infinite separation. Thus, the kinetic energy is responsible for bonding in these regions.

Finally, the elastic constants for each element are estimated by numerically taking the second derivative of the binding energy curves near the minimum. This calculation gives an additional comparison with experiment which tests some details of the curves near the minimum. The surface energy only gives a comparison with experiment of one point. These results and their comparison with experiment are presented in Table V.

Table V

Elastic Stiffness Constant
C'_{11} ((dynes/cm^2) x10^{12})

	Theory		Exp.
	Local	Nonlocal	
Al (111)	0.746	1.23	1.23 [57]
Zn (0001)	.680	.927	.688 [58]
Mg (0001)	.619	.666	.665 [59]
Na (110)	.183	.170	.133 [60]

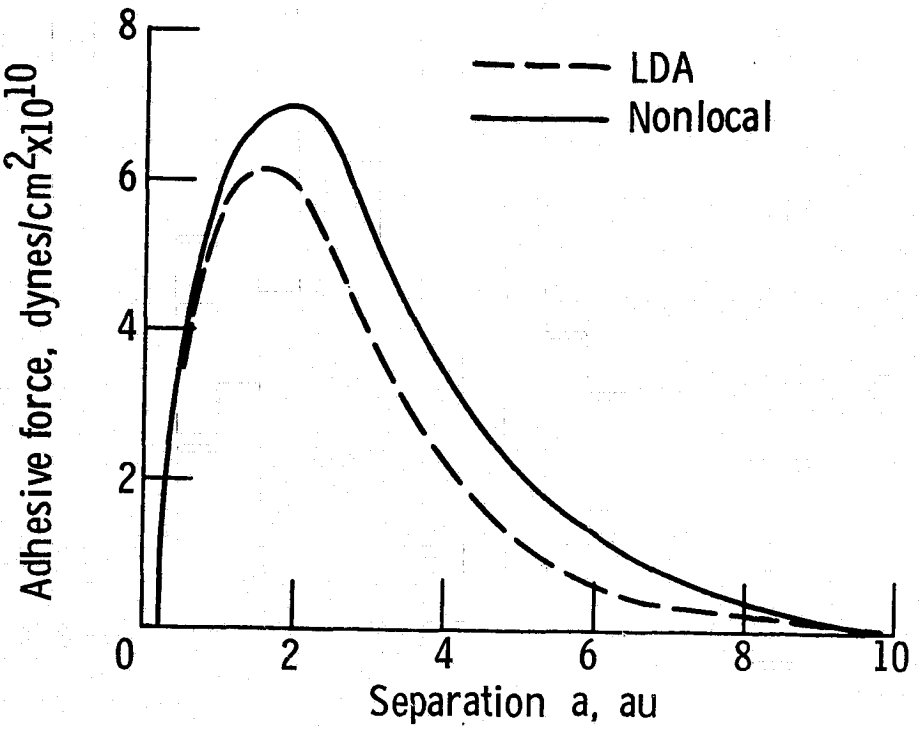


Fig. 17. - Adhesive force versus separation for a Mg(0001)-Mg(0001) contact for the LDA and including nonlocal terms in the exchange and correlation energies.

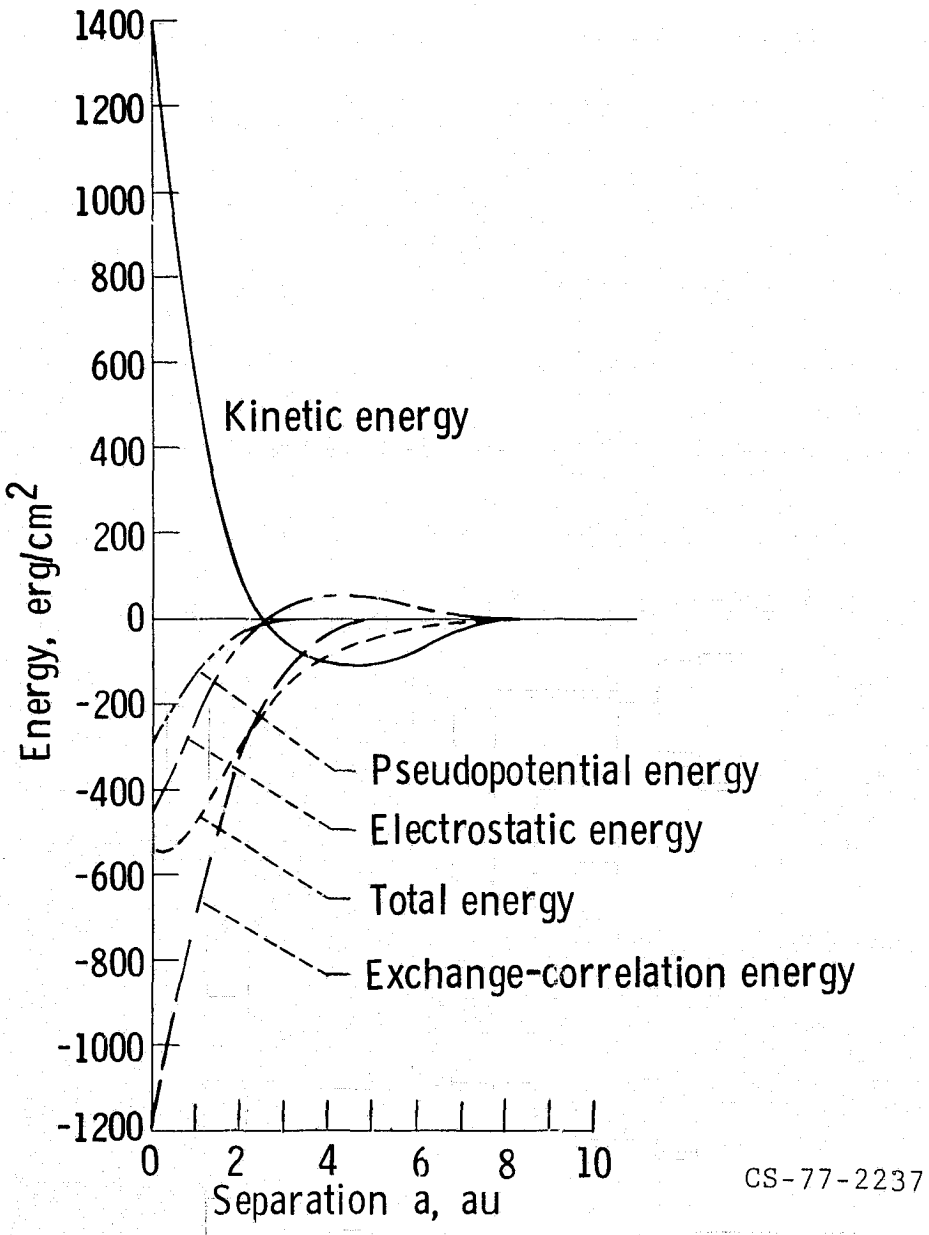


Fig. 18. - Self-consistent energy components of the binding energy for a Mg(0001)-Mg(0001) contact.

DISCUSSION

Having now presented the results of the metallic adhesion calculations, the implications and explanation of the results in terms of adhesion and their relationship to other similar surface calculations currently being conducted will be discussed. The format will follow that presented in the RESULTS section including general comments on certain aspects of the calculation. We should point out that the present work is an ab initio calculation which depends on no fitting parameters.

I - ELECTRON NUMBER DENSITY AND POTENTIAL ENERGIES

A. Electron Density

Figures 8 and 9 show some of the typical electron density profiles as a function of separation for aluminum and sodium. As we can see there are a number of features readily observable in these plots namely, that as the metals separate the electron number density in the intermediate region falls off rapidly and that the oscillations in the density increase with separation. The other interesting feature is that at a given separation the oscillations in the number density are larger for sodium than for aluminum. These oscillations are similar to the familiar Friedel oscillations [61] occurring with an impurity atom in a solid. They arise from the perturbations introduced into the potential by creating the surfaces. As would be expected the amplitude of the oscillations should in-

crease with the strength of the disturbance as is observed in Figures 8 and 9 corresponding to Figures 10 and 11 which show the increase of the potential barrier between the surfaces as a function of separation. For all separations the oscillations will have the general form given by Adawi as shown in the THEORY section and for large or infinite separation the number density should approach the form given by LK

$$n(x) \xrightarrow[x \to \pm\infty]{} n_+\left[1 + \frac{5}{(k_F x)^2}\cos(2k_F x - 2\gamma_F) + O\left(\frac{1}{x^3}\right)\right] \tag{80}$$

where γ_F is the phase shift at the Fermi momentum. A similar result is obtained for the infinite or square barrier model. If we examine this we see that $\frac{\Delta n}{n_+} \sim \frac{1}{k_F^2} \sim n_+^{-2/3}$, therefore, the amplitude of the oscillations should increase with decreasing n_+, the bulk electron density or conversely, increase with increasing r_s, the Wigner-Seitz radius. This effect is manifested in the larger oscillations for sodium and serves as a check on the results. Another perspective in explaining the oscillations is given in terms of the discontinuity in the slope of the dielectric function [61] which is due to the sharp cut off at the Fermi surface and produces oscillations in the potential of wave number $2k_F$. The wavelength of the Friedel oscillations was checked by examining $x^2(n(x) - n_+)$ near the slab boundary. In all cases it was found that near the boundary the oscillations had wavelengths very close to π/k_F ($\sim$1-2%).

Plots of the densities obtained from including gradient corrections to the potential were not included, because differences between these and the LDA densities were not perceptible with the scale used. Complete listings of these densities, however, are presented in Appendix V. This result is in agreement with that obtained by Rose, et al. [14] in their bare metal calculations who also used the Rasolt and Geldart gradient correction and also obtained only small differences in the electron number density.

B. Potential Energy

Figures 10 and 11 show the potential energy $v_{eff}(x)$ for separations of 0.25, 3, and 15 atomic units for both Al and Na. We see that the barrier increases in both height and range with separation as would be expected. In addition, we can again see that the oscillations in the potential display the same behavior as with the density, the oscillations increase with separation and with r_s.

Figure 13 shows a similar plot but for the gradient correction term included in the potential for aluminum at 15 au. In this figure, however, the potential is plotted from the end of the slab to the symmetry point. It can be seen that an anomolous depression appears in the potential. A similar behavior occurs in the potential for every value of r_s calculated. However, the potential is well behaved at 10 au. The behavior at 15 au is a result of the extrapolation of the Rasolt and Geldart [22] coefficient breaking down at these separations. Rasolt and Geldert have suggested that this coefficient is not accurate for values of r_s much greater

than six since the random phase approximation is used. At a separation of 15 au for aluminum the equivalent density falls to a minimum value equivalent to $r_s = 14.5$ whereas for a separation of 10 au the equivalent r_s value is 4.5. The comparison is similar for sodium. The behavior of $a = 15$ is therefore attributed to a breakdown of the expression. An examination of Equations (53) and (54) shows that the term multiplying $C_{xc}(n)$ is divergent as $n \to 0$ for an exponential fall-off in the density. This fact is well known and the general procedure in atomic calculations, Herman, Van Dyke, and Otenburger [41], has been to multiply the potential by a function which prevents this divergence. We can see for an exponential fall-off that although the potential is divergent, the contribution to the total energy (Eq. (67)) is convergent. The argument used is that although the potential is divergent or incorrect, the density is small in this region and thus gives a small contribution to the energy (Eq. (67)). Rose, et al. (private communication) experienced a similar problem in that they approximated $C_{xc}(n)$ by a linear fit. However, an additional function was also used to prevent divergence in their trial potential. This was the reason, in addition to the excellent curve fit, that a gaussian was chosen in the present work to fit $C_{xc}(n)$. As a test we see that in examining the binding energy curves (Fig. 15) that the binding energy has essentially saturated at a separation of 10 au and there is no strong effect at a separation of 15 au. This can be verified by the fact that the LDA binding energies which do not contain this term have similar behavior.

Figure 12 shows the increase in the barrier height versus separation in aluminum for the LDA and including the gradient terms. We can see that the two differ at small separations and approach one another at large separations. In addition, the work function has not saturated and is smaller than the Lang-Kohn (private communication) value for the jellium at a separation of 15 au. Although the differences in density are small between LDA and nonlocal and the binding energy has essentially saturated, this is not a surprising result. The electrostatic potential as determined from Poisson's Equation (Eq. (58c)) depends on differences between large numbers and thus small differences in density can be transformed to large differences in potential. Whereas, small differences in density will not be reflected as large differences in binding energy due to the variational principle as pointed out in Equation (42).

At this point some difficulties in determining the electrostatic potential should be mentioned. The self-consistent solution to the Kohn-Sham equations should require charge neutrality which is equivalent to requiring that $\frac{d\phi}{dx} \xrightarrow[x \to -\infty]{} 0$. Although this condition is imposed explicitly in the H-K formalism it does not arise as readily in the Kohn-Sham formalism and results in serious convergence problems in the self-consistent calculations because of the long-range nature of the coulomb interaction. Lang and Kohn used a variational technique which avoided this difficulty by starting with a neutralized trial density and then expanding the density in the surface region in terms of derivatives of harmonic oscillator wave

functions which preserved charge neutrality and then determining the expansion coefficients of these terms in such a way that self-consistency was required. The present author used this technique successfully on the bare-metal problem, but found it cumbersome for the bimetallic problem. Therefore, the approach described in the calculation section was attempted. First, neutrality in the slab was required, then this restriction was removed and the iterations were continued to convergence in the potential. Examination of the electrostatic potential energy near the slab bulk boundary demonstrated that $x^2\phi(x)$ had the correct behavior in this region for charge neutrality, i.e., sinusoidal oscillations. A further check of these results is obtained from the Budd-Vannemenus Theorem since the forces calculated in Table IV depend on the difference in electrostatic potential in the bulk and at the jellium surface. As can be seen the agreement is excellent. The result is not surprising since the self-consistent solution should be neutral over all space. Any solution which is not neutral would diverge. Another approach has been used in surface calculations to handle these problems by Perdew and Monnier [82] and Niemenen [32]. They modify Poisson's equation by addition a term which guarantees that the electrostatic potential satisfies the correct asymptotic boundary conditions. The Perdew-Monnier Results for the bare metal agree well with the present calculation at large separations, and therefore, both approaches serve as a mutual confirmation of each other.

II - BINDING ENERGIES FOR THE SIMPLE OVERLAP MODEL

The binding energies versus separation for the simple-overlap model are shown in Figure 14. The binding energies are given in Table III along with experimentally determined surface energies. This calculation was the first successful attempt to examine the adhesive interaction between two dissimilar clean metals. A number of interesting results are apparent; the range of the strong binding energy is approximately 4 au; the dissimilar metal nonregistry contacts (Wint = 0) were stronger than the weaker of the two metals; the minimum occurs at nonzero separation, and the binding energies are within reasonable agreement with experimental surface energies. The agreement with the qualitative and quantitative features of the self-consistent calculations (Fig. 15) is quite remarkable for such a crude approximation. In addition to reasonable values for the surface energies, the calculation gives good values for the range of the strong binding chemical forces and predicts that transfer of material from the lower surface energy to the higher surface energy can occur which is observed experimentally [4].

The simple overlap model is also important from two other theoretical aspects; in evaluating the success of Smith's surface energy calculations and in evaluating the importance of charge transfer to binding. Examination of Figure 14, curve II, shows that the simple surface energy calculation comparing zero and infinite separation which is the self-consistent Smith solution for

like metal pairs gives a poor result for the surface energy. Examining the binding energy versus separation in the spirit of cohesive energy calculations in which both energy and lattice constant are examined gives a different perspective on Smith's work in that it shows that the procedure can give better surface energies than expected. The present result shows that reasonable surface energies for similar metal contacts but poor lattice constants are obtained. Including the correct ion-ion interaction into the calculation (curve I) in effect improves the lattice constant and somewhat improves the binding energy. The question of the location of the minimum will be examined in detail later. The second result of importance especially to the dissimilar metal contacts is that binding is obtained without charge transfer and that indeed binding is obtained simply from electron-sharing. This will be important in evaluating self-consistent dissimilar metal contacts and helps separate the physical contribution necessary for binding.

A check of this calculation can be performed by a comparison with Heinrich and Kumar's [43] modification of the Budd-Vannemenus Theorem as presented in Eq. (75). This comparison is presented in Table II. As can be seen the results are remarkably good for dissimilar metals. Since the similar metal result is self-consistent at infinite separation the result for this case is not surprising. The good agreement is possibly a result of the argument in Eq. (42) concerning the effects of errors in the number density on the energy. Recently, Raykov [63] derived an expression for the difference in

electrostatic potential for the jellium model between dissimilar metal contacts as a function of separation from Heinrich's and Kumar's work. Raykov concluded that simple overlap did not correctly predict the difference in potential at the jellium surfaces for the simple overlap model in contraction to the good agreement with forces. This result is to be expected, since the calculation was not done self-consistently. Although the approach in this calculation is somewhat simple, it, in general, has produced some interesting and important results in metallic adhesion and have been used by other researchers in the field [14, 64, 65].

III - SELF-CONSISTENT BINDING ENERGIES

In this section of the paper there are a number of topics to be discussed such as comparisons with experiments for the binding energy, the location of the minimum in the binding energy curve, forces, and others. Each topic will, therefore, be discussed in a separate section for clarity.

A. Local and Nonlocal Contributions to the Binding Energy

Figure 15 shows the binding energy versus separation for Al, Zn, Mg, and Na both in the local density approximation and including the next higher order contribution to the exchange and correlation energy in the gradient expansion as determined by Rasolt and Geldart. We can see that the general features in these curves are quite similar to the simple overlap model. Quantitatively, however, the results are improved with regard to agreement with experiment and location of the minimum. The range of the strong bonding force

is still of the order of 4.0 au (defined as ~10% of the binding energy).

As can be seen in Table III, including the Rasolt-Geldart nonlocal contributions improves the agreement of the calculated surface energies with experiment (taken at the minimum in the binding energy curves). This result is in agreement with attempts by others to include such terms as discussed in the BACKGROUND section. In fact, the problem is not in the scatter in theoretical values for the surface energy, but rather the scatter in experimental values [51] for the surface energies. The experiments are usually performed of necessity at elevated temperatures and on liquid metals and the concomitant surface contamination problems often make the results of these difficult experiments questionable. An excellent review of these experiments is presented by Hondros [66]. In addition, the present and the other surface energy calculations are truly brittle fracture at 0 K models. Consequently, it is necessary to obtain surface energy measurements for solids of which there are few or to extrapolate from liquid metal values. The latter is the approach taken by Lang and Kohn, however, in performing the extrapolation they extrapolated through a phase change. In this paper, we choose instead the values published by Wawra [53], who derived the surface energies indirectly from solids at close to 0 K via ultrasonic attenuation. Wawra's method suffers from the same experimental uncertainty as other studies (~±20%) because it depends on the fact that the surface energy is proportional to the bulk modulus [67]. He uses this principle and the surface energy data of others in

order to determine the proportionality constants. His experiments are performed under the correct experimental conditions, i.e., solids at low temperature and thus require no extrapolation. Unfortunately, for Mg we could not find values for solids and have used the extrapolated values of Bohdansky and Shins [55] and compare to those of Tyson and Miller [56].

Evaluating these results in terms of adhesion experiments is quite difficult. Clean real surfaces in contact do not have well defined surface areas because of the asperity problem and consequently quantitative comparisons may be questionable. In addition, elastic recovery, ductile fracture in metals, and defects may make comparisons even more difficult. The practical importance of the present work is in setting bounds for studies of both breaking force and contact areas. When evaluating real surfaces the question must also be asked whether the strong short range is the dominant force in contacts, since the "true" contact is just over a fraction of the apparent area. In between it is not obvious whether the strong short range or the weaker long range Van der Waals forces dominate. Inglesfield [65] directed himself to this question using the results of Ferrante and Smith [28] and his own Van der Waals calculation and concludes that the long range forces make a negligible contribution in mechanical adhesion for aluminum based on estimates of the true contact area and an estimate of the average separation between asperities. In conclusion, it should be pointed out that the strong bonding forces are important in adhesive wear [4] where wear particles are generated because of adhesion and in brittle fracture of

metals at low temperatures [44].

B. Location of the Minimum in the Binding Energy

As stated previously the location of the minimum in surface energy calculations is analogous to examining the accuracy of the lattice constant in cohesive energy calculations. Therefore, the present work is a further check on surface energy calculations which evaluates the accuracy of how well it predicts the lattice constant. As we can seen in Fig. 15 for Al, Zn, and Mg we overestimate the interplanar spacing at the surface whereas for Na the calculation underestimates the surface lattice constants. It was speculated that the reason for nonzero minimum was that the bulk lattice constant (or n_+) must be chosen such that the cohesive energy is a minimum for the Ashcroft pseudopotential. The Ashcroft pseudopotential did not minimize the observed equilibrium bulk density for most bulk metals [62]. In order to accomplish this we use the expression for the ground state energy per atom for the solid obtained by Heine and Weaire [68].

$$U_o = \frac{1.105Z^{5/3}}{r_a^2} - \frac{0.458Z^{4/3}}{r_a} - \frac{0.44Z^{4/3}}{r_a + 7.8Z^{1/3}} - \frac{0.9Z^2}{r_a} + \frac{3Z^2}{2r_a}\left(\frac{r_m}{r_a}\right)^2 - A_o\left(\frac{r_m}{r_a}\right)^3 + (\alpha - 1.8)\frac{Z^2}{2r_a} \qquad (81)$$

Where $r_a = Z^{1/3} r_s$ and Z is the valence of the ion. The first term is the kinetic energy per electron. The second and third terms are the exchange and Wigner form for the correlation energy per particle. The next three terms are a combination of the poten-

tial for a uniform electron gas and the ionic pseudopotential which is averaged over the ion-core sphere. These terms correspond to the pseudopotential corrections presented earlier. The last term corrects for Ewald energy for point ions in a uniform electron gas and is similar to what we have previously called Wint. Therefore, it is a point ion correction where the constant α is given for a number of crystal structures in Reference [69]. The form for the energy presented in Eq. (81) is written in terms of the Abarenkov, Animalu, and Heine pseudopotential. In order to use the Ashcroft pseudopotential we set A_0, the value of the potential in the ion core, equal to zero and $r_m = r_c$. We proceed by finding the value of r_a and thus r_s which minimized U_0 by differentiating and finding the zeroes of dU_0/dr_a. In the subsequent calculation for the hcp metals the value of the axial ratio which minimized the Ewald energy is used, however, the difference between this and the ideal ratio is negligible in the present calculation. Having determined the r_s which minimized U_0 for the Ashcroft pseudopotential for each metal we repeat the self-consistent calculations for the binding energies. The results are shown in Figure 16. These can be compared with the results obtained for the experimental r_s values (Fig. 15) for both the LDA and with gradient corrections. We see that the minimum has moved and occurs at zero separation. This is somewhat difficult to judge for Al, Zn, and Mg because if we look at the binding energies for experimental r_s values we see that there is a very rapid rise from the minimum. Curve fitting the new binding energies in the region of the minimum and extrapolating to

$a < 0$ indicated that there was indeed a minimum. Also using the binding energy curves in Figure 15 near the minimum for comparison is convincing that there is indeed a minimum at these points. The results are most obvious with Na where the minimum for experimental values occur for $a < 0$ and the shift in the position of the minimum is toward the right. Therefore, it is apparent that a large portion of the discrepancy in the location of the minimum can be accounted for by the consistency between r_c and n_+ with regard to the cohesive energy.

C. Components of the Binding Energy and Forces

Appendix V gives the components of the binding energy for each material combination. The kinetic, exchange, and correlation total electrostatic (jellium + Wint), pseudopotential, nonlocal, and jellium components of the binding energy are presented for each separation referenced to a separation of 15 au. Since only the bare metal values for these quantities are available in the literature [7,14,62] we compare our values for the components of the surface energy with these values. The present results do not compare well with Lang and Kohn but agree extremely well with those of Perdew and Monnier [62]. The reason for the disagreement with Lang and Kohn and the agreement with Perdew and Monnier is that Lang and Kohn interpolated to obtain densities for nonintegral r_s values whereas Perdew and Monnier and the present author used the experimental values of r_s for each material. Perdew and Monnier had also come to the same conclusion. The fact that the surface energy

agreed well between the three even though the components did not is attributable to the argument given in Eq. (42) for the accuracy of simple overlap. That is, that the errors in the energy are second order in the number density. There is a disagreement with Perdew and Monnier's energies for zinc. The authors have checked their calculation (private communication) and now agree well with these results. As was mentioned, there was somewhat of a discrepancy with the results of Rose and Shore [14] concerning the nonlocal contributions to the energy, but these have also been resolved to be related to interpolation to obtain densities and a less accurate technique for obtaining numerical derivatives (private communication). It should be pointed out, therefore, that we get the correct separated solid limit for not only the surface energy but also the components of the surface energy.

A second point that should be addressed is the validity of using perturbation theory in order to evaluate the electron-ion contribution to the energy. This contribution is large and is needed for binding since the jellium is unbound. It is small compared to the kinetic energy. Perdew and Monnier found the perturbation theory to be fairly accurate (~10% error in surface energy for Al ranging to little effect of Na) but poor for lead by including the electron-ion pseudopotential self-consistently in their surface energies. That fact that it is poor for lead is not surprising since it is the only tetravalent metal tested, has more than one value for the ion core radius depending upon the property that is fit and and has by far the highest atomic num-

C2

ber of the elements examined. This was first pointed out by Lang and Kohn [7].

Figure 18 is a plot showing the breakdown of component energy versus separation for Mg relative to infinite separation (a = 15 au). Some interesting features appear in this figure, namely, that over a portion of the curve the kinetic energy is negative relative to infinite separation whereas the potential energy is positive. The total energy shows none of these interesting features as might be expected. Therefore, at large separations the change in kinetic energy is responsible for the binding. Before entering into a discussion of this behavior at this point a more general discussion concerning the details of the calculation is of interest.

It is interesting to examine the present calculation from the standpoint of the variational principle and of chemical binding to which the present work bears strong analogies. In order to have bonding it is necessary to have the energy lower at a finite separatio than at the separated solid limit as is the case in chemical bonding. Also by analogy to the chemical bond the bonding apparently arises from sharing electrons in the bond region. In chemical binding the energy lowers to a minimum value at the equilibrium separation and then rises beyond this point due to nuclear repulsion. Examining the binding energy curves simply from their qualitative aspects reveals that it would be difficult to distinguish them from those that would be expected for binding in a diatomic molecule. In a sense bimetallic adhesion can be looked upon in terms of the binding of two large molecules when brought into con-

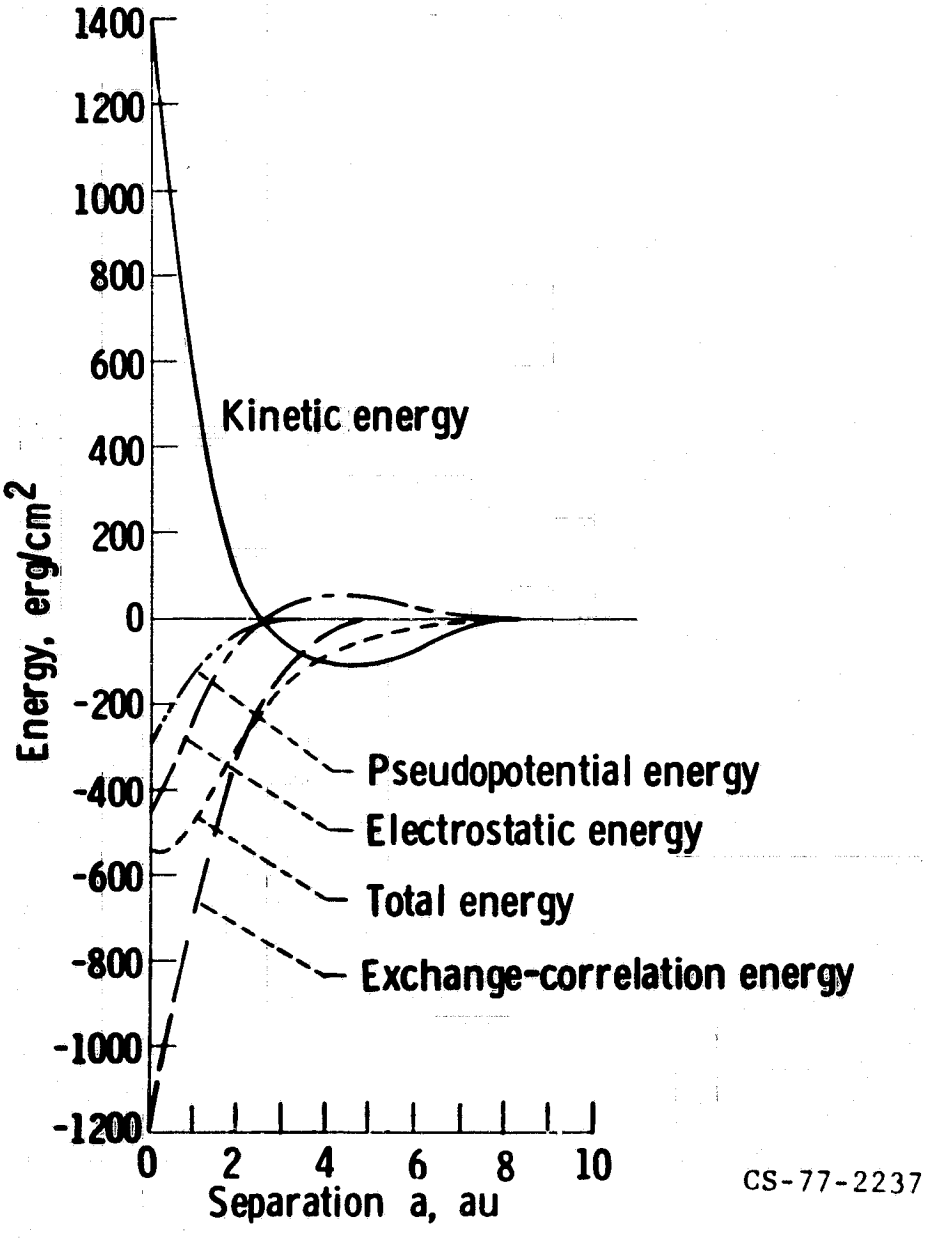


Fig. 18. - Self-consistent energy components of the binding energy for a Mg(0001)-Mg(0001) contact.

tact with one another and examining the effect of varying the charge density on the total energy. It is interesting to see how far the analogy will carry over. If we compare the components of the binding for simple overlap (Fig. 19) and for the self-consistent case we find that the kinetic and potential energies change monotonically. Thus, the behavior observed in the self-consistent case is not necessary for bonding and is a result of charge rearrangement. The fact that bonding occurs for simple overlap is sufficient to say that bonding will occur for dissimilar metals by the variational principle.

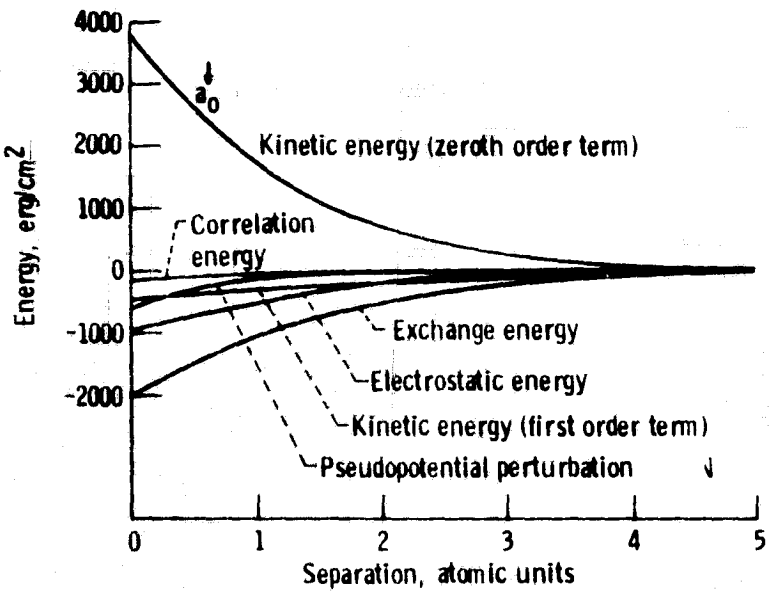


Fig. 19. - Energy components for the typical case of Al-Zn. a_0 is the location of the energy minimum.

In seeking an explanation for the behavior of the potential and kinetic energy we again find a direct analogy in the work of Feinberg and Ruedenberg (FR) [70] on the formation of a hydrogen molecule, H_2. FR solve the hydrogen molecule problem variationally

by use of trial wave functions. They then in a manner similar to the present calculation determine the kinetic, potential, and total energy as a function of separation. The same behavior for the kinetic and potential energy is observed in the hydrogen molecule as in the self-consistent, like-metal, bimetallic case. FR have an explanation of this behavior both in terms of the wave functions and the electronic charge density. The drop in the kinetic energy is a result of the symmetric wave functions in the bond region. The overlapping orbitals produces a smoothing of the wave functions in the bond region effectively destroying $d\psi/dx$ in this region. The $T_{||}$ component of the kinetic energy is reduced relative to the separated atom limit. The behavior of the potential energy is caused by charge transfer into the bonding region. In this case charge is transferred from a region where potential energy is low near the nuclei to a region where potential energy is higher in the bond. Since the kinetic energy effect dominates, kinetic energy is responsible for incipient bonding. It is this kinetic energy term which is also responsible for bonding at the equilibrium separation where the virial equation $T = -(1/2)V$ must be satisfied. The lowering of the kinetic energy pressure results in a charge contraction towards the nuclei thus lowering the potential energy and near equilibrium a subsequent increase in the kinetic energy because of the contraction. As a result of the combined effect the energy minimum is reached at a higher value of the kinetic energy. FR point out that in viewing the effects in terms of the density that the smoothing of the density in the bond region gives a decreased ki-

netic energy by virtue of the uncertainty principle.

The situation in the adhesion problem is similar to that in molecular bonding and gives the same qualitative behavior. Unfortunately, it is not possible to do a complete examination for adhesion, because of the self-consistent calculation. In molecular bonding with trial wave functions it is simple to fix certain properties such as spacing and examine the effects on the energy of others such as charge distribution. FR conclude that the difference in kinetic energy pressure in the molecule as opposed to the atom is essential to the formation of the covalent bond. This is not the case in adhesive bonding. The simple overlap model demonstrates that electron sharing is sufficient for bonding without the paradoxical effects in the kinetic and potential energies. The rate of loss in potential energy is simply greater than the rate increase in kinetic energy. Similar effects to molecular bonding occur in the self-consistent calculations but these must be a result of charge rearrangement analogous to those presented by FR for molecular bonding.

Finally, we show a plot of the adhesive force versus separation for the LDA and gradient expansion for Mg (0001) vs Mg (0001). This result is typical for all other materials. We can see that the force rises rapidly with separation to a maximum value which gives the force for brittle fracture. The nonlocal approximation gives a higher breaking force than the LDA in agreement with binding energy curves. The force achieves its maximum value at approximately 0.1 nanometers. Also included is Table IV which shows the jellium force at zero separation calculated for present results using

Eq. (72) and using the Budd-Vannemenus theorem (Eq. (74)). This table is actually a check on the self-consistency of the present calculation.

IV - ELASTIC STIFFNESS CONSTANTS

The elastic stiffness constants can be estimated from the binding energy curves by taking the second derivative as pointed out in the THEORY section. Comparing elastic constants with experiment is an important check on the Kohn-Sham formalism, since the only previous comparisons were with surface energies which only examines one point on the binding energy curves. The elastic constants check the behavior of the solution in the vicinity of the minimum. In addition, unlike surface energies, elastic constants can be determined very accurately experimentally. The results of the calculation as determined by a spline fit are presented in Table V along with experimental values [57,58,59,60], as can be seen the agreement is quite remarkable and is of the same order of accuracy as obtained from cohesive energy calculations [71,72]. The nonlocal values are better than the local with the exception of zinc which also deviates for the surface energy. Monnier and Perdew [62] point out that the Ashcroft pseudopotential may be in error for zinc and consequently this may account for the poorer agreement. The agreement for Na is quantitatively poor and probably is worse than the others since points are not available near the minimum for the spline fit. The trends in elastic constants are also predicted correctly.

The degree of agreement may have been somewhat fortuitous since there are not many values of binding energy available near the minimum. Obtaining binding energies for more separations near the minimum is difficult since it would require a variable mesh size with smaller intervals in the gap between the surfaces or a small uniform mesh size which would require large computer storage and long computation times. The spline fit is convenient since it is smooth, provides an analytic form, and can handle a variable spacing. In spite of the questionable accuracy the results are sufficiently good to encourage more sophisticated numerical techniques to obtain self-consistent solutions for small gap sizes.

CONCLUDING REMARKS

The adhesion of simple metals in contact (Al, Zn, Mg, and Na) has been examined by use of the Hohenberg and Kohn formalism and the Kohn and Sham formalism with and without gradient terms in the exchange and correlation energy. The spirit of this calculation is similar to cohesive energy calculations in which both the energy and lattice constant are investigated by examining binding energy versus separation. Strong analogies to molecular binding are also observed when examining both the binding energy curves and the component energies versus separation.

The results of the Hohenberg and Kohn simple overlap calculations (no relaxation or self-consistency), give reasonable quantitative and qualitative results. The surface energies are of the right order of magnitude, give the correct relative trends, and the range of strong chemical bonding forces is given. The model predicts transfer in dissimilar metal contacts in that interfacial energies are greater than binding energies in the weaker of the two materials. The possibility of incorrect lattice constants (nonzero minimum) is predicted as is observed in self-consistent calculations. In addition, the model demonstrates that charge transfer (relaxation is not necessary for bonding).

The self-consistent Kohn-Sham calculations for similar metal contacts are quite quantitative. Good agreement with experiment for

both surface energies and elastic stiffness constants are obtained when nonlocal terms in the exchange and correlation energy are included. The range of the strong chemical bonding forces is found to be 0.2 nanometers. Corrections to the lattice constant (nonzero minimum) are obtained by determining the bulk density which minimizes the cohesive energy for the Ashcroft pseudopotential. Excellent degrees of self-consistency are obtained as can be verified by comparison with the Budd-Vannemenus theorem. Strong analogies to molecular binding are observed when comparing the behavior of the kinetic and potential energies versus separation to similar results obtained for H_2 molecules by Feinberg and Ruedenberg. Crystallinity included in perturbation theory for the pseudopotential and a lattice sum for ionic potentials is found to be necessary for binding and agreement with experiment.

APPENDIX I

PSEUDOPOTENTIAL CORRECTION

We here present the derivations of Eqs. (70a) and (70b) for completeness since these derivations do not appear in the literature. The first term Eq. (69a) has a simple geometrical interpretation. The first term is the potential due to an array of sheets of charge with a surface density given by the proper planes of interest (e.g., fcc(111)). The second term is the potential due to the jellium charge density extending half an interplanar spacing on each side of a lattice plane. Thus the geometrical model for this term is a series of sheets of charge imbedded in the uniform distribution of charge with the jellium surface extending half an interplanar spacing beyond the first lattice plane. Let us first consider the first lattice plane since the extension to other planes is elementary. From elementary electrostatics and simple geometrical considerations the field due to the first sheet of charge is

$$E_1 = \mp 4\pi \frac{n_+ d}{2} \begin{cases} x > -d/2 \\ x < -d/2 \end{cases} \qquad \text{(I1)}$$

where d is the interplanar spacing and we are defining the electronic charge as positive. The field due to an element of jellium for $x > -d/2$.

$$E_2 = 4\pi n_+ \int_{-d/2}^{x} dx = 4\pi n_+ (x + d/2) \tag{I2}$$

The total field is

$$E = E_1 + E_2 = 4\pi n_+ x = -dV_1/dx \tag{I3}$$

For V = 0 at x = 0 we have

$$V_1 = -2\pi n_+ x^2 \qquad 0 > x > -d/2 \tag{I4}$$

for -d < x < -d/2, we again have

$$E_2 = 4\pi n_+ (x + d/2)$$

$$E = E_1 + E_2 = 4\pi n_+ (x+d) = -dV_2/dx \tag{I5}$$

Requiring continuity of the potential at x = -d/2 we get

$$V_2 = -2\pi n_+ (x+d)^2 \tag{I6}$$

Eq. (70a) follows simply by extending this results to other lattice planes.

The second term in the pseudopotential (Eq. (69b)) is a plane-wise average of the difference between the coulomb potential and Ashcroft pseudopotential [73]. Thus the term is zero outside the ion-cores and the plane wise average of the coulomb potential within the ion cores. Considering only the left-half and the first plane of pseudo-ions as an example we can evaluate this term. The integral we wish to evaluate is thus

$$\delta V_2 = \sum_{\nu} \int \frac{-Z \, dA}{[(x'-x_0)^2 + (y'-y_0)^2 + (z'-z_0)^2]^{1/2}} \tag{I7}$$

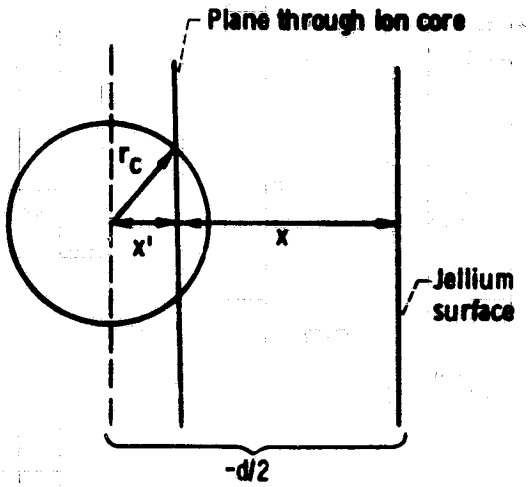
where A is the cross-sectional area and ν is a summation index that locates the centers of the ions. Since the integrals over each ion core are identical choosing now a single plane and atom we can write

$$\delta V_2 = -\frac{ZNd}{Ad} \int \frac{dy'dz'}{[x'^2 + y'^2 + z'^2]^{1/2}} \tag{I8}$$

where N is the total number of ion cores in the plane, A is the cross-sectional area and we are now integrating over a single ion core

$$n_+ d = \frac{ZNd}{Ad} \tag{I9}$$

We can now show the integration schematically with the following diagram



I.1. - Geometrical construction for the pseudo-potential contribution from the ion-core.

Transforming to cylindrical coordinates in the y-z plane we have

$$\delta V_2 = -n_+ d \int_0^{\sqrt{r_c^2-(x+d/2)^2}} \int_0^{2\pi} \frac{r\,dr\,d\phi}{[r^2+(x+d/2)^2]^{1/2}} \tag{I10}$$

integrating we get

$$\delta V_2 = 2\pi n_+ d\,(r_c - |x+\tfrac{1}{2}d|)\,\theta(r_c - |x+\tfrac{1}{2}d|) \tag{I11}$$

where the Heaviside function restricts the contribution to within the ion core. Again the extension to the whole lattice in order to obtain Eq. (73b) follows easily.

APPENDIX II

LATTICE SUM

In this Appendix a more detailed presentation of the techniques used to derive the expression for the lattice sums in Eqs. (40a), (40b), and (40c) is presented. This again is included for completeness since Ferrante and Smith [28] outlined the procedure in their initial adhesion calculations. The evaluation of these terms will be presented for the specific case of an fcc(111) versus fcc(111) interaction as an example.

As stated in Eq. (38) the interaction energy is given by

$$W_{int}(a) = \int \frac{\rho_1(\underline{r})\,\rho_2(\underline{r}')}{|\underline{r}-\underline{r}'|}\,d\underline{r}\,d\underline{r}' \qquad \text{(III)}$$

where the subscripts 1 and 2 refer to the half space and $\rho_i(\underline{r})$ is the net charge density ion minus jellium. The principle involved here is similar to the pseudopotential correction for the electron-ion interaction. The jellium-jellium interaction is subtracted out and the ion-ion interaction is added in. The difference in this case is that the result is exact. Thus we have a situation where calculationally we are evaluating the equivalent of the interaction energies of two periodic arrays of positive ions in a uniform distribution of negative charge. The primary contribution of this calculation is that it has extended the evalu-

ation of interaction energy to nonzero separation between the slabs which has been put to use in other calculations [32].

The charge density is given by

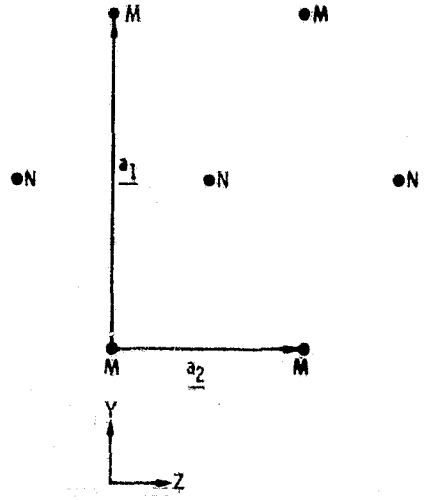
$$\rho(\underline{r}) = Z \sum_m \delta(x - x_m) \sum_\ell \sum_h \delta(y - y_\ell)\delta(z - z_h) - \sigma_1 \sum_m \delta(x - x_m) \qquad \text{(II2)}$$

where Z is the valence of the ions, the δ's are Dirac δ-functions and σ_1 is the charge per unit area of the jellium. The procedure applies only to the case in which the jellium from the two half-spaces do not overlap. The general procedure is to expand the density in a Fourier series giving

$$\rho(\underline{r}) = \sigma_1 \sum \delta(x - x_m) \sum_{\ell=-\infty}^{\infty}{}' \sum_{h=-\infty}^{\infty}{}' C_{m\ell h} e^{ig_\ell y} e^{ig_h z}$$

where g_ℓ and g_h are components of reciprocal lattice vectors, $C_{m\ell h}$ is a structure factor and the prime indicates that the terms $g_\ell = g_h = 0$ has been omitted. This term cancels out the jellium background and gives a convergent series.

We now proceed with an example calculation to demonstrate the procedure used. Taking an fcc(111) surface we choose an orthogonal coordinate system as shown.



II.1. - Breakdown of fcc(111) or hcp(0001) planes into two sublattices.

where $\underline{a}_1$ and $\underline{a}_2$ are basis vectors for the M mesh which has a unit cell area A1 where $\underline{a}_1 = c_1\sqrt{3}\,\hat{j}$; $\underline{a}_2 = c_1\hat{k}$ where $\hat{j}$ and $\hat{k}$ are unit vectors in the y and z directions and c_1 is the nearest neighbor distance. The N sublattice can be located with respect to the M using the translation vector $(\sqrt{3}/2)c_1\hat{j} + (1/2)c_1\hat{k}$, thus we have a two-dimensional lattice with a basis. The fcc structure has ABC stacking. Let $\rho^{(1A)}$ be the difference between the discrete charge density and the jellium charge density for the A-planes

$$\rho^{(1A)} = \underbrace{-\sigma_1 \sum_{m_1} \delta(x' - x_{m_1}^{(A)})}_{\text{jellium}}$$
$$+ \underbrace{Z_1 \sum_{m_1} \sum_{k_1'} \sum_{l_1'} \delta(x - x_{m_1}^{(A)})\,\delta(y' - \sqrt{3}c_1)\,\delta(z' - c_1 l_1')}_{\text{M-mesh}}$$
$$+ \underbrace{Z_1 \sum_{m_1} \sum_{k_1'} \sum_{l_1'} \delta(x - x_{m_1}^{(A)})\,\delta(y - \sqrt{3}c_1(k_1' + 1/2)) + \delta(z' - c_1 l_1')}_{\text{N-mesh}} \qquad \text{(II3)}$$

where the summation indices h_1' and ℓ_1' locate points in the direct lattice.

This can then be expanded in a Fourier series with reciprocal lattice vectors determined by the standard procedures given by $\underline{b}_1 = (\sqrt{3}/3c_1)\hat{j}$; $\underline{b}_2 = (1/c_1)\hat{k}$ for the A planes giving

$$\rho^{(1A)}(x',y',z') = -\sigma_1 \sum_{m_1}^{-} \delta(x-x_{m_1}^{(A)}) + \frac{\sigma_1}{2} \sum_{m_1} \sum_{\ell_1} \sum_{h_1} \delta(x-x_{m_1}^{(A)})$$
$$\cdot \exp\left[(i2\pi/3c_1) h_1 y'\right] \exp\left[(i2\pi/c_1)\ell_1 z'\right]$$
$$+ \sigma_1/2 \sum_{m_1} \sum_{\ell_1} \sum_{h_1} \delta(x-x_{m_1}) \exp\left[(i2\pi/3c_1)\sqrt{3}\, h_1 y'\right]$$
$$\cdot \exp\left[(i2\pi/c_1)\ell_1 z'\right) \exp\left[i\pi(h_1+\ell_1)\right]$$

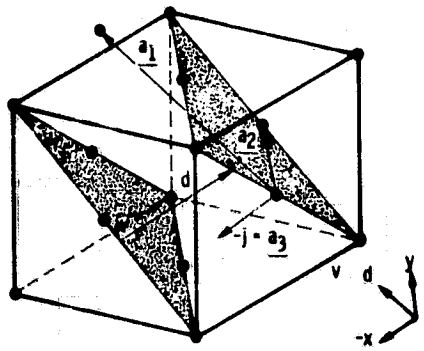
(II4)

where the h_1 and ℓ_1 summations locate points in the planar reciprocal lattice.

The B set of planes can be located with respect to the A by the direct lattice vector $(\sqrt{3}/3)c_1\hat{j}$ and the C set of planes by adding $(\sqrt{3}/6)c_1\hat{j} + (1/2)c_1\hat{k}$. For the total charge density which will be used in the potential we have

$$\rho^{(1)} = \rho^{(1A)} + \rho^{(1B)} + \rho^{(1C)} \tag{II5}$$

An example of the three-dimensional lattice is shown in Figure II-2.



II.2. - Three-dimensional drawing showing coordinate axes and basis vectors for fcc(111) planes.

The potential at a point outside of the metallic half space is given by

$$\delta\phi^{(i)} = \int d\underline{r}' \, \frac{\rho^{i}(\underline{r}')}{|\underline{r} - \underline{r}'|} \tag{II6}$$

evaluating this integral we get

$$\delta\phi^{(1)} = \frac{\sigma_i c_i}{2} \sum_{m_i} \sum_{h_i, \ell_i}{}' \left\{ \frac{1 + \exp[i\pi(h_i + \ell_i)]}{(\ell_i^2 + h_i^2/3)^{1/2}} \exp\left(i \frac{2\pi}{3c_i} \sqrt{3} h_i y\right) \right.$$

$$\cdot \exp\left[i \frac{2\pi}{c_i} h_i\right] \exp\left[-\frac{2\pi}{c_i}(x - x_{m_i}^{(A)})(\ell_i^2 + h_i^2/3)^{1/2}\right]$$

$$+ \exp\left[\frac{i2\pi}{c_i} h_i\right] \exp\left[-\frac{2\pi}{c_i}(x - x_{m_i}^{(B)})(\ell_i^2 + h_i^2/3)^{1/2}\right]$$

$$\left. + \exp[i\pi(h_i/3 + \ell_i)] \exp\left[-\frac{2\pi}{c_i}(x - x_{m_i}^{(C)})(\ell_i^2 + h_i^2/3)^{1/2}\right] \right. \tag{II7}$$

In performing these integrals the following relationships have been used

$$\int_0^\infty dx \; \frac{\cos(\alpha x)}{(\beta^2+x^2)^{1/2}} = K_0(\alpha\beta) \qquad \alpha,\beta > 0$$

$$\int_0^\infty dx \; K_0(\alpha^2(x^2+\beta^2))\cos(\gamma x) = \frac{\pi}{2} \; \frac{\exp[-\beta(\alpha^2+\gamma^2)^{1/2}]}{(\alpha^2+\beta^2)^{1/2}}$$

for $\mathrm{Re}\alpha > 0$; $\mathrm{Re}\beta > 0$, and $\gamma > 0$ where K_0 is the modified Bessel function of the second kind of order zero.

In order to calculate the interaction energy we perform the integral

$$W_{int}(a) = \int d\underline{r} \; \rho^2(\underline{r})\delta\phi^{(1)} \tag{II8}$$

where $\rho^{(2)}(\underline{r})$ is the charge density in the second slab.

Wint/A is composed of terms of the following form

$$\frac{\sigma C_1^2}{4} \sum_{m_2,m_1} \sum_{\ell_1,h_1}{}' \sum_{\ell_2,h_2}{}' \frac{(1+\exp[i\pi(h_2+\ell_2)])(1+\exp[i\pi(h_1+\ell_1)])}{(\ell_1^2+h_1^2/3)}$$
$$\cdot \exp\left[-\frac{2\pi}{C_1}(X^{(A)}_{m_2}-X^{(A)}_{m_1})(\ell_1^2+h_1^2/3)\right] \exp[i\pi(h_2/3+\ell_2)]$$
$$\cdot \iint \frac{dy\,dz}{A} \exp\left[\frac{2\pi i}{C_1}\left(\frac{h_1}{C_1}+\frac{h_2}{C_2}\right)\right] \exp\left[2\pi i\left(\frac{\ell_1}{C_1}+\frac{\ell_2}{C_2}\right)\right] \tag{II9}$$

where $X^{(A)}_{m1} = -3d(m_1 - 1) - (1/2)d$, $X^{(2)}_{m2} = 3d(m_2 - 1) + (1/2)d + a$ similar expressions can be derived for B and C planes [28]. We can see that the y-Z integrations give respectively Kronecker deltas in $h_1,-h_2$ and $\ell_1,-\ell_2$, respectively. Finally since the sums extend from $-\infty$ to ∞ the terms can be simplified by com-

bining positive and negative terms to give trigonometric functions and using the identity $\sum_{m_1=1}^{\infty}\sum_{m_2=1}^{\infty} g(m_1 + m_2) = \sum_{m=1}^{\infty} mg(m)$ for the planewise summations in the x-directions and considerable algebra we get Eq. (40a) for the fcc(111) lattice sum. The sums for the hcp(0001) and bcc(001) surfaces follow the same procedures with only the geometrical specifications of the lattice vectors and basis differing for these planes.

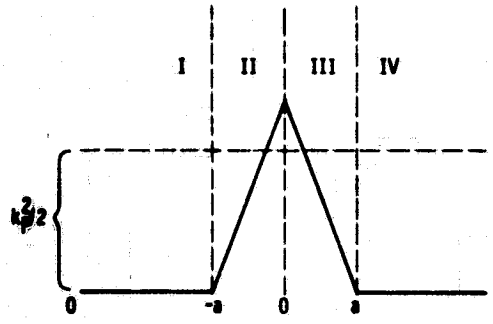
Another interesting aspect to this calculation is a consideration of what occurs in the lattice sum in the case that two dissimilar metals in contact. In this case we get nonregistry between the half spaces facing one another. This is equivalent to having h_2/c_2 and ℓ_2/c_2 in the integrations shown in Eq. (II9), consequently instead of getting Kronecker δ's in the integers h and ℓ we could only get a nonzero result for the lowest integer ratios $\frac{\ell_1}{\ell_2} = -\frac{c_1}{c_2} = \frac{h_1}{h_2}$ (a more general discussion of this point is presented by Ferrante and Smith [28].) Since for most dissimilar materials this would be quite a large number the contribution to Wint for dissimilar materials would be quite small because of the exponental fall off in Wint. Consequently, we have two extremes for the inclusion of the ion-ion interaction registry which applies to the case of separating a perfect solid to nonregistry which applies to dissimilar metals in contact and for which the principle ionic con-

tribution is the jellium-jellium interaction of the leading term in the lattice sum.

APPENDIX III

SOLUTION FOR THE TRIANGULAR POTENTIAL

There has been considerable interest in a linear ramp potential for simulation of the bare metal problem. Sahni and Grunebaum [74] have found the slope and barrier height which minimized the total Kohn-Sham energy and got good agreement with the self-consistent Lang-Kohn densities and energies. Although the solution for the triangular potential (Fig. III.1) was simply chosen to check the numerics in the present calculation inclusion of details of techniques used to solve the symmetric triangular potential are presented since they may be useful for metal-metal contact calculations.



III.1. - Triangular potential barrier.

The potential energy for this calculation is defined as follows.

$$V(x) = \begin{cases} 0 & x \leq -a \\ \alpha(x+a) & -a < x < 0 \\ \alpha(-x+a) & 0 \leq x \leq a \\ 0 & x > a \end{cases} \qquad \text{(III1)}$$

We have therefore for the Schroedinger equation in each region

$$\text{I} - \quad -\frac{1}{2}\frac{d^2\psi}{dx^2} = (k^2/2)\psi$$

$$\text{II} - \quad -\frac{1}{2}\frac{d^2\psi}{dx^2} + \alpha(x+a)\psi = (k^2/2)\psi$$

$$\text{III} - \quad -\frac{1}{2}\frac{d^2\psi}{dx^2} + \alpha(x+a)\psi = (k^2/2)\psi$$

$$\text{IV} - \quad -\frac{1}{2}\frac{d^2\psi}{dx^2} = \left(\frac{k^2}{2}\right)\psi \qquad \text{(III2)}$$

Considering Eqs. II and III we see that these can readily be cast in the form of Airy's equation [75] starting with region II we have

$$\frac{d^2\psi}{dx^2} - \gamma(x+a-E')\psi = 0 \qquad \text{(III3)}$$

where $\gamma = 2\alpha$ and $E' = k^2/2\alpha$. We next make a variable transformation $Z_1 = \gamma^{1/3}(x + \alpha - E')$ giving

$$\frac{d^2\psi}{dZ_1^2} - Z_1\psi = 0 \qquad \text{(III4)}$$

which is Airy's equation. Using a similar procedure for region III

we obtain

$$\frac{d^2\psi}{dz_2^2} - z_2\psi = 0 \qquad \text{(III5)}$$

where $z_2 = \gamma^{1/3}(-x + \alpha - E')$ following the procedure outlined in the THEORY section we have as one of the independent sets of solutions for a plane wave incident from the left

$$\psi_{kI} = Ae^{ikx} + Be^{-ikx} \qquad \text{(a.)}$$

$$\psi_{kII} = C\,A_i(z_1) + D\,B_i(z_1) \qquad \text{(b.)}$$

$$\psi_{kIII} = E\,A_i(z_2) + F\,B_i(z_2) \qquad \text{(c.)}$$

$$\psi_{kIV} = e^{ikx} \qquad \text{(d.)}$$

(III6)

The particular normalization chosen is to facilitate mathematical simplicity of the solution. The wave functions must be renormalized by dividing by A at the end to satisfy the requirements of unit incident flux. $A_i(z)$ and $B_i(z)$ are the two independent solutions to Airy's equation and some useful identities used in the calculation are presented:

$$A_i(z) = \frac{1}{3}\sqrt{z}\left[I_{-1/3}(\zeta) - I_{1/3}(\zeta)\right] \quad (a.)$$

$$A_i(-z) = \frac{1}{3}\sqrt{z}\left[J_{-1/3}(\zeta) + J_{1/3}(\zeta)\right] \quad (b.)$$

$$B_i(z) = \sqrt{z/3}\left[I_{-1/3}(\zeta) + I_{1/3}(\zeta)\right] \quad (c.)$$

$$B_i(-z) = \sqrt{z/3}\left[J_{1/3}(\zeta) - J_{1/3}(\zeta)\right] \quad (d.)$$

$$A_i'(z) = -\frac{1}{3}z\left[I_{-2/3}(\zeta) - I_{2/3}(\zeta)\right] \quad (e.)$$

$$A_i'(z) = -\frac{1}{3}z\left[J_{-2/3}(\zeta) - J_{2/3}(\zeta)\right] \quad (f.)$$

$$B_i'(z) = (z/\sqrt{3})\left[I_{-2/3}(\zeta) + I_{2/3}(\zeta)\right] \quad (g.)$$

$$B_i'(-z) = (z\sqrt{3})\left[J_{-2/3}(\zeta) + J_{2/3}(\zeta)\right] \quad (h.)$$

$$W\left\{A_i(z), B_i(z)\right\} = 1/\pi \quad (i)$$

(III7)

Where J and I are Bessel function and modified Bessel functions of the first kind, W is the Wronskian, $\zeta = (2/3)z^{3/2}$ and the prime denotes the derivative.

We now proceed to obtain a solution by requiring continuity of the slope and function at each boundary.

At x = -a

$$A e^{ika} + B e^{-ika} = C\,Ai_k(z_1(x=-a)) + D\,Bi_k(z_1(x=-a)) \quad (a.)$$

$$ikA e^{-ika} - ikB e^{ika} = \gamma^{1/3} C Ai_k(z_1(x=-a)) + \gamma^{1/3} B'(z_1(x=-a)) \quad (b.)$$

at x = 0

$$C\,Ai_k(z_1(x=0)) + D\,Bi_k(z_1(x=0)) = E\,Ai_k(z_2=0) + F\,Bi_k(z_2=0) \quad (c.)$$

$$C\,Ai_k'(z_1(x=0)) + D\,Bi_k'(z_1(x=0)) = E\,Ai_k'(z_2=0) + F\,Bi_k'(z_2=0) \quad (d.)$$

(III8)

at x = a

$$E\,A_{ik}(z_2=a) + F\,B_{ik}(z_2(x=a)) = e^{ika}$$

$$\gamma^{1/3} A'_{ik}(z_2(x=a)) + \gamma^{1/3} F B'_{ik}((z_2(x=a)) = ike^{ika}$$

Solving Eq. (III8) we get

$$E = \pi\left[e^{ika} B'_{ik}(z_2(x=a)) - ik\gamma^{1/3} B_{ik}(z_2(x=a))\right] \equiv r_1 \qquad (a.)$$

$$F = \pi\left[ik\gamma^{-1/3} A_{ik}(z_2(x=a)) - e^{ika} A_{ik}(z_2(x=a))\right] \equiv r_2 \qquad (b.)$$

$$r_3 \equiv r_1 A_{ik}(z_2(x=0)) + r_2 B_{ik}(z_2(x=0)) \qquad (c.)$$

$$r_4 \equiv r_1 A'_{ik}(z_2(x=0)) + r_2 B'_{ik}(z_2(x=0)) \qquad (d.)$$

$$C = \pi\left[r_3 B'_{ik}(z_1(x=0)) - r_4 B_{ik}(z_1(x=0)\right) \qquad (e.)$$

$$D = \pi\left[r_3 A_{ik}(z_1(x=0)) - r_4 A'_{ik}(z_1(x=0)\right) \qquad (f.)$$

$$r_7 \equiv r_5 A_{ik}(z_1(x=-a)) + r_6 B_{ik}(z_1(x=-a)) \qquad (g.)$$

$$r_8 \equiv \gamma^{1/3}\left[r_5 A'_{ik}(z_1(x=-a)) + r_6 B'_{ik}(z_1(x=-a))\right] \qquad (h.)$$

$$A = (e^{ika}/ik)(ikr_7 + r_8) \qquad (i.)$$

$$B = (e^{-ika}/ik)(ikr_7 - r_8) \qquad (j.)$$

(III9)

The results are then inserted into Eq. (58b) in order to calculate the number density. The resulting density is then compared with the number density obtained numerically (Fig. 7) for the same potential for $k_F = 1$ and $a = 1$ au. As can be seen the results are quite good.

APPENDIX IV

KINETIC ENERGY INTEGRALS

In this Appendix we will justify the approach used for calculation of the kinetic energy (Eq. (62)) and point out the differences with the Lang-Kohn [7] (Eq. (26)) approach which is a generalization of the Huntington [16] approach. An excellent discussion of the latter is given by Sugiyama [76]. The starting point for the two expressions is basically the same, namely, using the Schroedinger equation to define the single particle kinetic energy as the difference between the eigenvalue ϵ_i and the potential energy per particle. The approach, however, in obtaining the sums over the states is quite different in that the L-K approach is basically macroscopic and ours is basically microscopic. In the L-K expression the sum over eigenvalues is examined before and after creating the surface. Starting with particles in a box creating a surface in the middle of the box causes a shift in the density of states in k-space because the k-values undergo a shift in value $k \to k + \Delta k$. Therefore, for a crystal of length $2L$ the new values of k are given by

$$k = \frac{n\pi}{L} - \frac{\gamma\left(\frac{n\pi}{2L}\right)}{L}$$

or

$$k = k' - \frac{\gamma(k')}{L} \tag{IV1}$$

where n is an integer and $\gamma(k)$ is the phase shift in the wave function deep in the bulk caused by scattering from the surface potential (Eq. (19)) and the k' are the k-values before creation of the surface. The term $\gamma(k)/L$ is of order $1/L$. We can think of the change in terms of the infinite potential barrier as a change in the size of the box of the order of a lattice spacing. With a real potential, however, the phase shift depends on k, unlike the infinite potential barrier. L-K proceed to derive an expression for the kinetic energy in terms of the change in the sum over eigenvalues.

$$\sum_{\substack{k,k_y,k_z \\ occ.}} \frac{(k^2+k_y^2+k_z^2)}{2} \tag{IV2}$$

between the split and unsplit crystal and in terms of the phase shift $\gamma(k)$. For the bare metal calculation $\gamma(k)$ can be easily determined.

In this work the kinetic energy is determined in terms of a twofold integration in k and configuration space in terms of the exact wave functions (Eq. (60)). Proceeding in general for the k-space integration we have

$$\sum_{\substack{k,k_y,k_z \\ occ.}} f(k,x) \tag{IV3}$$

where f(k,x) is some function of k such as the arguments of the integrals presented in Eq. (60). In converting the sum to an integral using the Euler-McClaurin formula [75] we get

$\int_0^{n_m} dn\, f(k,x)$ ignorning higher order terms (referring now only to the x-direction) where n_m is the highest occupied state. The density of states in k-space $A_k'(n)$ has shifted from the profile in a box value to

$$\frac{dn}{dk} = \frac{2L}{\pi}\left(1 + \frac{1}{L}\frac{d\gamma}{dk}\right) = \frac{2L}{\pi}\left(1 + \frac{\gamma'}{L}\right) = \mathcal{D}_m(k) \qquad \text{(IV4)}$$

where γ' is the derivative with respect to k. In converting to a k-space integration we get

$$\frac{2L}{\pi}\int_0^{k_F} dk\, f(k,x) + \frac{2L}{\pi}\left\{\frac{1}{L}\int_0^{k_F} dk\,\gamma'(k)\, f(k,x)\right\} \qquad \text{(IV5)}$$

therefore, in using the particle in a box density of states we are ignoring terms of order 1/L (the second term in (IV5)). We must next consider the errors in the x-integration. We can assume $C = (x_0/L)$ is constant where x_0 is the length of the jellium in the computational space in order to neglect the effects of slab length on integrating the second term in configuration space (x-integration in Eq. (60)). The next consideration is selecting x_0 such that the deviation of the density from bulk conditions (Eq. (80)) is sufficiently small. This was checked by comparing the result of using Eq. (60) to the Lang-Kohn values of the kinetic energy for the bare metal case with integral values of r_s.

APPENDIX V

PROGRAMMERS MANUAL
LEWIS RESEARCH CENTER

11/70

Spline Curve

AUTHOR: R. Bruce Conright, Jr.

PURPOSE: To provide a function y = f(x) which interpolates for a given table of data points (x_i, y_i)

USAGE: To fit data, the call

CALL SPLIN1(X, Y, NPTS, BO, BN, J)

where

X - the array of points x_i in ascending order
Y - the array of corresponding y_i
NPTS - the number of these points
BO - the boundary condition at lower x boundary
BN - the boundary condition at upper x boundary
J - =1, the boundary conditions are the slopes dy/dx
=2, the boundary conditions are d^2y/dx^2

is required. After this, the spline fit is available through two entry points in SPLIN1:

YY = F(XX) where

XX independent variable, within the range of the x_i.
YY resultant interpolated Y value at XX.

and

DY = DF(XX) where

XX as above
DY approximate slope dy/dx at XX.

RESTRICTIONS:
1) $3 \leq NPTS \leq 50$
2) $X(1) \leq XX \leq X(NPTS)$

ERROR MESSAGES: When the input X is out of the range specified, a warning message is printed. The return is normal, but the answer is generally meaningless.

METHOD: The curve-fit is a set of cubic equations passed piece-wise through each pair of data points, constrained to match the derivatives at the data points. The fit is therefore very "smooth", excellent for interpolation or plotting. It is not to be used for extrapolation. Further this spline fit is not intended for large batches of data with scatter, noise, etc., because the fit passes exactly through every data point.

The method requires the boundary conditions to specify completely the solutions to the interpolation equations (reference). It is usually sufficient to say that the d^2y/dx^2 at the boundary are zero, whenever the boundary conditions are not known.

ACCURACY: Dependent on the input data. DF is about one s.f. less accurate than F.

SUBPROGRAMS USED: None

REFERENCE: Kopal, Zdenek: Numerical Analysis, Wiley & Sons, 1961.

APPENDIX VI

PROGRAMMERS MANUAL
LEWIS RESEARCH CENTER

11/70

QSF/DQSF

NUMERICAL INTEGRATION

IDENTIFICATION: IBM Scientific Subroutine Package

PURPOSE: To compute the vector of integral values for a given equidistant table of function values.

USAGE: CALL QSF(H, Y, Z, NDIM) for single precision, or

CALL DQSF(H, Y, Z, NDIM) for double precision.

where

H - The increment of argument values.
Y - The input vector of function values.
Z - The resulting vector of integral values. Z may be indentical with Y.
NDIM - The dimension of vectors Y and Z.

DOUBLE PRECISION: H, Y, and Z must be declared double precision in the calling program if the call is to DQSF.

RESTRICTIONS: NDIM must be 3 or greater.

METHOD: To compute the vector of integral values:

$$\left.\begin{aligned} z_i = z(x_i) &= \int_a^{x_i} y(x)\,dx \\ \text{with } x_i &= a + (i-1)\,h \end{aligned}\right\} \quad (i = 1, 2, \ldots, n)$$

for a table of function values $y_i (i = 1, 2, \ldots n)$, given at equidistant points $x_i = a + (i-1)\,h\ (i = 1, 2, \ldots n)$, Simpson's rule together with Newton's 3/8 rule or a combination of these two rules is used. Local truncation error is of the order h^5 in all cases with more than three points in the given table. No action takes place if the table consists of less than three sample points.

The function to be integrated is assumed to be continuous and differentiable (three or four times, depending on the rule used).

Formulas used in this subroutine (z_j are integral values, y_j function values) are:

$$z_j = z_{j-1} + \frac{h}{3}(1.25\,y_{j-1} + 2y_j - 0.25\,y_{j+1}) \qquad (1)$$

$$z_j = z_{j-2} + \frac{h}{3}(y_{j-2} + 4y_{j-1} + y_j) \quad \text{(Simpson's rule)} \qquad (2)$$

$$z_j = z_{j-3} + \frac{3}{8}h\,(y_{j-3} + 3y_{j-2} + 3y_{j-1} + y_j) \quad \text{(Newton's 3/8 rule)} \qquad (3)$$

PROGRAMMERS MANUAL
LEWIS RESEARCH CENTER

11/70

$$z_j = z_{j-5} + \frac{h}{3}(y_{j-5} + 3.875\, y_{j-4} + 2.625\, y_{j-3} + 2.625\, y_{j-2} + 3.875\, y_{j-1} + y_j) \qquad (4)$$

[combination of (2) and (3)]

Sometimes formula (2) is used in the following form:

$$z_j = z_{j+2} - \frac{h}{3}(y_j + 4\, y_{j+1} + y_{j+2}) \qquad (5)$$

ERROR MESSAGES: None

ACCURACY: Local truncation error is of the order h^5 in all cases with more than three points in the given table.

SUBPROGRAMS USED: None

REFERENCES: Hildebrand, F. B. Introduction to Numerical Analysis. McGraw-Hill, New York, 1956.

APPENDIX VII

PROGRAMMERS MANUAL
LEWIS RESEARCH CENTER

11/70

DET5/DDET5

NUMERICAL DIFFERENTIATION

IDENTIFICATION: IBM Scientific Subroutine Package

PURPOSE: To compute a vector of derivative values given a vector of function values whose entries correspond to equidistantly spaced argument values.

USAGE: CALL DET5 (H, Y, Z, NDIM, IER) for single precision, or

CALL DDET5 (H, Y, Z, NDIM, IER) for double precision.

where

- H - Constant difference between successive argument values. H is positive for increasing argument values and negative otherwise.
- Y - Given vector of function values (dimension NDIM).
- Z - Resulting vector of derivative values (dimension NDIM).
- NDIM - Dimension of vectors Y and Z.
- IER - Resulting error parameter.

  If IER = -1, NDIM is less than 5 and there is no computation.

  If IER = 0, there is no error.

  If IER = 1, H is equal to 0 and there is no computation.

DOUBLE PRECISION: H, Y, and Z must be declared double precision in the calling program if the call is to DDET5.

NOTE: Z can have the same storage location as Y. If Y is distinct from Z then it is not destroyed.

RESTRICTIONS: H must be greater than zero, and NDIM must be greater than 5.

METHOD: If X is the suppressed vector of argument values, then except at the points X(1), X(2), X(NDIM-1), and X(NDIM), Z(I) is the derivative at X(I) of the Lagrangian interpolation polynomial of degree 4. The polynomial is relevant to the 5 successive points (X(I+K), Y(I+K)) with K=-2, -1, 0, 1, 2.

ERROR MESSAGES: None

ACCURACY: Dependent upon the characteristics of the input data.

SUBPROGRAMS USED: None

REFERENCES: Hildebrand, F. B.: Introduction to Numerical Analysis, McGraw-Hill, 1956.

APPENDIX VIII

FORTRAN IV LISTING OF THE COMPUTER PROGRAM FOR OBTAINING SET CONSISTENT DENSITIES AND POTENTIALS

```
NUMEROV INTEGRATION COMPLEX WAVE FUNCTIONS
DIMENSION INT(252),VEFF(250),EX(250),ENERGL(250),RDENS(250),VEFF1(250)
DIMENSION RDENS1(250),VEFF2(250),VEFF3(250),RDENS2(250)
COMMON/FID/JJ,FK,PI
COMMON/SET/IX,NS,NT,IA,MP,AH,MDL
COMMON/WOW/CNPLUS,DELTA,A
REAL K,KK,KAP1,KAP2,CMIXC,RDENS(250),PHI(250),MUXC(250)
COMPLEX SLOPE,FUNC,U11,U22,U12,U21,AMP,PSI2(250)
DIMENSION WAVE(7),DWAVE(7),WAVE1(7),DWAVE1(7)
DIMENSION EN1(250),EN2(250),PAD1(250),ENRG3(250)
DIMENSION ENRG1(250),ENRG2(250),POD(250),PAD(250)
DIMENSION ENG(250),ENG1(250),PAD11(250),PAD22(250)
DIMENSION ENG11(250),ENG22(250),POD1(250)
DIMENSION ENL(250),ENL1(250)
DIMENSION EXC(250),CMC(250),D1DENS(250)
DOUBLE PRECISION DENS(250)
DIMENSION EN12(250),ENL3(250)
COMPLEX AII,BII,AIII,BIII
COMPLEX PSI(250),Z(250),J,PSI1(250),TEMP1,TEMP2,TEMP3
COMPLEX G1,G2,G3,G4
COMPLEX TEM1,TEM2,D1,D2,D3,D4,D5,D6,B1,B2,B3,B4
DELK=2.E-2
DELTA=.25E0
PI=4.E0*ATAN(1.E0)
RS=2.070
RS1=2.070
C9=3./(4.*PI)
CNPLUS=3.E0/(4.E0*PI*RS*RS*RS)
CNPL2=3.E0/(4.E0*RS1*RS1*RS1)
FK1=(3.E0*PI*PI*CNPL2)**(1./3.)
FK=(3.E0*PI*PI*CNPLUS)**(1./3.)
OMEG=FK*FK/(FK1*FK1)
OMEG=1.0000000
AP=FK**5.
J=(0.,1.)
N3=120
N4=N3/2
AH=.25000000
EX(1)=22.25
A=2.00000000
IA=A/AH
MX=EX(1)/AH
NS=MX-IA+1
NT=NS+2*IA
IX=2*MX+1
L=IX-4
NR=IX-NT
MDL=MX+1
MDL1=MDL1-1
IK=50
MI1=MDL/8
MI2=MDL/5
MAX1=9*MI1+8
MAX2=5*MI2+5
```

```
      EKIN1=.3*(3.*PI*PI)**(2./3.)*(EX(1)-A)
      EKIN1=EKIN1*CNPLUS**(5./3.)*1.557E6
      MICKEY=5*MI2
      IF(MICKEY.EQ.MDL) MAX2=MDL
      IB=2*IA+1
      ALEPH=.5550634
      Y0=0.
      Y1=2.05E-4
      DO 1 I=1,IX
      EX(I+1)=EX(I)-AH
    1 CONTINUE
      AQ=.3*(3.*PI*PI)**(2./3.)*CNPLUS**(5./3.)
      DO 1115 I=1,MDL
      IF(I.LE.NS) ENRG3(I)=AQ
      IF(I.GT.NS) ENRG3(I)=0.0000000
 1115 CONTINUE
      DO 91 I=1,IX
      IF(I.LE.NS) PDENS(I)=CNPLUS
      IF(I.GT.NS.AND.I.LT.NT) PDENS(I)=0.EC
      IF(I.GE.NT) PDENS(I)=CNPLUS
   91 CONTINUE
      BETA=1.24
      CENTER=5.25
 1050 CONTINUE
      DO 73 I=1,IX
      X=EX(I)
      TOMP1=ALEPH*(X-5.25)
      TOMP1=TOMP1*TOMP1
      TOMP2=ALEPH*(X+5.25)
      TOMP2=TOMP2*TOMP2
      IF(TOMP1.GT.50.) TOMP1=50.
      IF(TOMP2.GT.50.) TOMP2=50.
      B1=Y1*EXP(-TOMP1)
      B2=Y0*EXP(-TOMP2)
      TEMT1=EXP(BETA*(X+A))
      TEMT2=EXP(BETA*(X-A))
      TEMT3=EXP(-BETA*(X+A))
      TEMT4=EXP(-BETA*(X-A))
      IF(I.LE.NS) EDENS(I)=B1+B2+CNPLUS*(1.+TEMT3/2.-TEMT4/2.)
      IF(I.GE.NS.AND.I.LE.NT) EDENS(I)=B1+B2+CNPLUS*(TEMT3+TEMT2)/2.
      IF(I.GT.NT) EDENS(I)=B1+B2+CNPLUS*(1.-TEMT1+TEMT2)/2.
   73 CONTINUE
      MM=0
 1000 MM=MM+1
      IF(MM.GT.59) DELK=2.E-2
      IF(MM.GT.59) IK=50
      CONF=.0000000000
      IF(MM.EQ.2) CONF=.00000
      IF(MM.EQ.21) CONF=.1525
      IF(MM.GT.21) CONF=.00375
      IF(MM.EQ.41) CONF=.5
      IF(MM.GT.41.AND.MM.LT.51) CONF=.00275
      IF(MM.EQ.61) CONF=.05387
      IF(MM.GT.61) CONF=.003750000
```

```
      IF(MM.EQ.81) CONF=.5
      IF(MM.GT.81.AND.MM.LT.101) CONF=.005
      IF(MM.EQ.101) CONF=.1
      IF(MM.GT.1) MIT=1
      DO 200 I=1,IX
      EDENS1(I)=EDENS(I)
  200 CONTINUE
      IF(MM.GT.1) GO TO 3000
      DO 2 I=1,MDL
      T1=.5*(EX(I)-CENTER)
      T1=T1*T1
      IF(T1.GT.50.) T1=50.
      T2=Y1*EXP(-T1)
      T3=.5*(EX(I)+CENTER)
      T3=T3*T3
      IF(T3.GT.50.) T3=50.
      T4=Y1*EXP(-T3)
      IF(I.GT.NS.AND.I.LE.MDL) PHI(I)=T2+T4+FUN2(EX(I))
      IF(I.LE.NS) PHI(I)=T2+T4+FUN2(A)
    2 CONTINUE
      DUMB=PHI(1)
      DO 3 I=1,MDL
      PHI(I)=PHI(I)-DUMB
    3 CONTINUE
 3000 CONTINUE
      IF(MM.EQ.1) GO TO 8052
      JJ=0
 1001 JJ=JJ+1
      IF(JJ.GT.MIT) GO TO 8052
 1002 CONTINUE
      CALL CHARGE(EDENS1,PDENS,IX,Q,AH,NS,NT,IA,IB,NR,MDL,EX,PHI)
      Q=ABS(Q)
      IF(JJ.EQ.1) A2=Q
      A1=Q
 5555 CONTINUE
      WRITE(6,400) A1
  400 FORMAT(1H ,3HA1=,E16.8)
      Q=1.0000000
      DO 201 I=1,IX
      EDENS1(I)=EDENS(I)*Q
  201 CONTINUE
      GO TO 1001
 8052 WRITE(6,352) MM
  352 FORMAT(7H  EDENS,2X,3HMM=,I3)
      IF(MM.NE.N3) GO TO 156
      NF=0
  155 NF=NF+1
      KMAX=5*NF
      KINT=KMAX-4
      IF(KINT.GE.MAX2) GO TO 156
      KMIN=KMAX-4
      IF(NF.EQ.1) NG=1
      IF(NF.GT.1) NG=KMIN
      WRITE(6,151) NG,(EDENS(I),I=KMIN,KMAX)
```

```
151 FORMAT(1H ,23,7(E16.8))
    GO TO 155
 156 CONTINUE
 300 CONTINUE
    CALL XC(DENS1,MUXC,IX,CMPLUS,CMUXC)
    IF(MM.EQ.1) GO TO 3111
3111 CONTINUE
    DO 20 I=1,IX
    II=IX-I+1
    IF(I.LE.MDL) VEFF1(I)=-(EK*EK/2.)-0.50*PI*PHI(I)+MUXC(I)-MUXC(IX)+BXC(I)-BXC(IX)
    IF(I.GT.MDL) VEFF1(I)=VEFF1(II)
  20 CONTINUE
    POTAV=(VEFF1(11)-VEFF1(1))/(10.*AH)
    DELTV=VEFF(1)-VEFF1(1)
    DVDZ=(VEFF(1)-VEFF(11))/(10.*AH)
    WRITE(6,2000) POTAV,DELTV,DVDZ,NS
2000 FORMAT(1H ,'POTAV=',E15.4,2X,'SHDELTV=',E16.8,2X,'SHDVDZ=',E16.8,2X,'SHNS= ',I3)
  26 CONTINUE
    IF(MM.GT.1) CALL MIX(VEFF,VEFF1,IX,MDL,MM,N3,N4,MAX2,PIGEPS)
    IF(PIGEPS.GT.10.) GO TO 503
    IF(MM.EQ.1) READ(7,8) (VEFF(I),I=1,MAX2)
   8 FORMAT(5(E15.8))
    IF(MM.GT.1) GO TO 29
    DO 27 I=1,IX
    II=IX-I+1
    IF(I.LE.MDL) VEFF(I)=OMEG*VEFF(I)
    IF(I.GT.MDL) VEFF(I)=VEFF(II)
   27 CONTINUE
  29 CONTINUE
    DO 30 I=1,IX
    VEFF6(I)=VEFF(I)
    DENS6(I)=DENS(I)
  30 CONTINUE
    IF(MM.EQ.1) GO TO 29
2001 CONTINUE
    DO 21 I=1,IX
    VEFF(I)=VEFF(I)+CONF*(VEFF1(I)-VEFF(I))
    IF(MM.EQ.1) VEFF(I)=VEFF1(I)
  21 CONTINUE
  29 CONTINUE
    IF(MM.NE.N3) GO TO 1777
    WRITE(6,8) (VEFF1(I),I=1,MAX2)
1777 CONTINUE
    IF(MM.EQ.N3) GO TO 31
    IF(MM.EQ.1) GO TO 175
    IF(MM.LE.500) GO TO 33
  31 DO 32 I=1,IX
    VEFF(I)=VEFF6(I)
  32 CONTINUE
    WRITE(71,43) (VEFF6(I),I=1,MAX2)
    WRITE(72,43) (FDENS(I),I=1,MAX2)
    WRITE(6,43) (PHI(I),I=1,MAX2)
    WRITE(6,43) (BXC(I),I=1,MAX2)
  43 FORMAT(5(E15.8))
```

```
   33 CONTINUE
      IF(MM.LE.100) GO TO 1004
      DO 1003 I=1,TX
      IF(MM.EQ.1) VEFF(I)=VEFF1(I)
 1003 CONTINUE
 1004 CONTINUE
      IF(MM.NE.N3) GO TO 165
      WRITE(6,351)
  351 FORMAT(6H  VEFF)
      NK=0
  160 NK=NK+1
      LMAX=5*NK
      LINT=LMAX-4
      IF(LINT.GE.MAX2) GO TO 165
      LMIN=LMAX-4
      IF(NK.EQ.1) NL=1
      IF(NK.GT.1) NL=LMIN
      WRITE(6,168) NL,(VEFF(I),I=LMIN,LMAX)
      GO TO 160
  168 FORMAT(1H ,I3,5(E10.6))
  165 CONTINUE
  175 CONTINUE
      IF(MM.EQ.N3) GO TO 503
      DO 90 I=1,IX
      INTGRL(I)=0.0
      DENS(I)=0.0
      ENRG1(I)=0.0
      ENRG2(I)=0.0
      PSD(I)=0.0
      PAB(I)=0.0
   90 CONTINUE
      DO 120 M=1,IK
      ARG=XWALK*ELGAI(M)
      KAP1=SQRT(2.0*VEFF(1)+(EK+KK)*(EK-KK))
      KAP2=SQRT(2.0*VEFF(1)+(EK+KK)*(EK-KK))
      KAP1=SQRT(KAP1)
      KAP2=SQRT(KAP2)
      PSI(1)=CEXP(ARG*KAP1)
      PSI(2)=CEXP(ARG*KAP2)
      CALL WAVE(KK,EK,AM,J,DELK,PSI(1),PSI(2),VEFF,PSI,IX)
      WAVE(1)=REAL(PSI(L+3))
      WAVE(2)=REAL(PSI(L+2))
      WAVE(3)=REAL(PSI(L+1))
      WAVE(4)=REAL(PSI(L))
      WAVE(5)=REAL(PSI(L-1))
      WAVE(6)=REAL(PSI(L-2))
      WAVE(7)=REAL(PSI(L-3))
      WAVE1(1)=AIMAG(PSI(L+3))
      WAVE1(2)=AIMAG(PSI(L+2))
      WAVE1(3)=AIMAG(PSI(L+1))
      WAVE1(4)=AIMAG(PSI(L))
      WAVE1(5)=AIMAG(PSI(L-1))
      WAVE1(6)=AIMAG(PSI(L-2))
      WAVE1(7)=AIMAG(PSI(L-3))
```

```
      CALL DETS(AH,WAVE,DWAVE,7,IER)
      CALL DETS(AH,WAVE1,DWAVE1,7,IER)
      SLOPE =DWAVE(4)+J*DWAVE1(4)
      FUNC=WAVE(4)+J*WAVE1(4)
      CALL FFNORM(SLOPE,FUNC,EX(L),KK,PI,J,AMP,U11)
      BAH=CABS(U11)
      U22=REAL(U11)-J*AIMAG(U11)
      T1=(CABS(1.E0/AMP))**2
      T2=1.E0-(CABS(U11))**2
      IF(M.EQ.IK) WRITE(6,301) AMP
  301 FORMAT(1H ,3HDS=,2E16.7)
      DO 75 I=1,IX
      PSI(I)=PSI(I)/AMP
   75 CONTINUE
      T7=CABS(AMP)
      T7=T7*T7
      DO 81 I=1,IX
      II=IX-I+1
      PSI2(II)=PSI(I)
   81 CONTINUE
      DO 95 I=1,IX
      DK=KK/FK
      T3=CABS(PSI(I))
      T3=T3*T3
      T4=CABS(PSI2(I))
      T4=T4*T4
      COEF=4.E0
      IF(MOD(M,2).EQ.0) COEF=2.E0
      ENTGRL(I)=CNPLUS*(1.-DK)*(1.+DK)*(T3+T4)*DELK/4.E0
      EDENS(I)=COEF*ENTGRL(I)+EDENS(I)
      TERM1=(1.+DK)*(1.-DK)
      TERM2=TERM1*TERM1
      EN1(I)=AP*DELK*DK*DK*TERM1*(T3+T4)/3.E0
      EN2(I)=AP*DELK*TERM2*(T3+T4)/3.E0
      ENRG1(I)=ENRG1(I)+COEF*EN1(I)
      ENRG2(I)=ENRG2(I)+COEF*EN2(I)
   95 CONTINUE
  100 CONTINUE
      DO 1111 I=1,MDL
      II=I-NS+1
      POD(I)=(-FK*FK/2.-VEFF(I))*EDENS(I)
      IF(I.LE.NS) PAD(I)=PHI(I)*(EDENS(I)-PDENS(I))
      IF(I.GE.NS) PAD1(II)=PHI(I)*EDENS1(I)
 1111 CONTINUE
      NDIM=IA+1
  179 CONTINUE
      IF(MM.EQ.0) CALL GRD(EX,EDENS,BXC,CXC,D1DENS,IX,MDL,AH)
  180 CONTINUE
      DO 1112 I=1,MDL
      II=I-NS+1
      IF(I.LE.NS) ENG(I)=(ENRG1(I)+.5*ENRG2(I))/(8.*PI*PI)+POD(I)-ENRG3(I)
      IF(I.GE.NS) ENG1(II)=(ENRG1(I)+.5*ENRG2(I))/(8.*PI*PI)+POD(I)
      ENL(I)=1.5576*CXC(I)*D1DENS(I)*D1DENS(I)/(EDENS(I)**(4./3.))
      T=EDENS(I)
```

```
      T1=D1DENS(I)
      T2=(EDENS(I)/C9)**(1./3.)
      T3=T2*T2
      T4=(.0126+.013*T2+.0349*T3)*C9**(4./3.)
      ENL2(I)=.5*1.557E6*T4*T1*T1/(T**(4./3.))
 1112 CONTINUE
      CALL QSF(AH,ENG,ENG11,NS)
      CALL QSF(AH,ENG1,ENG22,NDIM)
      CALL QSF(AH,PAD,PAD11,NS)
      CALL QSF(AH,PAD1,PAD22,NDIM)
      CALL QSF(AH,POD,POD1,MDL)
      CALL QSF(AH,ENL,ENL1,MDL)
      CALL QSF(AH,ENL2,ENL3,MDL)
      IF(NDIM.LT.3) ENG22(NDIM)=(ENG1(NDIM)+ENG1(NDIM-1))*AH/2.
      IF(NDIM.LT.3) PAD22(NDIM)=(PAD1(NDIM)+PAD1(NDIM-1))*AH/2.
      ESE=2.*DI*(PAD11(NS)+PAD22(NDIM))*1.557E6
      EKIN=(ENG11(NS)+ENG22(NDIM))*1.557E6
      PKIN2=A2*(EKIN+EKIN1)-EKIN1
      WRITE(6,1113) ENG1(1),ENG1(2),PKIN2,EKIN
 1113 FORMAT(15H KINETIC ENERGY,2X,E12.6,2X,E12.6,2X,E13.7,2X,E13.7)
      WRITE(6,1114) MDL,POD1(MDL),PAD1(1),PAD1(2)
 1114 FORMAT(9H ESTAT EN,2X,E13.7,2X,E13.6,2X,E13.6,2X,E13.6)
      A5=2.*A
      N25=N3-1
      IF(MM.EQ.N25) WRITE(6,1116) A5,ES,EX(1),Q
 1116 FORMAT(1H ,3HA= ,E12.6,2X,3HES= ,E13.7,2X,4HX0= ,E12.6,2X,3HQ= ,E13.7)
      WRITE(6,1117) ENL1(MDL),ENL3(MDL)
 1117 FORMAT(1H ,12HNONRELCL EN=,E14.7,2X,E14.7)
   74 CONTINUE
  502 CONTINUE
      IF(MM.LE.N3) GO TO 1000
  503 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE CHARGE(PDENS1,PDENS,IX,Q,AH,NS,NT,IA,ID,NP,MDL,EX,PHI)
      DIMENSION PDENS1(250),PDENS(250),QNET(250),PHI(250)
      DIMENSION QNET1(250),QNET2(250),QNET3(250),DIP1(250),DIP2(250),DIP3(250)
      DIMENSION QNET(250),EX(250),DIP(250)
     COMMON/BLD/JJ,PK,PI
      M=MDL+1
      N=PI/(PK*AH)
      N=N+1
      MM=N+1
      A=PI/PK
      B=A-AH*FLOAT(N-1)
      D=0.
      C=IA
      CALL AINT(PDENS1,PDENS,DIP1,AH,MDL)
      DO 97 I=1,MDL
      II=I+MDL-1
      III=MDL-I+1
      QNET(II)=DIP1(I)*(EX(II)+C*AH)*PDENS(II)
      QNET(III)=QNET(II)
   97 CONTINUE
      DO 98 I=1,MDL
      II=I+MDL-1
      DIP(II)=DIP1(I)
   98 CONTINUE
      DO 101 I=1,MDL
      III=MDL-I+1
      DIP(III)=DIP1(I)
  101 CONTINUE
      DEN=DIP(IX)
      CALL AINT(DIP,PDENS,PHI,AH,MDL)
    1 CONTINUE
      W=PHI(MDL)
      DO 99 I=1,MDL
      II=I+MDL-1
      TEMP1=.5*(EX(II)+C*AH)*(EX(II)+C*AH)
      PHI(II)=PHI(I)-TEMP1*PDENS(II)
   99 CONTINUE
      PHI(IX)=W-.5*(EX(IY)+C*AH)*(EX(IX)+C*AH)*PDENS(IX)
      DO 102 I=1,MDL
      II=MDL+I-1
      III=MDL-I+1
      PHI(III)=PHI(II)
  102 CONTINUE
      V=PHI(IX)
      DO 100 I=1,IX
      PHI(I)=PHI(I)-V
  100 CONTINUE
      L=IX
      IIII=IX-1
      IF(JJ.LT.3) GO TO 1001
      DO 1000 I=1,MM
      COEFF=2.
      IF(MOD(I,2).EQ.0) COEFF=4.
      IF(I.EQ.1) COEFF=1.
```

```
      IF(I.EQ.N) COEFF=1.
      TEMP1=EX(I)*EX(I)*COS(2.*FK*EX(I))/(EX(I)*EX(I))
      D=D+COEFF*TEMP1
 1000 CONTINUE
      QNET(MM)=COS(2.*FK*EX(MM))/(EX(MM)*EX(MM))
      QNET(N)=COS(2.*FK*EX(N))/(EX(N)*EX(N))
      F=EX(MM)*EX(MM)*QNET(MM)-EX(N)*EX(N)*QNET(N)
      F=(B/AH)*F+EX(M)*EX(N)*QNET(N)
      TEMP2=(EX(MM)*EX(MM)*QNET(MM)*F)*(B-A)/2.+D*AH/3.
      G=(EX(1)-A)**3.-EX(1)**3.
      H=3.*TEMP2/G
      WRITE(6,1002) H
 1002 FORMAT(9H CCHARGE=,2X,E15.8)
 1001 CONTINUE
      ALPH=PDINS(L)*(EX(L)+C*AH)
      Q=ALPH/DEN
      Q=ABS(Q)
      RETURN
      END
```

```
      SUBROUTINE RENORM(SLOPE,FUNC,X,KK,PI,J,AMP,U11)
      COMPLEX SLOPE,FUNC,J,AMP,U11,PSI,PSIP,D1,D2,D3
      REAL KK
      PSI=FUNC
      PSIP=SLOPE
      COEF=SQRT(2.E0*PI*KK)
      COEF=1.E0
      D1=CEXP(J*KK*X)
      D2=CEXP(-J*KK*X)
      D3=2.E0*KK*J
      AMP=COEF*((D3*PSI/2.E0)+PSIP)/(D1*D3)
      U11=COEF*((D3*PSI/2.E0)-PSIP)/(D2*D3*AMP)
      RETURN
```

```
      SUBROUTINE WAVE(KK,FK,AH,J,DELK,P1,P2,VEFF,PST,IX)
      REAL KK
      INTEGER Q
      DIMENSION VEFF(250)
      COMPLEX P1,P2,J,PSI(250)
      PSI(1)=P1
      PSI(2)=P2
      DO 15 I=2,IX
      PSI(I+1)=2.*PSI(I)-PSI(I-1)
      Q=0
    6 A=REAL(PSI(I+1))
      Q=Q+1
      T1=REAL(PSI(I+1))
      T2=REAL(PSI(I))
      T3=REAL(PSI(I-1))
      T1=2.*T2-T3+(1./12.)*AH*AH*(FK+KK)*(FK-KK)*(T1+10.*T2+T3)
     *+(1./6.)*AH*AH*(VEFF(I+1)*T1+10.*VEFF(I)*T2+VEFF(I-1)*T3)
      Y=ABS((T1-A)/A)
      PSI(I+1)=T1+J*AIMAG(PST(I+1))
      IF(Q.GT.9) GO TO 10
      IF(Y.GT..00001) GO TO 6
   10 CONTINUE
      N=0
    7 B=AIMAG(PSI(I+1))
      N=N+1
      T4=AIMAG(PSI(I+1))
      T5=AIMAG(PSI(I))
      T6=AIMAG(PSI(I-1))
      T4=2.*T5-T6+(1./12.)*AH*AH*(FK+KK)*(FK-KK)*(T4+10.*T5+T6)
     *+(1./6.)*AH*AH*(VEFF(I+1)*T4+10.*VEFF(I)*T5+VEFF(I-1)*T6)
      W=ABS((T4-B)/B)
      PST(I+1)=REAL(PSI(I+1))+J*T4
      IF(N.GT.9) GO TO 11
      IF(W.GT..00001) GO TO 7
   11 CONTINUE
      PSI(I+1)=T1+J*T4
   15 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE DETS(H,Y,Z,NDIM,IER)

      DIMENSION Y(1),Z(1)

         TEST OF DIMENSION
      IF(NDIM-5)4,1,1

         TEST OF STEPSIZE
    1 IF(H)2,5,2

         PREPARE DIFFERENTIATION LOOP
    2 HH=.08333333/H
      YY=Y(NDIM-4)
      B=HH*(-25.*Y(1)+48.*Y(2)-36.*Y(3)+16.*Y(4)-3.*Y(5))
      C=HH*(-3.*Y(1)-10.*Y(2)+18.*Y(3)-6.*Y(4)+Y(5))

         START DIFFERENTIATION LOOP
      DO 3 I=5,NDIM
      A=B
      B=C
      C=HH*(Y(I-4)-Y(I)+8.*(Y(I-1)-Y(I-3)))
    3 Z(I-4)=A
         END OF DIFFERENTIATION LOOP

         NORMAL EXIT
      IER=0
      A=HH*(-YY+6.*Y(NDIM-3)-18.*Y(NDIM-2)+10.*Y(NDIM-1)+3.*Y(NDIM))
     0Z(NDIM)=HH*(3.*YY-16.*Y(NDIM-3)+36.*Y(NDIM-2)-48.*Y(NDIM-1)
     1            +25.*Y(NDIM))
      Z(NDIM-1)=A
      Z(NDIM-2)=C
      Z(NDIM-3)=B
      RETURN

         ERROR EXIT IN CASE NDIM IS LESS THAN 5
    4 IER=-1
      RETURN

         ERROR EXIT IN CASE OF ZERO STEPSIZE
    5 IER=1
      RETURN
      END
```

```
      SUBROUTINE XC(ZLAMS,MUXC,IX,CNPLUS,CMUXC)
      REAL MUXC(250),ZLAMS(250)
      P3=2.50
      P6=.384397610
      P7=.9457014510
      P8=.2972704971
      ATA=1.00/3.00
      DO 2 I=1,IX
      TEMP1=ZLAMS(I)**ATA
      TEMP2=1.00+.1273837+3*TEMP1
      MUXC(I)=-P6*(1-P7*TEMP1/TEMP2+P8*(TEMP1**P5)/(TEMP2**P5)
    2 CONTINUE
      TEMP3=CNPLUS**P3
      TEMP4=1.50+.1577+TEMP3
      CMUXC=-P6*(1-P7*(TEMP3)/TEMP4+P8*(TEMP3**P5/TEMP4**P5)
      RETURN
      END
```

```
      FUNCTION GAM1(X)
      DELTA=.25E0
      TEMP1=DELTA*X**X
      IF(TEMP1.GT.50.) GAM1=0.E0
      IF(TEMP1.LE.50.) GAM1=EXP(-TEMP1)
      RETURN
      END
```

```
      SUBROUTINE AINT(X,Y,Z,AH,N)
      DIMENSION X(250),Y(250),Z(250)
      A0=251./720.
      A1=646./720.
      A2=-264./720.
      A3=106./720.
      A4=-19./720.
      Z(1)=0.0
      NAT=N+1
      DO 1 I=1,NAT
      II=I+N
      T0=X(II)
      T1=X(II-1)
      T2=X(II-2)
      T3=X(II-3)
      T4=X(II-4)
      Z(I+1)=Z(I)+AH*(A0*T0+A1*T1+A2*T2+A3*T3+A4*T4)
    1 CONTINUE
      RETURN
      END
```

```
FUNCTION FUN1(X)
COMMON/WOW/CNPLUS,BETA,A
T1=(X-A)*BETA
T1=EXP(-T1)
T2=(X+A)*BETA
T2=EXP(-T2)
T3=1.-EXP(-2.*BETA*A)
FUN1=CNPLUS*(-T1+T2+T3)/(2.*BETA*BETA)
RETURN
END
```

```
FUNCTION FUN2(X)
COMMON/WOW/CNPLUS,BETA,A
T1=EXP(-BETA*(X+A))
T2=EXP(BETA*(X-A))
T3=2.*EXP(-BETA*A)
FUN2=CNPLUS*(T1+T2-T3)/(2.*BETA*BETA)
RETURN
END
```

```
      SUBROUTINE GRD(EX,EDENS,BXC,CXC,D1DENS,IX,MDL,AH)
      DIMENSION EX(250),EDENS(250),BXC(250),D1DENS(250),CXC(250),S(250)
      DIMENSION D2DENS(250)
      CALL DET5(AH,EDENS,D1DENS,IX,IEP)
      CALL DET5(AH,D1DENS,D2DENS,IX,IER)
      A=2.69412789E-3
      B=2.612933E-3
      C=.1033
      DO 1 I=1,IX
      T=EDENS(I)
      S(I)=(C-4.+2.*B*(T**(-2./3.)))/(3.*T)
      CXC(I)=A*(T**(C/3.))*EXP(-B*(T**(-2./3.)))
      T1=D1DENS(I)*D1DENS(I)
      T2=D2DENS(I)
      T3=CXC(I)/(T**(4./3.))
      BXC(I)=-T3*(2.*T2+S(I)*T1)
    1 CONTINUE
    2 CONTINUE
      RETURN
      END
```

```
      FUNCTION FP(X1)
      DIMENSION A1(102),B1(102),C1(102),D1(102)
      DIMENSION A(102),B(102),C(102),D(102)
      IENTRY = 1
      GO TO 15
      ENTRY SPLIN1(X,Y,N,BC,BN,J)
      DIMENSION X(1),Y(1),DY(102)
      N1 = N-1
      GO TO (4,5),J
    4 B(1) = 1.0
      C(1) = 0.0
      D(1) = BC
      A(N) = 0.0
      B(N) = 1.0
      D(N) = BN
      GO TO 6
    5 B(1) = 2.0
      C(1) = 1.0
      D(1) = 3.0*(Y(2)-Y(1))/(X(2)-X(1))-0.5*(X(2)-Y(1))*BC
      A(N) = 1.0
      B(N) = 2.0
      D(N) = 3.0*(Y(N)-Y(N1))/(X(N)-X(N1))+0.5*(Y(N)-X(N1))*BN
    6 DO 1 I=2,N1
      A(I) = X(I+1)-X(I)
      B(I) = 2.0*(X(I+1)-X(I-1))
      C(I) = Y(I)-Y(I-1)
    1 D(I) = 3.0*(Y(I+1)*C(I)**2+Y(I)*(A(I)**2-C(I)**2)-Y(I-1)*A(I)**2)/-
     *(C(I)*A(I))
      D(1) = D(1)/B(1)
      DO 2 I=2,N
      B(I) = B(I)-A(I)*C(I-1)/B(I-1)
    2 D(I) = (D(I)-A(I)*D(I-1))/B(I)
      DY(N) = D(N)
      DO 3 I=1,N1
      K = N-I
    3 DY(K) = D(K)-C(K)*DY(K+1)/B(K)
      A(1) = X(2)-X(1)
      DO 8 I=1,N1
      D(I) = (2.0*Y(I)-2.0*Y(I+1)+A(I)*DY(I)+A(I)*DY(I+1))/A(I)**3
      C(I) = (-3.0*Y(I)+3.0*Y(I+1)-2.0*A(I)*DY(I)-A(I)*DY(I+1))/A(I)**2
      B(I) = DY(I)
      A(I) = Y(I)+X(I)*(-B(I)+X(I)*(C(I)-X(I)*D(I)))
      B(I) = B(I)+X(I)*(-2.0*C(I)+X(I)*3.0*D(I))
    8 C(I) = C(I)-3.0*D(I)*X(I)
      DO 4500 I=1,N
      A1(I)=A(I)
      B1(I)=B(I)
      C1(I)=C(I)
      D1(I)=D(I)
 4500 CONTINUE
      GO TO 20
      ENTRY DF(X1)
      IENTRY = 2
   15 IF(X1.LT.X(1))   WRITE (6,201)
```

```
      DO 16 I=2,N
      K = I-1
      IF(X1.LE.X(I)) GO TO (17,18),IENTRY
   16 CONTINUE
      WRITE (6,202)
      GO TO (17,18),IENTRY
   17 F2 = A(K)+X1*(B(K)+X1*(C(K)+X1*D(K)))
      GO TO 20
   18 F2 = B(K)+X1*(2.0*C(K)+X1*3.0*D(K))
   20 RETURN
  201 FORMAT(36H **WARNING** X BELOW XMIN IN F OR DF  )
  202 FORMAT(36H **WARNING** X ABOVE XMAX IN F OR DF  )
      END
```

```
      SUBROUTINE ERR(VEFF,VEFF1,TX,MDL,MM,N3,NG,MAX2,BIGERR)
      DIMENSION VEFF(250),VEFF1(250),ER(250),D(2),WRO(250)
      X=0.
      BIGERR=0.
      DO 1 I=50,MDL
      TEMP1=VEFF(I)-VEFF1(I)
      TEMP1=ABS(TEMP1)
      ER(I)=TEMP1*TEMP1
      WRO(I)=TEMP1
      X=X+TEMP1*TEMP1
      IF(I.GT.50) D(1)=SQRT(ER(I-1))
      IF(D(1).GE.BIGERR) BIGERR=D(1)
      D(2)=TEMP1
      IF(D(2).GT.BIGERR) M=I
      IF(D(2).GT.BIGERR) BIGERR=D(2)
    1 CONTINUE
      R=FLOAT(MDL-50)
      STDERR=SQRT(X/R)
      WRITE(6,2) STDERR,BIGERR,M
    2 FORMAT(1H ,8H STDERR=,E16.7,8H BIGERR=,E16.7,3H M=,I3)
      IF(MM.NE.N3)  GO TO 4
      DO 6 I=1,MDL
      WRO(I)=ABS(VEFF(I)-VEFF1(I))
    6 CONTINUE
      WRITE(6,5) MDL
      NF=0
  155 NF=NF+1
      KMAX=5*NF
      KINT=KMAX-4
      IF(KINT.GE.MAX2) GO TO 4
      KMIN=KMAX-4
      IF(NF.EQ.1) NG=1
      IF(NF.GT.1) NG=KMIN
      WRITE(6,151) NG,(WRO(I),I=KMIN,KMAX)
  151 FORMAT(1H ,I3,5(E16.7))
      GO TO 155
    4 CONTINUE
    5 FORMAT(1H ,2X,5HMDL= ,I3)
      RETURN
      END
```

```
LOGON FSRRANTE,,,1800
FTNLIB
DDEF FT06F001,VS,EDGAR,RET=T
DDEF FT07F001,VS,POTE1
DDEF FT71F001,VS,VEFF6
DDEF FT72F001,VS,SNEDE,RET=T
BIAD
PRINT EDGAR,PRTSP=EDIT,ERASE=Y
RECAT VEFF6,POTE1
PUNCH POTE1
PUNCH SNEDE
PUNCH POTE1
PUNCH SNEDE
LOGOFF
```

APPENDIX IX

COMPONENTS OF BINDING ENERGY

This Appendix contains tables of the components of the binding energies for each material and each separation used. All energies are references to the 15 atomic units separation values at which point the adhesive energy had essentiahly saturated. The following defines the symbols.

a	Separation between slabs in atomic units
σ_s	The kinetic energy in ergs/cm^2
σ_{xc}	The sum of the exchange and correlation energies in ergs/cm^2
σ_{es}	The sum of the electrostatic energy and Wint in ergs/cm^2
σ_{ps}	The pseudopotential contribution to the energy in ergs/cm^2
σ_{NL}	The nonlocal contribution to the energy in ergs/cm^2
$\sigma_u = \sigma_s + \sigma_{xc} + \sigma_{es} - \text{Wint}$	The jellium contribution to the energy in ergs/cm^2
σ_T	The total adhesive bonding energy in ergs/cm^2

Aluminum r_s=2.07

a	σ_S	σ_{XC}	σ_{eS}	σ_{PS}	σ_U	σ_T
0	4717.7	-2850.4	-1522.1	-1055.1	753.4	-710
0.25	3882.4	-2470.4	-1364.6	-762.2	340.4	-714.7
0.50	3156.7	-2122.3	-1183.8	-533.8	60.45	-683.3
0.75	2506.9	-1812.7	-972.4	-362.2	-127.9	-640.5
1.0	1960.7	-1531.9	-792.1	-230.4	-255.6	-593.8
1.5	1175.5	-1093.3	-483.1	-67.74	-345.8	-468.7
2.0	597.9	-727.2	-231.3	-9.30	-332.44	-353.4
2.5	270.1	-486.4	-95.17	54.8	-297.0	-256.6
3.0	65.0	-313.1	-3.54	64.0	-244.24	-187.7
4.0	-149.2	-87.0	74.5	57.6	-151.9	-96.2
5.0	-173.7	-5.22	84.7	38.5	-83.7	-45.7
10.0	-54.9	27.6	12.5	5.0	-14.8	-9.8
15.0	0	0	0	0	0	0

Aluminum Nonlocal r_s=2.07

a	σ_S	σ_{XC}	σ_{eS}	σ_{PS}	σ_U	σ_{NL}	σ_T
0	4915.5	-2954.8	-1618.9	-1094.2	750.4	-323.8	-1075.9
0.25	4067.8	-2569.7	-1459.6	-800.7	331.3	-322.8	-1084.7
0.50	3347.0	-2221.4	-1274.2	-570.0	61.2	-318.3	-1037.0
0.75	2687.4	-1911.2	-1069.5	-394.3	-142.9	-311.4	-999.1
1.0	2140.8	-1633.6	-870.8	-259.7	-255.9	-302.4	-925.8
1.5	1302.0	-1770.9	-534.4	-82.0	-347.7	-278.9	-763.8
2.0	726.6	-813.8	-285.1	2.5	-344.2	-250.1	-620.0
2.5	357.1	-554.5	-105.0	54.1	-287.7	-220.3	-468.3
3.0	119.4	-366.4	-1.3	64.8	-240.9	-189.0	-372.5
4.0	-132.3	-121.2	108.4	68.9	-142.9	-135.7	-229.7
5.0	-165.1	-23.8	116.4	50.3	-72.0	-91.5	-113.9
10.0	-39.5	-7.8	18.2	6.7	-13.5	-6.0	-26.6
15.0	0	0	0	0	0	0	0

Aluminum* r_s=2.097238

a	σ_S	σ_{XC}	σ_{eS}	σ_{pS}	σ_U	σ_T
0	4408.9	-2714.6	-1438.2	-1032.8	652.1	-776.7
0.25	3624.5	-2351.6	-1286.8	-741.9	270.0	-756.2
0.50	2950.2	-2024.9	-1115.1	-516.8	14.3	-706.6
0.75	2340.6	-1731.6	-918.2	-347.5	-162.6	-656.7
1.0	1830.0	-1462.2	-774.0	-218.5	-278.1	-601.7
2.0	541.6	-693.2	-215.9	16.4	-339.6	-351.1
3.0	52.6	-305.4	-0.6	65.0	-204.8	-187.2
5.0	-136.1	-18.8	77.5	36.0	-76.9	-41.0
10.0	-27.6	9.0	7.6	2.3	-10.9	-8.6
15.0	0	0	0	0	0	0

Aluminum* Nonlocal r_s=2.097238

a	σ_S	σ_{XC}	σ_{eS}	σ_{pS}	σ_U	σ_{NL}	σ_T
0	4598.3	-2811.0	-1528.8	-1073.9	654.5	-312.2	-1127.6
0.25	3811.8	-2451.3	-1376.0	-782.4	268.7	-310.9	-1108.9
0.50	3134.5	-2118.5	-1200.3	-553.3	19.8	-307.0	-1044.7
0.75	2509.8	-1818.9	-1005.8	-377.7	-168.3	-300.6	-993.2
1.0	1995.0	-1554.3	-818.4	-245.2	-272.6	-292.0	-915.0
2.0	667.1	-774.5	-264.5	11.2	-344.0	-300.6	-602.9
3.0	87.0	-342.8	9.2	72.4	-239.2	-242.1	-358.2
5.0	-190.2	-8.5	120.2	54.7	-78.0	-184.1	-113.7
10.0	-52.6	23.7	22.0	7.0	-6.96	-89.4	-6.02
15.0	0	0	0	0	0	0	0

Zinc r_s=2.30

a	σ_S	σ_{XC}	σ_{eS}	σ_{pS}	σ_U	σ_T
0	2835.1	-1993.6	-759.1	-557.9	183.1	-475.5
0.25	2339.5	-1740.1	-704.0	-426.9	-34.3	-531.6
0.50	1913.0	-1513.1	-625.5	-318.3	-176.4	-543.9
0.75	1536.6	-1316.5	-527.3	-231.3	-273.3	-538.5
1.0	1203.3	-1121.8	-426.2	-160.6	-320.8	-505.4
1.5	703.7	-807.8	-267.0	-63.7	-366.1	-441.6
2.0	379.4	-579.7	-119.3	-12.51	-313.8	-332.1
2.5	149.7	-392.5	-44.4	19.7	-284.2	-267.4
3.0	24.1	-264.1	21.8	27.5	-216.7	-190.7
4.0	-100.8	-100.2	50.3	37.9	-158.9	-121.5
5.0	-118.3	-32.0	66.6	21.2	-83.5	-62.6
10.0	-12.0	-13.2	3.7	.69	2.90	3.21
15.0	0	0	0	0	0	

Zinc Nonlocal r_s=2.3

q	σ_S	σ_{XC}	σ_{ES}	σ_{PS}	σ_U	σ_{NL}	σ_T
0	2942.4	-2045.3	-821.3	-569.4	176.4	-240.3	-734
0.25	2446.8	-1796.0	-766.1	-441.4	-45.0	-239.4	-795.2
0.50	2014.5	-1564.6	-685.6	-335.3	-186.7	-236.7	-807.6
0.75	1623.2	-1356.0	-584.9	-248.8	-283.8	-232.3	-798.64
1.0	1288.8	-1167.0	-482.8	-178.5	-337.0	-226.3	-765.9
1.5	768.6	-848.5	-301.1	-80.5	-369.2	-210.4	-635.0
2.0	418.2	-606.8	-153.8	-22.6	-336.6	-190.7	-555.7
2.5	177.2	-412.8	-85.8	9.31	-282.4	-169.4	-408.5
3.0	-25.3	-275.9	21.5	25.1	-227.7	-144.8	-351.9
4.0	-123.3	-107.2	84.9	37.7	-145.1	-108.2	-179.2
5.0	-162.3	-17.7	94.8	28.8	-85.0	-74.6	-131.0
10.0	-10.0	4.2	11.5	3.00	-5.93	-4.87	3.81
15.0	0	0	0	0	0	0	0

Zinc* r_s=2.61389

q	σ_S	σ_{XC}	σ_{ES}	σ_{PS}	σ_U	σ_T
0	1466.3	-1224.1	-475.2	-343.4	99.9	-576.5
0.25	1202.3	-1070.1	-427.9	-261.3	-197.5	-557.1
0.50	973.1	-928.3	-373.0	-193.6	-255.3	-521.4
0.75	767.4	-802.4	-310.7	-139.2	-292.2	-484.9
1.0	590.2	-685.0	-250.7	-95.3	-306.1	-440.9
2.0	130.7	-337.9	-66.9	-.21	-262.4	-273.9
3.0	-50.3	-147.2	26.9	23.1	-167.2	-147.5
5.0	-111.4	-4.3	54.5	19.9	-58.1	-39.5
10.0	-9.63	6.4	4.36	1.25	1.13	2.21
15.0	0	0	0	0	0	0

Zn* Nonlocal r_s=2.61389

q	σ_S	σ_{XC}	σ_{ES}	σ_{PS}	σ_U	σ_{NL}	σ_T
0	1557.1	-1227.2	-516.7	-353.3	103.7	-166.4	-756.5
0.25	1289.1	-1123.2	-469.3	-271.8	-205.1	-165.8	-740.8
0.5	1066.5	-985.1	-413.2	-204.9	-259.2	-164.2	-700.8
0.75	852.9	-854.3	-350.2	-149.7	-298.1	-161.5	-662.8
1.0	671.2	-734.1	-287.1	-105.0	-310. 6	-157.9	-613.0
2.0	187.7	-378.5	-88.6	-4.86	-267.7	-135.9	-420.1
3.0	-24.6	-175.1	18.5	24.5	-177.8	-108.0	-264.8
5.0	-121.2	-2.00	63.7	23.9	-59.2	-57.1	-92.8
10.0	-24.86	10.0	9.55	2.55	-5.32	-3.97	-6.75
15.0	0	0	0	0	0	0	0

Magnesium r_s=2.65

a	σ_S	σ_{XC}	σ_{ES}	σ_{PS}	σ_U	σ_T
0	1373.4	-1173.2	-450.1	-291.2	120.0	-541.0
0.25	128.1	-1030.4	-404.8	-243.1	-210.8	-550.1
0.50	913.3	-893.4	-352.3	-199.6	-261.0	-531.9
0.75	721.2	-774.7	-293.2	-161.4	-293.9	-508.1
1.0	556.1	-663.2	-235.9	-128.1	-303.7	-471.0
1.5	300.7	-481.3	-143.9	-75.8	-302.8	-400.1
2.0	122.9	-330.1	-61.9	-40.55	-257.2	-309.6
2.5	19.0	-229.8	-16.4	-17.3	-220.7	-244.4
3.0	-48.9	-146.9	27.6	-8.58	-164.6	-176.8
4.0	-100.6	-52.9	34.4	9.50	-112.7	-104.3
5.0	-107.9	0.117	46.9	5.38	-60.6	-55.5
6.0	-87.8	17.3	28.3	6.9	-42.1	-35.3
10.0	-6.90	-0.235	4.20	.53	2.93	-2.41
15.0	0	0	0	0	0	0

Magnesium Nonlocal r_s=2.65

a	σ_S	σ_{XC}	σ_{ES}	σ_{PS}	σ_U	σ_{NL}	σ_T
0	1460.3	-1225.4	-489.3	-282.9	124.6	-159.8	-697.0
0.25	1209.4	-1078.5	-444.1	-237.0	-216.9	-159.2	-709.4
0.50	1001.9	-949.2	-391.6	-197.1	-267.6	-157.7	-693.8
0.75	798.5	-819.6	-331.2	-160.9	-299.5	-155.2	-668.4
1.0	633.7	-711.4	-272.8	-129.3	-311.4	-151.7	-631.5
1.5	367.8	-527.1	-168.1	-80.9	-305.9	-142.5	-550.8
2.0	186.8	-379.7	-85.3	-45.6	-266.4	-130.8	-454.7
2.5	57.4	-262.8	-23.3	-23.1	-222.3	-117.9	-369.8
3.0	-25.0	-172.41	15.6	-8.97	-178.3	-104.2	-296.1
4.0	-97.8	-67.0	55.8	6.78	-107.1	-78.4	-179.8
5.0	-117.4	-2.9	57.2	8.44	-62.3	-55.4	-109.5
6.0	-110.4	22.9	52.8	9.11	-34.3	-38.0	-63.3
10.0	-23.15	1.9	7.60	1.47	-13.7	-3.92	-16.2
15.0	0	0	0	0	0	0	0

Magnesium r_s=2.78926

a	σ_S	σ_{XC}	σ_{ES}	σ_{PS}	σ_U	σ_T
0	1059.7	-985.3	-356.9	-274.9	173	-557.5
0.25	868.9	-866.6	-320.8	-217.6	-236	-536.2
0.50	704.1	-757.4	-279.3	-169.1	-270.6	-501.6
0.75	554.3	-659.6	-233.2	-128.8	-291.9	-476.2
1.0	424.9	-567.0	-187.7	-95.4	-294.7	-425.7
2.0	87.23	-293.6	-50.54	-16.2	-245.7	-273.1
3.0	-54.4	-132.4	25.1	9.32	-161.4	-155.6
5.0	-98.6	-2.99	38.7	12.7	-62.8	-50.2
10.0	-23.5	6.34	1.90	.92	-15.2	-14.3
15.0	0	0	0	0	0	0

Magnesium r_s=2.78926

a	σ_S	σ_{XC}	σ_{ES}	σ_{PS}	σ_U	σ_{NL}	σ_T
0	1112.7	-1025.7	-388.2	-277.9	191.6	-137.5	-716.7
0.25	921.7	-907.7	-352.1	-221.9	-255.6	-137.1	-697.0
0.50	753.7	-795.4	-310.2	-173.9	-289.9	-135.8	-661.6
0.75	600.5	-694.9	-262.8	-134.2	-310.6	-133.8	-625.2
1.0	469.2	-603.3	-216.2	-101.1	-315.3	-131.0	-582.4
2.0	116.2	-320.2	-66.3	-20.3	-265.1	-113.7	-410.3
3.0	-53.6	-150.9	16.4	9.6	-184.4	-91.5	-269.8
5.0	-124.4	-5.0	52.5	16.2	-76.6	-49.6	-110.3
10.0	-42.0	-3.2	8.7	2.1	-30.1	-3.60	-31.6
15.0	0	0	0	0	0	0	0

Sodium r_s=3.99

a	σ_S	σ_{XC}	σ_{ES}	σ_{PS}	σ_U	σ_T
0	144.3	-257.4	-77.3	-38.2	-157.5	-228.6
0.25	108.7	-228.4	-69.1	-36.3	-160.4	-223.0
0.50	83.8	-200.4	-60.4	-34.3	-156.1	-211.3
0.75	57.6	-174.1	-51.3	-32.1	-151.2	-199.9
1.0	35.6	-151.0	-42.1	-29.8	-144.3	-187.4
2.0	-26.9	-74.0	-13.2	-21.0	-108.9	-131.1
3.0	-48.4	-35.1	5.4	-15.3	-76.1	-93.4
5.0	-46.4	3.72	12.4	-6.7	-29.9	-36.9
10.0	-6.5	1.32	1.87	-.45	-3.31	-3.78
15.0	0	0	0	0	0	0

Sodium Nonlocal r_s=3.99

a	σ_S	σ_{xc}	σ_{es}	σ_{ps}	σ_U	σ_{NL}	σ_T
0	169.8	-279.4	-82.8	-34.9	-159.5	-45.7	-273.1
0.25	137.8	-251.3	-74.8	-33.4	-162.1	-45.6	-267.4
0.50	109.8	-223.2	-66.1	-31.7	-158.6	-45.4	-256.6
0.75	83.6	-198.7	-56.9	-29.8	-155.4	-44.9	-246.6
1.0	60.3	-173.5	-47.6	-28.0	-147.6	-44.2	-233.1
2.0	-5.86	-95.5	-16.20	-20.5	-112.3	-40.0	-178.0
3.0	-42.6	-40.6	3.91	-15.1	-77.2	-33.9	-128.3
5.0	-44.4	-4.2	15.5	-6.9	-32.7	-20.7	-60.6
10.0	-15.0	10.8	3.18	-0.5	-1.02	-1.87	-3.39
15.0	0	0	0	0	0	0	0

Sodium* r_s=3.88127

a	σ_S	σ_{xc}	σ_{es}	σ_{ps}	σ_U	σ_T
0	170.1	-289.9	-84.4	-38.0	-168.4	-242.2
0.25	131.7	-258.8	-75.2	-38.3	-173.2	-239.8
0.50	100.2	-225.5	-65.8	-37.9	-168.7	-229.0
0.75	70.1	-196.0	-55.7	-36.9	-163.9	-218.5
1.0	44.6	-170.3	-45.5	-35.5	-157.2	-206.8
2.0	-25.9	-86.0	-13.3	-27.7	-119.7	-152.9
3.0	-52.5	-40.0	6.48	-21.5	-84.0	-107.6
5.0	-50.3	2.49	13.8	-10.0	-33.7	-44.1
10.0	-8.54	2.04	1.74	-0.66	-4.75	-5.42
15.0	0	0	0	0	0	0

Sodium* Nonlocal r_s=3.88127

a	σ_S	σ_{xc}	σ_{es}	σ_{ps}	σ_U	σ_{NL}	σ_T
0	199.3	-312.2	-92.5	-32.8	-169.6	-50.0	-288.1
0.25	162.1	-279.4	-83.5	-33.5	-172.4	-49.9	-284.1
0.50	128.8	-247.6	-73.8	-33.3	-170.1	-49.5	-275.4
0.75	97.8	-217.3	-63.2	-33.1	-165.0	-49.0	-264.8
1.0	71.3	-190.6	-52.8	-32.2	-158.2	-48.3	-252.8
2.0	-4.70	-103.6	-17.5	-26.3	-120.4	-43.5	-195.7
3.0	-40.5	-51.9	4.6	-21.0	-85.7	-36.8	-145.5
5.0	-523.0	1.54	17.4	-10.4	-33.4	-22.2	-66.3
10.0	-12.9	5.73	3.41	-0.89	-3.71	-2.00	-6.60
15.0	0	0	0	0	0	0	0

APPENDIX X

SELF-CONSISTENT POTENTIALS AND DENSITIES

In this Appendix the self-consistent potentials and densities are listed in order of increasing r_s values. Each element is treated as a section. The ordering is LDA followed by nonlocal values. The superscript + indicates self-consistent densities obtained by minimizing the cohesive energy. Each element is presented in order of increasing separation. The first entry is the first point at the computational space-bulk boundary. The x-values are readily obtained knowing the x-value of the first entry and the mesh spacing which are included in the following table. The symmetry point is readily recognized as the minimum in the density or the maximum in the potential. Each listing contains a few entries past the symmetry point. The maximum number of separations were calculated for Mg in order to Separate Force Curves.

Separation, au	x-value of first entry, au	Mesh size, au	Entry of symmetry point
0.25	-15.0	0.125	121
.50	-15.0	.25	61
.75	-15.125	.125	122
1.0	-15.25	.25	62
1.5	-20.75	.25	84
2.0	-15.75	.25	64
2.5	-21.5	.25	87
3.0	-21.5	.25	87
4.0	-22.25	.25	90
5.0	-22.25	.25	90
6.0	-25.0	.25	101
10.0	-25.0	.25	101
15.0	-27.5	.25	111

```
redit pote2
LOADING POTE2        AL LDA a=0.25
REKEYED
EDIT                 DENS
p99
       TOP RECORD
0000100 0.26912708E-01 0.26912525E-01 0.26912440E-01 0.26912481E-01 0.26912633E-01
0000200 0.26912950E-01 0.26913393E-01 0.26913948E-01 0.26914626E-01 0.26915342E-01
0000300 0.26916128E-01 0.26916951E-01 0.26917722E-01 0.26918441E-01 0.26919067E-01
0000400 0.26919544E-01 0.26919860E-01 0.26919968E-01 0.26919913E-01 0.26919633E-01
0000500 0.26919156E-01 0.26918478E-01 0.26917633E-01 0.26916634E-01 0.26915558E-01
0000600 0.26914440E-01 0.26913334E-01 0.26912276E-01 0.26911311E-01 0.26910547E-01
0000700 0.26910007E-01 0.26909757E-01 0.26909813E-01 0.26910201E-01 0.26910912E-01
0000800 0.26911914E-01 0.26913159E-01 0.26914582E-01 0.26916131E-01 0.26917756E-01
0000900 0.26919331E-01 0.26920751E-01 0.26921999E-01 0.26922952E-01 0.26923593E-01
0001000 0.26923835E-01 0.26923683E-01 0.26923094E-01 0.26922088E-01 0.26920740E-01
0001100 0.26919041E-01 0.26917148E-01 0.26915103E-01 0.26913065E-01 0.26911177E-01
0001200 0.26909515E-01 0.26908219E-01 0.26907388E-01 0.26907105E-01 0.26907414E-01
0001300 0.26908360E-01 0.26909899E-01 0.26912056E-01 0.26914667E-01 0.26917555E-01
0001400 0.26920877E-01 0.26924156E-01 0.26927274E-01 0.26930064E-01 0.26932295E-01
0001500 0.26933812E-01 0.26934419E-01 0.26934035E-01 0.26932530E-01 0.26929896E-01
0001600 0.26926160E-01 0.26921414E-01 0.26915804E-01 0.26909564E-01 0.26902962E-01
0001700 0.26896294E-01 0.26889924E-01 0.26884202E-01 0.26879489E-01 0.26876088E-01
0001800 0.26874293E-01 0.26874281E-01 0.26876125E-01 0.26879810E-01 0.26885118E-01
0001900 0.26891697E-01 0.26899003E-01 0.26906323E-01 0.26912753E-01 0.26917178E-01
0002000 0.26919389E-01 0.26914928E-01 0.26905350E-01 0.26888050E-01 0.26861444E-01
0002100 0.26824001E-01 0.26774235E-01 0.26710853E-01 0.26632786E-01 0.26539274E-01
0002200 0.26429903E-01 0.26304714E-01 0.26164267E-01 0.26009571E-01 0.25842309E-01
0002300 0.25664750E-01 0.25479771E-01 0.25290940E-01 0.25102392E-01 0.24918959E-01
0002400 0.24745937E-01 0.24589259E-01 0.24455283E-01 0.24350792E-01 0.24282809E-01
0002500 0.24259482E-01 0.24282809E-01 0.24350792E-01 0.24455283E-01 0.24589259E-01
EOF
q
redit pote3
LOADING POTE3
REKEYED              VEFF
EDIT
p99
       TOP RECORD
0000100-0.42978472E 00-0.42979503E 00-0.42979437E 00-0.42980540E 00-0.42980504E 00
0000200-0.42980474E 00-0.42981696E 00-0.42981708E 00-0.42981941E 00-0.42981029E 00
0000300-0.42981291E 00-0.42981595E 00-0.42980635E 00-0.42980945E 00-0.42979962E 00
0000400-0.42980152E 00-0.42980242E 00-0.42979062E 00-0.42978978E 00-0.42979842E 00
0000500-0.42979383E 00-0.42980039E 00-0.42980641E 00-0.42979974E 00-0.42980456E 00
0000600-0.42980027E 00-0.42981440E 00-0.42981941E 00-0.42981476E 00-0.42979836E 00
0000700-0.42979443E 00-0.42979193E 00-0.42979032E 00-0.42978984E 00-0.42979008E 00
0000800-0.42979079E 00-0.42979252E 00-0.42979473E 00-0.42979717E 00-0.42979920E 00
0000900-0.42980134E 00-0.42980301E 00-0.42980379E 00-0.42980373E 00-0.42981523E 00
0001000-0.42981291E 00-0.42981923E 00-0.42982364E 00-0.42982674E 00-0.42984051E 00
0001100-0.42984056E 00-0.42983305E 00-0.42983228E 00-0.42983103E 00-0.42982942E 00
0001200-0.42982739E 00-0.42982578E 00-0.42982322E 00-0.42982179E 00-0.42982012E 00
0001300-0.42981851E 00-0.42981732E 00-0.42981678E 00-0.42981601E 00-0.42981648E 00
0001400-0.42981732E 00-0.42981845E 00-0.42982019E 00-0.42982203E 00-0.42982405E 00
0001500-0.42982537E 00-0.42982727E 00-0.42982924E 00-0.42982829E 00-0.42982680E 00
0001600-0.42982376E 00-0.42981990E 00-0.42981143E 00-0.42980236E 00-0.42979936E 00
0001700-0.42977452E 00-0.42975706E 00-0.42973791E 00-0.42971557E 00-0.42969221E 00
0001800-0.42966729E 00-0.42964125E 00-0.42961556E 00-0.42958863E 00-0.42956275E 00
0001900-0.42953563E 00-0.42950624E 00-0.42947626E 00-0.42944050E 00-0.42939800E 00
0002000-0.42934310E 00-0.42927772E 00-0.42918020E 00-0.42905700E 00-0.42894425E 00
0002100-0.42868042E 00-0.42840332E 00-0.42804743E 00-0.42759603E 00-0.42703104E 00
0002200-0.42633146E 00-0.42547548E 00-0.42444021E 00-0.42320067E 00-0.42173278E 00
0002300-0.42001057E 00-0.41800076E 00-0.41570753E 00-0.41308147E 00-0.41011390E 00
0002400-0.40678856E 00-0.40300882E 00-0.39903700E 00-0.39485843E 00-0.39017178E 00
0002500-0.38813120E 00-0.39017178E 00-0.39485843E 00-0.39903700E 00-0.40300882E 00
EOF
```

```
redit pote4
LOADING POTE4        AL LDA a=0.5
REKEYED
EDIT                 DENS
p99
        TOP RECORD
0000100 0.26914787E-01 0.26912760E-01 0.26911974E-01 0.26912652E-01 0.26914705E-01
0000200 0.26917730E-01 0.26921030E-01 0.26923869E-01 0.26925504E-01 0.26925500E-01
0000300 0.26923597E-01 0.26920032E-01 0.26915483E-01 0.26910733E-01 0.26906732E-01
0000400 0.26904460E-01 0.26904553E-01 0.26907124E-01 0.26911795E-01 0.26917715E-01
0000500 0.26923664E-01 0.26928298E-01 0.26930418E-01 0.26929196E-01 0.26924513E-01
0000600 0.26917037E-01 0.26908148E-01 0.26899744E-01 0.26893795E-01 0.26892021E-01
0000700 0.26895367E-01 0.26903775E-01 0.26915964E-01 0.26929591E-01 0.26941650E-01
0000800 0.26948899E-01 0.26948690E-01 0.26939612E-01 0.26922006E-01 0.26898265E-01
0000900 0.26872642E-01 0.26850540E-01 0.26837591E-01 0.26838008E-01 0.26853193E-01
0001000 0.26880205E-01 0.26910678E-01 0.26930418E-01 0.26919931E-01 0.26856028E-01
0001100 0.26714239E-01 0.26472472E-01 0.26114963E-01 0.25636472E-01 0.25045827E-01
0001200 0.24368566E-01 0.23647904E-01 0.22944100E-01 0.22331871E-01 0.21896090E-01
0001300 0.21741942E-01 0.21896090E-01 0.22331871E-01 0.22944100E-01 0.23647904E-01
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT                 VEFF
p99
        TOP RECORD
0 00120-0.42976809E 00-0.42977315E 00-0.42975879E 00-0.42976171E 00-0.42975825E 00
0000200-0.42977029E 00-0.42977124E 00-0.42977089E 00-0.42976665E 00-0.42978036E 00
0000300-0.42   554E 00-0.42976439E 00-0.42977273E 00-0.42977995E 00-0.42976660E 00
0000400-0.42  5926E 00-0.42976028E 00-0.42975914E 00-0.42975408E 00-0.42975301E 00
0000500-0.42975271E 00-0.42975879E 00-0.42977858E 00-0.42978579E 00-0.42979294E 00
0000600-0.42979079E 00-0.42978454E 00-0.42977506E 00-0.42976379E 00-0.42975217E 00
0000700-0.42974287E 00-0.42973793E 00-0.42974007E 00-0.42974776E 00-0.42976224E 00
0000800-0.42977941E 00-0.42979592E 00-0.42980582E 00-0.42980313E 00-0.42978209E 00
0000900-0.42974001E 00-0.42967820E 00-0.42959940E 00-0.42950982E 00-0.42941546E 00
0001000-0.42931658E 00-0.42920393E 00-0.42904651E 00-0.42878920E 00-0.42833465E 00
0001100-0.42753863E 00-0.42620176E 00-0.42406666E 00-0.42081749E 00-0.41609442E 00
0001200-0.40951037E 00-0.40068942E 00-0.38930118E 00-0.37602210E 00-0.35573930E 00
0001300-0.35166734E 00-0.35573930E 00-0.37602210E 00-0.38930118E 00-0.40068942E 00
EOF
q
-
```

```
redit pote6
LOADING POTE6   AL LDA  a=075
REKEYED
EDIT            DENS.
p99
        TOP RECORD
0000100 0.26911855E-01 0.26910156E-01 0.26908793E-01 0.26907846E-01 0.26907388E-01
0000200 0.26907496E-01 0.26908163E-01 0.26909381E-01 0.26911102E-01 0.26913267E-01
0000300 0.26915759E-01 0.26918419E-01 0.26921157E-01 0.26923783E-01 0.26926164E-01
0000400 0.26928134E-01 0.26929587E-01 0.26930410E-01 0.26930548E-01 0.26929915E-01
0000500 0.26928589E-01 0.26926544E-01 0.26923884E-01 0.26920736E-01 0.26917193E-01
0000600 0.26913520E-01 0.26909843E-01 0.26906371E-01 0.26903320E-01 0.26900832E-01
0000700 0.26899122E-01 0.26898302E-01 0.26898388E-01 0.26899502E-01 0.26901580E-01
0000800 0.26904564E-01 0.26908342E-01 0.26912719E-01 0.26917487E-01 0.26922423E-01
0000900 0.26927222E-01 0.26931670E-01 0.26935425E-01 0.26938297E-01 0.26940081E-01
0001000 0.26940603E-01 0.26939776E-01 0.26937544E-01 0.26933994E-01 0.26929233E-01
0001100 0.26923474E-01 0.26916973E-01 0.26910041E-01 0.26903082E-01 0.26896466E-01
0001200 0.26890580E-01 0.26885808E-01 0.26882529E-01 0.26880968E-01 0.26881330E-01
0001300 0.26883744E-01 0.26888195E-01 0.26894569E-01 0.26902590E-01 0.26911952E-01
0001400 0.26922211E-01 0.26932783E-01 0.26943140E-01 0.26952613E-01 0.26960567E-01
0001500 0.26966430E-01 0.26969653E-01 0.26969802E-01 0.26966598E-01 0.26959915E-01
0001600 0.26949760E-01 0.26936464E-01 0.26920397E-01 0.26902214E-01 0.26882730E-01
0001700 0.26862916E-01 0.26843809E-01 0.26826534E-01 0.26812166E-01 0.26801709E-01
0001800 0.26796062E-01 0.26795801E-01 0.26801307E-01 0.26812498E-01 0.26828893E-01
0001900 0.26849478E-01 0.26872784E-01 0.26896726E-01 0.26918713E-01 0.26935611E-01
0002000 0.26943803E-01 0.26939329E-01 0.26917834E-01 0.26874863E-01 0.26805874E-01
0002100 0.26706506E-01 0.26572667E-01 0.26400808E-01 0.26188016E-01 0.25932346E-01
0002200 0.25632851E-01 0.25289796E-01 0.24904366E-01 0.24481151E-01 0.24023246E-01
0002300 0.23537274E-01 0.23030836E-01 0.22512972E-01 0.21994010E-01 0.21485459E-01
0002400 0.20999838E-01 0.20550523E-01 0.20151682E-01 0.19818146E-01 0.19565381E-01
0002500 0.19408360E-01 0.19355498E-01 0.19408360E-01 0.19565381E-01 0.19819146E-01
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT            VEFF
p99
        TOP RECORD
0000100-0.42978603E 00-0.42977911E 00-0.42978424E 00-0.42977977E 00-0.42977625E 00
0000200-0.42977619E 00-0.42976683E 00-0.42976993E 00-0.42976409E 00-0.42977059E 00
0000300-0.42977643E 00-0.42977387E 00-0.42978072E 00-0.42977846E 00-0.42978477E 00
0000400-0.42979121E 00-0.42978507E 00-0.42978656E 00-0.42978758E 00-0.42978388E 00
0000500-0.42978984E 00-0.42979360E 00-0.42978537E 00-0.42978460E 00-0.42978346E 00
0000600-0.42978323E 00-0.42978108E 00-0.42978030E 00-0.42976910E 00-0.42977047E 00
0000700-0.42976886E 00-0.42976576E 00-0.42976427E 00-0.42976266E 00-0.42975962E 00
0000800-0.42975891E 00-0.42975974E 00-0.42976052E 00-0.42976350E 00-0.42976618E 00
0000900-0.42977011E 00-0.42977422E 00-0.42977738E 00-0.42979175E 00-0.42979735E 00
0001000-0.42979879E 00-0.42980373E 00-0.42980856E 00-0.42982131E 00-0.42982394E 00
0001100-0.42982054E 00-0.42981780E 00-0.42981398E 00-0.42980796E 00-0.42980087E 00
0001200-0.42979342E 00-0.42978531E 00-0.42977625E 00-0.42976755E 00-0.42975944E 00
0001300-0.42975163E 00-0.42974555E 00-0.42974156E 00-0.42973930E 00-0.42974037E 00
0001400-0.42974293E 00-0.42974895E 00-0.42975700E 00-0.42976803E 00-0.42977953E 00
0001500-0.42979306E 00-0.42980650E 00-0.42981887E 00-0.42982984E 00-0.42983752E 00
0001600-0.42984110E 00-0.42983961E 00-0.42983127E 00-0.42981553E 00-0.42979205E 00
0001700-0.42975998E 00-0.42972046E 00-0.42967242E 00-0.42961782E 00-0.42955667E 00
0001800-0.42949057E 00-0.42942142E 00-0.42934924E 00-0.42927575E 00-0.42920172E 00
0001900-0.42913570E 00-0.42906872E 00-0.42900485E 00-0.42894160E 00-0.42887604E 00
0002000-0.42862326E 00-0.42844540E 00-0.42821157E 00-0.42790043E 00-0.42748642E 00
0002100-0.42694008E 00-0.42622530E 00-0.42530173E 00-0.42413198E 00-0.42263442E 00
0002200-0.42078167E 00-0.41850179E 00-0.41572815E 00-0.41239047E 00-0.40841824E 00
0002300-0.40373927E 00-0.39828259E 00-0.39127946E 00-0.38476640E 00-0.37659293E 00
0002400-0.36741567E 00-0.35718977E 00-0.34588569E 00-0.33351010E 00-0.32062685E 00
0002500-0.31345046E 00-0.31237358E 00-0.31345046E 00-0.32062685E 00-0.33351010E 00
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.26912140E-01 0.26907042E-01 0.26903961E-01 0.26903689E-01 0.26906397E-01
0000200 0.26911654E-01 0.26918326E-01 0.26924960E-01 0.26930016E-01 0.26932161E-01
0000300 0.26930571E-01 0.26925262E-01 0.26917070E-01 0.26907481E-01 0.26898421E-01
0000400 0.26892010E-01 0.26880861E-01 0.26892789E-01 0.26900634E-01 0.26912056E-01
0000500 0.26924893E-01 0.26936360E-01 0.26943821E-01 0.26945077E-01 0.26939288E-01
0000600 0.26926968E-01 0.26910253E-01 0.26892539E-01 0.26877829E-01 0.26869979E-01
0000700 0.26871782E-01 0.26894187E-01 0.26905794E-01 0.26932906E-01 0.26959963E-01
0000800 0.26980419E-01 0.26983219E-01 0.26979096E-01 0.26951980E-01 0.26909709E-01
0000900 0.26859142E-01 0.26810352E-01 0.26774757E-01 0.26762608E-01 0.26779957E-01
0001000 0.26825558E-01 0.26888430E-01 0.26946526E-01 0.26967004E-01 0.26908517E-01
0001100 0.26725531E-01 0.26374519E-01 0.25821425E-01 0.25049284E-01 0.24064880E-01
0001200 0.22902999E-01 0.21627396E-01 0.20327833E-01 0.19114256E-01 0.18110029E-01
0001300 0.17442420E-01 0.17213940E-01 0.17442420E-01 0.18110029E-01 0.19114256E-01
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.42978472E 00-0.42977970E 00-0.42975873E 00-0.42975128E 00-0.42974359E 00
0000200-0.42974782E 00-0.42974460E 00-0.42974293E 00-0.42974663E 00-0.42975407E 00
0000300-0.42975050E 00-0.42974478E 00-0.42975104E 00-0.42975205E 00-0.42973292E 00
0000400-0.42973226E 00-0.42972296E 00-0.42971909E 00-0.42971969E 00-0.42972022E 00
0000500-0.42972463E 00-0.42973381E 00-0.42975265E 00-0.42975885E 00-0.42978358E 00
0000600-0.42978299E 00-0.42978114E 00-0.42977345E 00-0.42976141E 00-0.42974716E 00
0000700-0.42973489E 00-0.42972821E 00-0.42973101E 00-0.42974478E 00-0.42977047E 00
0000800-0.42980164E 00-0.42983335E 00-0.42985481E 00-0.42985624E 00-0.42982596E 00
0000900-0.42975903E 00-0.42965537E 00-0.42952037E 00-0.42936665E 00-0.42920756E 00
0001000-0.42905188E 00-0.42889386E 00-0.42869550E 00-0.42837703E 00-0.42779469E 00
0001100-0.42672503E 00-0.42484778E 00-0.42173576E 00-0.41685247E 00-0.40956539E 00
0001200-0.39917463E 00-0.38496584E 00-0.36627662E 00-0.34257770E 00-0.31427461E 00
0001300-0.28790154E 00-0.28405017E 00-0.28790164E 00-0.31427461E 00-0.34257770E 00
EOF
q
redit pote
```

AL LDA a=1.0
DENS.

VEFF

```
redit pote10
LOADING POTE10   AL LDA a=1.5
REKEYED
EDIT             DENS.
p99
       TOP RECORD
0000100 0.26915044E-01 0.26919775E-01 0.26923783E-01 0.26926138E-01 0.26926231E-01
0000200 0.26923809E-01 0.26919287E-01 0.26913505E-01 0.26907593E-01 0.26902888E-01
0000300 0.26900474E-01 0.26901077E-01 0.26904773E-01 0.26910976E-01 0.26918646E-01
0000400 0.26926283E-01 0.26932277E-01 0.26935451E-01 0.26935097E-01 0.26931211E-01
0000500 0.26924629E-01 0.26916791E-01 0.26909497E-01 0.26904576E-01 0.26903488E-01
0000600 0.26906878E-01 0.26914418E-01 0.26924904E-01 0.26936263E-01 0.26946060E-01
0000700 0.26952021E-01 0.26952509E-01 0.26946843E-01 0.26935719E-01 0.26920926E-01
0000800 0.26905283E-01 0.26891969E-01 0.26883777E-01 0.26882671E-01 0.26889261E-01
0000900 0.26902370E-01 0.26910264E-01 0.26936132E-01 0.26948765E-01 0.26953556E-01
0001000 0.26948240E-01 0.26932605E-01 0.26908886E-01 0.26881453E-01 0.26856069E-01
0001100 0.26838854E-01 0.26834879E-01 0.26846930E-01 0.26874509E-01 0.26913530E-01
0001200 0.26956562E-01 0.26994176E-01 0.27015509E-01 0.27015623E-01 0.26987497E-01
0001300 0.26933633E-01 0.26861712E-01 0.26784956E-01 0.26720025E-01 0.26683658E-01
0001400 0.26688438E-01 0.26739115E-01 0.26823733E-01 0.26920751E-01 0.26988667E-01
0001500 0.26973218E-01 0.26811637E-01 0.26440825E-01 0.25807586E-01 0.24870791E-01
0001600 0.23656081E-01 0.22172436E-01 0.20503417E-01 0.18757012E-01 0.17064653E-01
0001700 0.15568528E-01 0.14406454E-01 0.13676345E-01 0.13430823E-01 0.13676345E-01
EOF
q
redit potell
LOADING POTE11
REKEYED
EDIT             VEFF
p99
       TOP RECORD
0000100-0.42978477E 00-0.42977709E 00-0.42977440E 00-0.42976787E 00-0.42977393E 00
0000200-0.42976826E 00-0.42977047E 00-0.42977381E 00-0.42976409E 00-0.42976528E 00
0000300-0.42976451E 00-0.42976689E 00-0.42976987E 00-0.42977005E 00-0.42977524E 00
0000400-0.42979467E 00-0.42980009E 00-0.42980736E 00-0.42982502E 00-0.42983133E 00
0000500-0.42984951E 00-0.42985952E 00-0.42985606E 00-0.42985964E 00-0.42986050E 00
0000600-0.42986411E 00-0.42986733E 00-0.42986822E 00-0.42988282E 00-0.42988485E 00
0000700-0.42988348E 00-0.42989337E 00-0.42989437E 00-0.42989008E 00-0.42985439E 00
0000800-0.42983400E 00-0.42981213E 00-0.42979442E 00-0.42974246E 00-0.42971224E 00
0000900-0.42969960E 00-0.42967814E 00-0.42966741E 00-0.42966384E 00-0.42963300E 00
0001000-0.42967307E 00-0.42966634E 00-0.42965545E 00-0.42963964E 00-0.42961800E 00
0001100-0.42956.645 00-0.42957455E 00-0.42956638E 00-0.42957544E 00-0.42960626E 00
0001200-0.42965776E 00-0.42972481E 00-0.42979538E 00-0.42985400E 00-0.42989062E 00
0001300-0.42985743E 00-0.42976910E 00-0.42961102E 00-0.42939472E 00-0.42913735E 00
0001400-0.42886823E 00-0.42861587E 00-0.42830515E 00-0.42818487E 00-0.42791325E 00
0001500-0.42742634E 00-0.42646241E 00-0.42462873E 00-0.42137134E 00-0.41507056E 00
0001600-0.40754944E 00-0.39510024E 00-0.37759769E 00-0.35400532E 00-0.32343490E 00
0001700-0.28620762E 00-0.25354928E 00-0.23174685E 00-0.22810340E 00-0.23174685E 00
EOF
e
-
```

```
redit potel2
LOADING POTE12
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.26916306E-01 0.26903037E-01 0.26891887E-01 0.26885301E-01 0.26884705E-01
0000200 0.26890382E-01 0.26901212E-01 0.26914058E-01 0.26928633E-01 0.26939100E-01
0000300 0.26943702E-01 0.26940949E-01 0.26930895E-01 0.26915267E-01 0.26897103E-01
0000400 0.26880383E-01 0.26869085E-01 0.26866302E-01 0.26873503E-01 0.26890196E-01
0000500 0.26913382E-01 0.26938811E-01 0.26961002E-01 0.26974626E-01 0.26975762E-01
0000600 0.26962917E-01 0.26937570E-01 0.26904188E-01 0.26869554E-01 0.26841521E-01
0000700 0.26827395E-01 0.26832171E-01 0.26857238E-01 0.26898397E-01 0.26951108E-01
0000800 0.27001504E-01 0.27038299E-01 0.27050465E-01 0.27030814E-01 0.26978400E-01
0000900 0.26899703E-01 0.26808418E-01 0.26723545E-01 0.26665706E-01 0.26652202E-01
0001000 0.26691426E-01 0.26777677E-01 0.26887383E-01 0.26977722E-01 0.26988462E-01
0001100 0.26847456E-01 0.26479702E-01 0.25819354E-01 0.24821974E-01 0.23477152E-01
0001200 0.21816365E-01 0.19014739E-01 0.17885659E-01 0.15968112E-01 0.14010439E-01
0001300 0.12453668E-01 0.11302382E-01 0.10600980E-01 0.10367565E-01 0.10600980E-01
EOF
q
redit potel3
LOADING POTE13
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.42978632E 00-0.42975020E 00-0.42971045E 00-0.42968661E 00-0.42967314E 00
0000200-0.42967546E 00-0.42967170E 00-0.42967278E 00-0.42968035E 00-0.42970270E 00
0000300-0.42971414E 00-0.42972249E 00-0.42973775E 00-0.42975050E 00-0.42974263E 00
0000400-0.42973828E 00-0.42972970E 00-0.42972219E 00-0.42971402E 00-0.42970854E 00
0000500-0.42971146E 00-0.42972332E 00-0.42975557E 00-0.42977881E 00-0.42981344E 00
0000600-0.42982537E 00-0.42983097E 00-0.42982256E 00-0.42979956E 00-0.42976451E 00
0000700-0.42972273E 00-0.42968291E 00-0.42965627E 00-0.42964965E 00-0.42967016E 00
0000800-0.42971617E 00-0.42978245E 00-0.42985547E 00-0.42991716E 00-0.42994392E 00
0000900-0.42991632E 00-0.42981988E 00-0.42965120E 00-0.42941809E 00-0.42914057E 00
0001000-0.42883021E 00-0.42852652E 00-0.42818370E 00-0.42774355E 00-0.42705959E 00
0001100-0.42588162E 00-0.42381948E 00-0.42031837E 00-0.41463232E 00-0.40582305E 00
0001200-0.39277983E 00-0.37427396E 00-0.34905022E 00-0.31594390E 00-0.27402645E 00
0001300-0.23062002E 00-0.20203561E 00-0.19318188E 00-0.17989537E 00-0.19318188E 00
EOF
q
-
```

```
redit pote2
LOADING POTE2
READY
EDIT
p20
        TOP RECORD
0000100 0.26901942E-01 0.26907846E-01 0.26915487E-01 0.26923317E-01 0.26920677E-01
0000200 0.26933104E-01 0.26932642E-01 0.26929198E-01 0.26920442E-01 0.26910238E-01
0000300 0.26901335E-01 0.26899273E-01 0.26899371E-01 0.26901451E-01 0.26897166E-01
0000400 0.26906516E-01 0.26917592E-01 0.26927067E-01 0.26935294E-01 0.26937216E-01
0000500 0.26934605E-01 0.26926063E-01 0.26913605E-01 0.26899982E-01 0.26887912E-01
0000600 0.26880264E-01 0.26879124E-01 0.26885185E-01 0.26897691E-01 0.26914436E-01
0000700 0.26932102E-01 0.26946973E-01 0.26955694E-01 0.26956033E-01 0.26947424E-01
0000800 0.26931275E-01 0.26910830E-01 0.26895018E-01 0.26874974E-01 0.26863358E-01
0000900 0.26873127E-01 0.26889414E-01 0.26914656E-01 0.26944142E-01 0.26971664E-01
0001000 0.26999002E-01 0.26996627E-01 0.26986141E-01 0.26960053E-01 0.26922580E-01
0001100 0.26880931E-01 0.26843987E-01 0.26820607E-01 0.26817545E-01 0.26837680E-01
0001200 0.26873001E-01 0.26933840E-01 0.26990883E-01 0.27036205E-01 0.27056586E-01
0001300 0.27042594E-01 0.26991340E-01 0.26980312E-01 0.26807430E-01 0.26700370E-01
0001400 0.26637659E-01 0.26613284E-01 0.26649261E-01 0.26739642E-01 0.26844830E-01
0001500 0.26970312E-01 0.27018309E-01 0.26902467E-01 0.26547637E-01 0.25870031E-01
0001600 0.24840787E-01 0.23419663E-01 0.21644160E-01 0.19501942E-01 0.17391657E-01
0001700 0.15150104E-01 0.13076715E-01 0.11272542E-01 0.98380446E-02 0.88108666E-02
0001800 0.81970431E-02 0.79042271E-02 0.81970431E-02 0.88108666E-02 0.98380446E-02
0001900
EOF
q
redit pote3
LOADING POTE3
READY
EDIT
p20
        TOP RECORD
0000100-0.42078364E 00-0.42079282E 00-0.42078060E 00-0.42078519E 00-0.42078346E 00
0000200-0.42079121E 00-0.42078489E 00-0.42078841E 00-0.42079085E 00-0.42077941E 00
0000300-0.42077452E 00-0.42076803E 00-0.42076141E 00-0.42075277E 00-0.42074705E 00
0000400-0.42074305E 00-0.42075241E 00-0.42075152E 00-0.42075253E 00-0.42076481E 00
0000500-0.42076326E 00-0.42077053E 00-0.42077476E 00-0.42076200E 00-0.42076046E 00
0000600-0.42075500E 00-0.42075000E 00-0.42074651E 00-0.42074621E 00-0.42076052E 00
0000700-0.42077160E 00-0.42078191E 00-0.42081011E 00-0.42082352E 00-0.42084557E 00
0000800-0.42085010E 00-0.42086006E 00-0.42086647E 00-0.42086351E 00-0.42084907E 00
0000900-0.42084068E 00-0.42085064E 00-0.42085517E 00-0.42086870E 00-0.42088705E 00
0001000-0.42091300E 00-0.42094314E 00-0.42095363E 00-0.42095350E 00-0.42093794E 00
0001100-0.42090488E 00-0.42085624E 00-0.42079690E 00-0.42073703E 00-0.42069565E 00
0001200-0.42065364E 00-0.42064488E 00-0.42066233E 00-0.42069884E 00-0.42074484E 00
0001300-0.42078320E 00-0.42078145E 00-0.42075329E 00-0.42065409E 00-0.42049641E 00
0001400-0.42032600E 00-0.42034711E 00-0.42078045E 00-0.42055382E 00-0.42028643E 00
0001500-0.42702219E 00-0.42730075E 00-0.42514013E 00-0.42405153E 00-0.42041427E 00
0001600-0.41444606E 00-0.40515362E 00-0.39135557E 00-0.37174886E 00-0.34409309E 00
0001700-0.30820057E 00-0.26548266E 00-0.22009388E 00-0.19594266E 00-0.16138023E 00
0001800-0.14531026E 00-0.14229635E 00-0.14531026E 00-0.16138023E 00-0.19594266E 00
EOF
e
-
```

AL LDA a=2.5

DENS.

ORIGINAL PAGE IS
OF POOR QUALITY

VEFF

```
redit pote4
LOADING POTE4
RETYED
EDIT
p99
        TOP RECORD
0000100 0.26903141E-01 0.26912268E-01 0.26922312E-01 0.26931159E-01 0.26937015E-01
0000200 0.26933520E-01 0.26935212E-01 0.26927646E-01 0.26917297E-01 0.26906326E-01
0000300 0.26897054E-01 0.26891552E-01 0.26891235E-01 0.26896395E-01 0.26906140E-01
0000400 0.26918557E-01 0.26930995E-01 0.26940737E-01 0.26945431E-01 0.26943702E-01
0000500 0.26935595E-01 0.26922412E-01 0.26906766E-01 0.26891921E-01 0.26881326E-01
0000600 0.26877545E-01 0.26881011E-01 0.26893040E-01 0.26911531E-01 0.26931204E-01
0000700 0.26948754E-01 0.26960108E-01 0.26962288E-01 0.26954144E-01 0.26936650E-01
0000800 0.26912991E-01 0.26887968E-01 0.26867002E-01 0.26855160E-01 0.26855015E-01
0000900 0.26868815E-01 0.26895221E-01 0.26927263E-01 0.26950255E-01 0.26963872E-01
0001000 0.26964795E-01 0.26948115E-01 0.26925635E-01 0.26905020E-01 0.26892912E-01
0001100 0.26937744E-01 0.26899022E-01 0.26892007E-01 0.26921114E-01 0.26865166E-01
0001200 0.26927089E-01 0.26904539E-01 0.27052086E-01 0.27064209E-01 0.27078822E-01
0001300 0.27030740E-01 0.26943915E-01 0.26832089E-01 0.26717239E-01 0.26625760E-01
0001400 0.26582617E-01 0.26604287E-01 0.26691073E-01 0.26825622E-01 0.26961170E-01
0001500 0.27031370E-01 0.26951309E-01 0.26628710E-01 0.25978010E-01 0.24936601E-01
0001600 0.23480702E-01 0.21635536E-01 0.19470490E-01 0.17136585E-01 0.14760185E-01
0001700 0.12510173E-01 0.10527680E-01 0.88083908E-02 0.76504424E-02 0.67782886E-02
0001800 0.62648617E-02 0.60961507E-02 0.62648617E-02 0.67782886E-02 0.76504424E-02
EOF
9
redit pote5
LOADING POTE5
RETYED
EDIT
p99
        TOP RECORD
0000100-0.42977071E 00-0.42979491E 00-0.42981631E 00-0.42982203E 00-0.42982119E 00
0000200-0.42982829E 00-0.42983222E 00-0.42981088E 00-0.42981809E 00-0.42981166E 00
0000300-0.42980289E 00-0.42979443E 00-0.42978364E 00-0.42977607E 00-0.42976987E 00
0000400-0.42977512E 00-0.42977262E 00-0.42977238E 00-0.42978734E 00-0.42978764E 00
0000500-0.42979902E 00-0.42980403E 00-0.42980427E 00-0.42978900E 00-0.42978412E 00
0000600-0.42977715E 00-0.42978364E 00-0.42977981E 00-0.42977500E 00-0.42977823E 00
0000700-0.42979544E 00-0.42980212E 00-0.42980939E 00-0.42982256E 00-0.42982775E 00
0000800-0.42981666E 00-0.42980623E 00-0.42979109E 00-0.42977190E 00-0.42975265E 00
0000900-0.42973596E 00-0.42972815E 00-0.42973077E 00-0.42975444E 00-0.42977357E 00
0001000-0.42980650E 00-0.42982465E 00-0.42983586E 00-0.42983383E 00-0.42981578E 00
0001100-0.42978621E 00-0.42974716E 00-0.42970920E 00-0.42968315E 00-0.42967772E 00
0001200-0.42970608E 00-0.42974883E 00-0.42981808E 00-0.42988104E 00-0.42994084E 00
0001300-0.42996514E 00-0.43001519E 00-0.43003537E 00-0.43002764E 00-0.42999250E 00
0001400-0.42993733E 00-0.42985157E 00-0.42973525E 00-0.42807132E 00-0.42774497E 00
0001500-0.42722321E 00-0.42623425E 00-0.42434740E 00-0.42003509E 00-0.41514075E 00
0001600-0.40580602E 00-0.38181121E 00-0.35171888E 00-0.32382612E 00-0.30680382E 00
0001700-0.25891815E 00-0.21314377E 00-0.17550284E 00-0.14673656E 00-0.12640760E 00
0001800-0.11334204E 00-0.11067319E 00-0.11334204E 00-0.12640760E 00-0.14673656E 00
EOF
9
-
```

```
redit pote6
LOADING POTE6
REVERSED
PRINT
p00
        TOP RECORD
0000100 0.26804521E-01 0.26830338E-01 0.26907876E-01 0.26918415E-01 0.26928745E-01
0000200 0.26936475E-01 0.26930668E-01 0.26937306E-01 0.26924468E-01 0.26917484E-01
0000300 0.26903506E-01 0.26800658E-01 0.26881382E-01 0.26877888E-01 0.26881143E-01
0000400 0.26890703E-01 0.26904732E-01 0.26920274E-01 0.26933960E-01 0.26942663E-01
0000500 0.26944119E-01 0.26937609E-01 0.26924020E-01 0.26905935E-01 0.26887093E-01
0000600 0.26871625E-01 0.26863214E-01 0.26864160E-01 0.26875015E-01 0.26894074E-01
0000700 0.26917744E-01 0.26941244E-01 0.26959471E-01 0.26968136E-01 0.26964832E-01
0000800 0.26940570E-01 0.26925001E-01 0.26896376E-01 0.26869714E-01 0.26851512E-01
0000900 0.26846778E-01 0.26857027E-01 0.26883041E-01 0.26920468E-01 0.26960347E-01
0001000 0.26995100E-01 0.27016530E-01 0.27013618E-01 0.26998230E-01 0.26960880E-01
0001100 0.26910566E-01 0.26858840E-01 0.26817605E-01 0.26797742E-01 0.26806377E-01
0001200 0.26844785E-01 0.26907459E-01 0.26993374E-01 0.27052801E-01 0.27100984E-01
0001300 0.27111143E-01 0.27074486E-01 0.26991751E-01 0.26974751E-01 0.26745453E-01
0001400 0.26632264E-01 0.26564095E-01 0.26562784E-01 0.26635099E-01 0.26765786E-01
0001500 0.26913572E-01 0.27010970E-01 0.26969420E-01 0.26899641E-01 0.26876455E-01
0001600 0.25056455E-01 0.23595244E-01 0.21710418E-01 0.19476194E-01 0.17017074E-01
0001700 0.14490452E-01 0.12061519E-01 0.98754056E-02 0.30139204E-02 0.65100867E-02
0001800 0.53584203E-02 0.45961400E-02 0.39274066E-02 0.35028397E-02 0.34826819E-02
EOR
0
redit pote7
LOADING POTE7
REVERSED
PRINT
p00
        TOP RECORD
0000100-0.42078472E 00-0.42078466E 00-0.42077142E 00-0.42076022E 00-0.42075229E 00
0000200-0.42075575E 00-0.42074561E 00-0.42074621E 00-0.42074520E 00-0.42072958E 00
0000300-0.42072612E 00-0.42071605E 00-0.42070319E 00-0.42069203E 00-0.42068041E 00
0000400-0.42067307E 00-0.42067074E 00-0.42067331E 00-0.42067051E 00-0.42067087E 00
0000500-0.42067814E 00-0.42068708E 00-0.42068197E 00-0.42068392E 00-0.42068076E 00
0000600-0.42067373E 00-0.42066861E 00-0.42065972E 00-0.42065400E 00-0.42066712E 00
0000700-0.42067421E 00-0.42068702E 00-0.42071444E 00-0.42073316E 00-0.42076213E 00
0000800-0.42077220E 00-0.42079131E 00-0.42079670E 00-0.42079467E 00-0.42077601E 00
0000900-0.42077262E 00-0.42078170E 00-0.42078370E 00-0.42078068E 00-0.42077346E 00
0001000-0.42075630E 00-0.42074470E 00-0.42073908E 00-0.42074496E 00-0.42076640E 00
0001100-0.42077008E 00-0.42078565E 00-0.42080539E 00-0.42081148E 00-0.42082263E 00
0001200-0.42080164E 00-0.42080402E 00-0.42083580E 00-0.42085020E 00-0.42085390E 00
0001300-0.43000954E 00-0.43003190E 00-0.42900566E 00-0.42088318E 00-0.42068845E 00
0001400-0.42042110E 00-0.42010575E 00-0.41977525E 00-0.41945637E 00-0.41914320E 00
0001500-0.42777848E 00-0.42721772E 00-0.42510569E 00-0.42429477E 00-0.42089820E 00
0001600-0.41516334E 00-0.40600470E 00-0.39210832E 00-0.37187590E 00-0.34401402E 00
0001700-0.30680507E 00-0.25006503E 00-0.20087244E 00-0.16852030E 00-0.13432121E 00
0001800-0.10681623E 00-0.85503402E-01-0.70503655E-01-0.59962372E-01-0.58752984E-01
EOR
0
```

AL LDA a=4.0

DENS.

VEFF

```
redit pete9
LOADING POINTS
REVERSE
EDIT
p99
        TOP RECORD
0000100 0.26905507E-01 0.26916396E-01 0.26922138E-01 0.26937995E-01 0.26943500E-01
0000200 0.26943313E-01 0.26936850E-01 0.26935284E-01 0.26910763E-01 0.26896343E-01
0000300 0.26885150E-01 0.26879840E-01 0.26891918E-01 0.26901261E-01 0.26905341E-01
0000400 0.26924133E-01 0.26940975E-01 0.26953131E-01 0.26957676E-01 0.26953254E-01
0000500 0.26940300E-01 0.26921946E-01 0.26899904E-01 0.26880353E-01 0.26868436E-01
0000600 0.26865820E-01 0.26874108E-01 0.26902390E-01 0.26917055E-01 0.26943173E-01
0000700 0.26964081E-01 0.26977412E-01 0.26977055E-01 0.26963089E-01 0.26937671E-01
0000800 0.26905607E-01 0.26873875E-01 0.26840256E-01 0.26838247E-01 0.26844107E-01
0000900 0.26867047E-01 0.26903328E-01 0.26945052E-01 0.26955571E-01 0.27013231E-01
0001000 0.27021363E-01 0.27006373E-01 0.26969444E-01 0.26916966E-01 0.26859500E-01
0001100 0.26800845E-01 0.26780350E-01 0.26780158E-01 0.26812546E-01 0.26873663E-01
0001200 0.26952323E-01 0.27031738E-01 0.27002610E-01 0.27117226E-01 0.27093761E-01
0001300 0.27020052E-01 0.26905496E-01 0.26770715E-01 0.26644207E-01 0.26557090E-01
0001400 0.26534330E-01 0.26587207E-01 0.26705224E-01 0.26851181E-01 0.26960220E-01
0001500 0.26944097E-01 0.26701963E-01 0.26130769E-01 0.25152326E-01 0.23722604E-01
0001600 0.21950776E-01 0.19604716E-01 0.17136250E-01 0.14514378E-01 0.11999696E-01
0001700 0.97144870E-02 0.77512786E-02 0.61346851E-02 0.48477352E-02 0.38535986E-02
0001800 0.31103360E-02 0.25777433E-02 0.22221008E-02 0.20187066E-02 0.19526286E-02
EOF
9
redit pete9
LOADING POINTS
REVERSE
EDIT
p99
        TOP RECORD
0000100-0.42972696E 00-0.42972201E 00-0.42972511E 00-0.42972869E 00-0.42973626E 00
0000200-0.42974246E 00-0.42975288E 00-0.42976505E 00-0.42977178E 00-0.42978054E 00
0000300-0.42977542E 00-0.42978333E 00-0.42977670E 00-0.42977278E 00-0.42977050E 00
0000400-0.42976308E 00-0.42976403E 00-0.42976863E 00-0.42977786E 00-0.42978114E 00
0000500-0.42978019E 00-0.42978407E 00-0.42978986E 00-0.42979044E 00-0.42979190E 00
0000600-0.42978054E 00-0.42977020E 00-0.42975044E 00-0.42974877E 00-0.42975160E 00
0000700-0.42975602E 00-0.42976373E 00-0.42978230E 00-0.42978932E 00-0.42980605E 00
0000800-0.42980713E 00-0.42980515E 00-0.42979150E 00-0.42978224E 00-0.42975241E 00
0000900-0.42973363E 00-0.42972740E 00-0.42972153E 00-0.42973303E 00-0.42976516E 00
0001000-0.42978836E 00-0.42982131E 00-0.42984003E 00-0.42984664E 00-0.42983520E 00
0001100-0.42980400E 00-0.42975748E 00-0.42970628E 00-0.42966139E 00-0.42963547E 00
0001200-0.42963830E 00-0.42967337E 00-0.42973483E 00-0.42980029E 00-0.42982200E 00
0001300-0.42980087E 00-0.42984131E 00-0.42983685E 00-0.42981906E 00-0.42981817E 00
0001400-0.42985643E 00-0.42985003E 00-0.42983089E 00-0.42979326E 00-0.42984200E 00
0001500-0.42979552E 00-0.42985813E 00-0.42985806E 00-0.41513055E 00-0.40640139E 00
0001600-0.39305675E 00-0.37352061E 00-0.36637080E 00-0.38985085E 00-0.26955509E 00
0001700-0.21030051E 00-0.16786594E 00-0.13342507E 00-0.10275275E 00-0.77071607E-01
0001800-0.56697190E-01-0.41114400E-01-0.29894695E-01-0.22862524E-01-0.21335058E-01
EOF
9
-
```

AL LDA a=5.0
DENS.

VEFF

```
redit potel0
LOADING POTE10
REKEYED
EDIT
p99
```

AL LDA a=100

DENS

```
       TOP RECORD
0000100 0.26820785E-01 0.26899636E-01 0.26913285E-01 0.26928924E-01 0.26943170E-01
0000200 0.26952796E-01 0.26955302E-01 0.26940898E-01 0.26937302E-01 0.26910689E-01
0000300 0.26900619E-01 0.26894124E-01 0.26873857E-01 0.26872281E-01 0.26880052E-01
0000400 0.26895951E-01 0.26916772E-01 0.26938211E-01 0.26955575E-01 0.26964806E-01
0000500 0.26963398E-01 0.26951090E-01 0.26929048E-01 0.26904114E-01 0.26878969E-01
0000600 0.26860103E-01 0.26851986E-01 0.26856985E-01 0.26874743E-01 0.26902139E-01
0000700 0.26933696E-01 0.26962645E-01 0.26982453E-01 0.26988178E-01 0.26977643E-01
0000800 0.26952125E-01 0.26916385E-01 0.26877690E-01 0.26844561E-01 0.26824708E-01
0000900 0.26823897E-01 0.26843477E-01 0.26880715E-01 0.26928663E-01 0.26977308E-01
0001000 0.27015720E-01 0.27034301E-01 0.27027205E-01 0.26993781E-01 0.26938359E-01
0001100 0.26874494E-01 0.26813190E-01 0.26769921E-01 0.26756581E-01 0.26779257E-01
0001200 0.26836406E-01 0.26918095E-01 0.27007509E-01 0.27083822E-01 0.27126603E-01
0001300 0.27120542E-01 0.27059942E-01 0.26951231E-01 0.26913606E-01 0.26675187E-01
0001400 0.26560381E-01 0.26524853E-01 0.26557669E-01 0.26662342E-01 0.26806138E-01
0001500 0.26927039E-01 0.26937556E-01 0.26733087E-01 0.26211642E-01 0.25283206E-01
0001600 0.23897983E-01 0.22057418E-01 0.19822825E-01 0.17311778E-01 0.14682315E-01
0001700 0.12107816E-01 0.97462460E-02 0.76959878E-02 0.59856176E-02 0.46000108E-02
0001800 0.35019931E-02 0.26464551E-02 0.19885558E-02 0.14878456E-02 0.11090051E-02
0001900 0.82655414E-03 0.61533600E-03 0.45871246E-03 0.34320052E-03 0.25256914E-03
0002000 0.19715617E-03 0.15328986E-03 0.12286451E-03 0.10299911E-03 0.91795780E-04
0002100 0.88177767E-04 0.91795780E-04 0.10299911E-03 0.12286451E-03 0.15328986E-03
EOF
q
redit potell
LOADING POTE11
REKEYED
EDIT
p99
```

VEFF

```
       TOP RECORD
0000100-0.42978263E 00-0.42976075E 00-0.42976689E 00-0.42975879E 00-0.42975223E 00
0000200-0.42975456E 00-0.42975467E 00-0.42974889E 00-0.42974788E 00-0.42974389E 00
0000300-0.42973781E 00-0.42972726E 00-0.42971841E 00-0.42970544E 00-0.42969549E 00
0000400-0.42969346E 00-0.42968505E 00-0.42968273E 00-0.42969030E 00-0.42969352E 00
0000500-0.42970061E 00-0.42970753E 00-0.42971188E 00-0.42970550E 00-0.42970079E 00
0000600-0.42969185E 00-0.42968905E 00-0.42967963E 00-0.42967105E 00-0.42966706E 00
0000700-0.42967767E 00-0.42968369E 00-0.42969191E 00-0.42971241E 00-0.42972865E 00
0000800-0.42973030E 00-0.42973346E 00-0.42972916E 00-0.42971541E 00-0.42970127E 00
0000900-0.42968243E 00-0.42966966E 00-0.42966419E 00-0.42967653E 00-0.42969340E 00
0001000-0.42972857E 00-0.42975402E 00-0.42978263E 00-0.42980057E 00-0.42980427E 00
0001100-0.42978948E 00-0.42975765E 00-0.42971355E 00-0.42966758E 00-0.42962986E 00
0001200-0.42961204E 00-0.42962021E 00-0.42965621E 00-0.42971355E 00-0.42977905E 00
0001300-0.42983198E 00-0.42984074E 00-0.42980844E 00-0.42970002E 00-0.42951411E 00
0001400-0.42926276E 00-0.42906521E 00-0.42863911E 00-0.42827791E 00-0.42783225E 00
0001500-0.42717540E 00-0.42607588E 00-0.42415018E 00-0.42087648E 00-0.41544414E 00
0001600-0.40684390E 00-0.39378768E 00-0.37474298E 00-0.34797513E 00-0.31160653E 00
0001700-0.26364499E 00-0.21353668E 00-0.17131243E 00-0.13537848E 00-0.10490828E 00
0001800-0.78850448E-01-0.56421235E-01-0.36979370E-01-0.20012908E-01-0.51123090E-02
0001900 0.80463775E-02 0.19717075E-01 0.30003435E-01 0.39316837E-01 0.47585666E-01
0002000 0.54619595E-01 0.60725570E-01 0.65721035E-01 0.69473386E-01 0.71836531E-01
0002100 0.72620630E-01 0.71836531E-01 0.69473386E-01 0.65721035E-01 0.60725570E-01
EOF
e
```

```
redit potel2
LOADING POTE12
REVEED
EDIT
p99
      TOP RECORD
0000100 0.26887931E-01 0.26893660E-01 0.26914436E-01 0.26932187E-01 0.26948337E-01
0000200 0.26950546E-01 0.26963286E-01 0.26958469E-01 0.26945930E-01 0.26928056E-01
0000300 0.26908495E-01 0.26891354E-01 0.26880465E-01 0.26879357E-01 0.26885834E-01
0000400 0.26901502E-01 0.26922446E-01 0.26943985E-01 0.26961446E-01 0.26970670E-01
0000500 0.26969116E-01 0.26956432E-01 0.26934747E-01 0.26908185E-01 0.26883354E-01
0000600 0.26862916E-01 0.26854411E-01 0.26859280E-01 0.26877202E-01 0.26904978E-01
0000700 0.26937053E-01 0.26966535E-01 0.26986752E-01 0.26992600E-01 0.26981872E-01
0000800 0.26955750E-01 0.26919123E-01 0.26879385E-01 0.26845142E-01 0.26824456E-01
0000900 0.26822899E-01 0.26842232E-01 0.26879698E-01 0.26928320E-01 0.26977677E-01
0001000 0.27016953E-01 0.27036238E-01 0.27029490E-01 0.26996002E-01 0.26941117E-01
0001100 0.26875477E-01 0.26813209E-01 0.26769128E-01 0.26755232E-01 0.26777940E-01
0001200 0.26835471E-01 0.26918177E-01 0.27008876E-01 0.27086519E-01 0.27130208E-01
0001300 0.27124558E-01 0.27063336E-01 0.26953001E-01 0.26813594E-01 0.26671170E-01
0001400 0.26562080E-01 0.26514802E-01 0.26545057E-01 0.26650608E-01 0.26796225E-01
0001500 0.26920829E-01 0.26936390E-01 0.26738589E-01 0.26221650E-01 0.25207448E-01
0001600 0.23914587E-01 0.22074405E-01 0.19839000E-01 0.17356098E-01 0.14696471E-01
0001700 0.12121800E-01 0.97595789E-02 0.77073202E-02 0.59337984E-02 0.46044365E-02
0001800 0.35025806E-02 0.26434977E-02 0.19825178E-02 0.14792394E-02 0.10991630E-02
0001900 0.81403321E-03 0.60125324E-03 0.44314004E-03 0.32605138E-03 0.23858508E-03
0002000 0.17587577E-03 0.12901930E-03 0.94607880E-04 0.69365764E-04 0.50867267E-04
0002100 0.37321777E-04 0.27411370E-04 0.20170177E-04 0.14891225E-04 0.11060219E-04
0002200 0.82996021E-05 0.63386005E-05 0.49840783E-05 0.41033109E-05 0.36079964E-05
0002300 0.34482428E-05 0.36079964E-05 0.41033109E-05 0.49840783E-05 0.63386005E-05
EOF
9
redit potel3
LOADING POTE13
REVEED
EDIT
p99
      TOP RECORD
0000100-0.42978358E 00-0.42979872E 00-0.42982327E 00-0.42982978E 00-0.42983413E 00
0000200-0.42984611E 00-0.42985481E 00-0.42984623E 00-0.42984450E 00-0.42983681E 00
0000300-0.42982876E 00-0.42981440E 00-0.42979860E 00-0.42978472E 00-0.42977226E 00
0000400-0.42977154E 00-0.42976236E 00-0.42975742E 00-0.42976874E 00-0.42976683E 00
0000500-0.42977822E 00-0.42978603E 00-0.42978734E 00-0.42977148E 00-0.42976105E 00
0000600-0.42974687E 00-0.42974365E 00-0.42972755E 00-0.42971748E 00-0.42971164E 00
0000700-0.42972273E 00-0.42972976E 00-0.42973906E 00-0.42975074E 00-0.42977715E 00
0000800-0.42977494E 00-0.42977625E 00-0.42976743E 00-0.42974943E 00-0.42972767E 00
0000900-0.42970550E 00-0.42969000E 00-0.42968404E 00-0.42970270E 00-0.42972428E 00
0001000-0.42976624E 00-0.42979467E 00-0.42982298E 00-0.42983925E 00-0.42983842E 00
0001100-0.42981696E 00-0.42977685E 00-0.42972493E 00-0.42967301E 00-0.42963523E 00
0001200-0.42962128E 00-0.42963755E 00-0.42968565E 00-0.42975545E 00-0.42983115E 00
0001300-0.42989759E 00-0.42989923E 00-0.42984170E 00-0.42970073E 00-0.42947471E 00
0001400-0.42918015E 00-0.42884490E 00-0.42849517E 00-0.42813271E 00-0.42771327E 00
0001500-0.42711216E 00-0.42609370E 00-0.42427325E 00-0.42107719E 00-0.41570514E 00
0001600-0.40710270E 00-0.39395070E 00-0.37474293E 00-0.34776551E 00-0.31129378E 00
0001700-0.26366007E 00-0.21408623E 00-0.17199975E 00-0.13622099E 00-0.10569477E 00
0001800-0.79514027E-01-0.56920640E-01-0.37287492E-01-0.20108264E-01-0.49736127E-02
0001900 0.84450282E-02 0.20411488E-01 0.31136371E-01 0.40787969E-01 0.49516004E-01
0002000 0.57377700E-01 0.64500809E-01 0.70930362E-01 0.76707661E-01 0.81863821E-01
0002100 0.86417735E-01 0.90741873E-01 0.94951630E-01 0.98947287E-01 0.10261661E 00
0002200 0.10607421E 00 0.10929698E 00 0.11355424E 00 0.11530411E 00 0.11637890E 00
0002300 0.11682564E 00 0.11637890E 00 0.11530411E 00 0.11355424E 00 0.10929698E 00
EOF
9
-
```

AL LDA a=15.0

DENS.

VEFF

```
redit note2
LOADING NOTE2
RETRIEVED
EDIT
p99
        TOP RECORD
0000100 0.26911784E-01 0.26911039E-01 0.26910361E-01 0.26909836E-01 0.26909463E-01
0000200 0.26909281E-01 0.26909325E-01 0.26909560E-01 0.26910003E-01 0.26910614E-01
0000300 0.26911393E-01 0.26912291E-01 0.26913226E-01 0.26914187E-01 0.26915114E-01
0000400 0.26915982E-01 0.26916716E-01 0.26917301E-01 0.26917715E-01 0.26917923E-01
0000500 0.26917923E-01 0.26917726E-01 0.26917331E-01 0.26916787E-01 0.26916098E-01
0000600 0.26915353E-01 0.26914593E-01 0.26913822E-01 0.26913106E-01 0.26912563E-01
0000700 0.26912134E-01 0.26911970E-01 0.26911985E-01 0.26912298E-01 0.26912820E-01
0000800 0.26913557E-01 0.26914526E-01 0.26915580E-01 0.26916765E-01 0.26917975E-01
0000900 0.26919149E-01 0.26920222E-01 0.26921112E-01 0.26921798E-01 0.26922159E-01
0001000 0.26922215E-01 0.26921898E-01 0.26921224E-01 0.26920203E-01 0.26918873E-01
0001100 0.26917234E-01 0.26915457E-01 0.26913550E-01 0.26911639E-01 0.26909862E-01
0001200 0.26908312E-01 0.26907060E-01 0.26906211E-01 0.26905864E-01 0.26906062E-01
0001300 0.26906807E-01 0.26908092E-01 0.26909929E-01 0.26912190E-01 0.26914813E-01
0001400 0.26917670E-01 0.26920568E-01 0.26923418E-01 0.26925992E-01 0.26928168E-01
0001500 0.26929736E-01 0.26930588E-01 0.26930597E-01 0.26929639E-01 0.26927862E-01
0001600 0.26925124E-01 0.26921518E-01 0.26917234E-01 0.26912410E-01 0.26907295E-01
0001700 0.26902124E-01 0.26897244E-01 0.26892886E-01 0.26889332E-01 0.26886884E-01
0001800 0.26885677E-01 0.26885893E-01 0.26887566E-01 0.26890561E-01 0.26894715E-01
0001900 0.26899625E-01 0.26904754E-01 0.26909459E-01 0.26912827E-01 0.26913863E-01
0002000 0.26911397E-01 0.26904140E-01 0.26890706E-01 0.26869673E-01 0.26839621E-01
0002100 0.26799008E-01 0.26746932E-01 0.26681643E-01 0.26602585E-01 0.26509028E-01
0002200 0.26400659E-01 0.26277561E-01 0.26140261E-01 0.25989812E-01 0.25827844E-01
0002300 0.25656447E-01 0.25479438E-01 0.25297116E-01 0.25116455E-01 0.24940945E-01
0002400 0.24775635E-01 0.24626050E-01 0.24498239E-01 0.24398625E-01 0.24333801E-01
0002500 0.24311572E-01 0.24333801E-01 0.24398625E-01 0.24498239E-01 0.24626050E-01
EOF
q
redit note3
LOADING NOTE3
RETRIEVED
EDIT
p99
        TOP RECORD
0000100-0.42978442E 00-0.42977327E 00-0.42975461E 00-0.42975175E 00-0.42974067E 00
0000200-0.42973191E 00-0.42973363E 00-0.42972666E 00-0.42973083E 00-0.42972529E 00
0000300-0.42973214E 00-0.42974037E 00-0.42973626E 00-0.42974633E 00-0.42974395E 00
0000400-0.42975175E 00-0.42975897E 00-0.42975456E 00-0.42976284E 00-0.42977434E 00
0000500-0.42977202E 00-0.42978209E 00-0.42978996E 00-0.42978626E 00-0.42979157E 00
0000600-0.42979753E 00-0.42980391E 00-0.42980766E 00-0.42980993E 00-0.42979926E 00
0000700-0.42979819E 00-0.42980051E 00-0.42980117E 00-0.42980111E 00-0.42980015E 00
0000800-0.42979926E 00-0.42979771E 00-0.42979664E 00-0.42979240E 00-0.42978829E 00
0000900-0.42978686E 00-0.42978430E 00-0.42978132E 00-0.42977971E 00-0.42979115E 00
0001000-0.42979044E 00-0.42979121E 00-0.42979175E 00-0.42979115E 00-0.42980522E 00
0001100-0.42980552E 00-0.42980331E 00-0.42980266E 00-0.42980236E 00-0.42980170E 00
0001200-0.42980117E 00-0.42980051E 00-0.42979920E 00-0.42979777E 00-0.42979616E 00
0001300-0.42979389E 00-0.42979145E 00-0.42978883E 00-0.42978597E 00-0.42978287E 00
0001400-0.42978084E 00-0.42977890E 00-0.42977756E 00-0.42977679E 00-0.42977720E 00
0001500-0.42977786E 00-0.42978001E 00-0.42978328E 00-0.42978662E 00-0.42979079E 00
0001600-0.42979532E 00-0.42980051E 00-0.42980486E 00-0.42980974E 00-0.42981088E 00
0001700-0.42981225E 00-0.42981112E 00-0.42980862E 00-0.42980218E 00-0.42979372E 00
0001800-0.42978114E 00-0.42976469E 00-0.42974502E 00-0.42972040E 00-0.42969036E 00
0001900-0.42965442E 00-0.42961103E 00-0.42956007E 00-0.42949796E 00-0.42942333E 00
0002000-0.42933124E 00-0.42921978E 00-0.42908049E 00-0.42890877E 00-0.42869804E 00
0002100-0.42843163E 00-0.42810565E 00-0.42770416E 00-0.42721200E 00-0.42661333E 00
0002200-0.42588955E 00-0.42502111E 00-0.42398673E 00-0.42276424E 00-0.42133141E 00
0002300-0.41966456E 00-0.41774142E 00-0.41553974E 00-0.41303939E 00-0.41022217E 00
0002400-0.40707242E 00-0.40357971E 00-0.39973116E 00-0.39580405E 00-0.39035749E 00
0002500-0.38942015E 00-0.39035749E 00-0.39580405E 00-0.39973116E 00-0.40357971E 00
eof
```

AL NL a=0.25
DENS.

VEFF

```
redit note2
LOADING NOTE2
REVERSED
EDIT
p00
        TOP RECORD
0000100 0.26911784E-01 0.26911039E-01 0.26910361E-01 0.26909836E-01 0.26909463E-01
0000200 0.26909281E-01 0.26909325E-01 0.26909560E-01 0.26910003E-01 0.26910614E-01
0000300 0.26911393E-01 0.26912291E-01 0.26913226E-01 0.26914187E-01 0.26915114E-01
0000400 0.26915982E-01 0.26916716E-01 0.26917301E-01 0.26917715E-01 0.26917923E-01
0000500 0.26917923E-01 0.26917726E-01 0.26917331E-01 0.26916787E-01 0.26916098E-01
0000600 0.26915353E-01 0.26914593E-01 0.26913822E-01 0.26913106E-01 0.26912563E-01
0000700 0.26912134E-01 0.26911970E-01 0.26911985E-01 0.26912298E-01 0.26912820E-01
0000800 0.26913557E-01 0.26914526E-01 0.26915580E-01 0.26916765E-01 0.26917975E-01
0000900 0.26919149E-01 0.26920222E-01 0.26921112E-01 0.26921798E-01 0.26922159E-01
0001000 0.26922215E-01 0.26921898E-01 0.26921224E-01 0.26920203E-01 0.26918873E-01
0001100 0.26917234E-01 0.26915457E-01 0.26913550E-01 0.26911639E-01 0.26909862E-01
0001200 0.26908312E-01 0.26907060E-01 0.26906211E-01 0.26905864E-01 0.26906062E-01
0001300 0.26906807E-01 0.26908093E-01 0.26909929E-01 0.26912190E-01 0.26914813E-01
0001400 0.26917670E-01 0.26920568E-01 0.26923419E-01 0.26925992E-01 0.26928169E-01
0001500 0.26929736E-01 0.26930589E-01 0.26930597E-01 0.26929699E-01 0.26927862E-01
0001600 0.26925124E-01 0.26921518E-01 0.26917234E-01 0.26912410E-01 0.26907295E-01
0001700 0.26902124E-01 0.26897244E-01 0.26892886E-01 0.26889332E-01 0.26886884E-01
0001800 0.26885677E-01 0.26885893E-01 0.26887566E-01 0.26890561E-01 0.26894715E-01
0001900 0.26899625E-01 0.26904754E-01 0.26909459E-01 0.26912927E-01 0.26913863E-01
0002000 0.26911397E-01 0.26904140E-01 0.26890706E-01 0.26869673E-01 0.26839621E-01
0002100 0.26799098E-01 0.26746932E-01 0.26681643E-01 0.26602585E-01 0.26509028E-01
0002200 0.26400659E-01 0.26277561E-01 0.26140261E-01 0.25989812E-01 0.25827844E-01
0002300 0.25656447E-01 0.25479438E-01 0.25297116E-01 0.25116455E-01 0.24940945E-01
0002400 0.24775635E-01 0.24626050E-01 0.24499239E-01 0.24398625E-01 0.24333801E-01
0002500 0.24311572E-01 0.24333801E-01 0.24398625E-01 0.24499239E-01 0.24626050E-01
EOF
q
redit note3
LOADING NOTE3
REVERSED
EDIT
p00
```

VEFF

```
        TOP RECORD
0000100-0.42978442E 00-0.42977327E 00-0.42975461E 00-0.42975175E 00-0.42974067E 00
0000200-0.42973191E 00-0.42973363E 00-0.42972666E 00-0.42973083E 00-0.42972529E 00
0000300-0.42973214E 00-0.42974037E 00-0.42973626E 00-0.42974633E 00-0.42974395E 00
0000400-0.42975175E 00-0.42975897E 00-0.42975456E 00-0.42976284E 00-0.42977434E 00
0000500-0.42977202E 00-0.42978209E 00-0.42978996E 00-0.42978626E 00-0.42979157E 00
0000600-0.42979753E 00-0.42980391E 00-0.42980766E 00-0.42980993E 00-0.42979926E 00
0000700-0.42979819E 00-0.42980051E 00-0.42980117E 00-0.42980111E 00-0.42980015E 00
0000800-0.42979926E 00-0.42979771E 00-0.42979664E 00-0.42979240E 00-0.42978829E 00
0000900-0.42978686E 00-0.42978430E 00-0.42978132E 00-0.42977971E 00-0.42979115E 00
0001000-0.42979044E 00-0.42979121E 00-0.42979175E 00-0.42979115E 00-0.42980522E 00
0001100-0.42980552E 00-0.42980331E 00-0.42980266E 00-0.42980236E 00-0.42980170E 00
0001200-0.42980117E 00-0.42980051E 00-0.42979920E 00-0.42979777E 00-0.42979616E 00
0001300-0.42979399E 00-0.42979145E 00-0.42978883E 00-0.42978597E 00-0.42978287E 00
0001400-0.42978084E 00-0.42977899E 00-0.42977756E 00-0.42977679E 00-0.42977720E 00
0001500-0.42977786E 00-0.42978001E 00-0.42978328E 00-0.42978662E 00-0.42979079E 00
0001600-0.42979533E 00-0.42980051E 00-0.42980486E 00-0.42980974E 00-0.42981089E 00
0001700-0.42981225E 00-0.42981112E 00-0.42980862E 00-0.42980218E 00-0.42979372E 00
0001800-0.42978114E 00-0.42976469E 00-0.42974502E 00-0.42972040E 00-0.42969036E 00
0001900-0.42965442E 00-0.42961103E 00-0.42956007E 00-0.42949796E 00-0.42942333E 00
0002000-0.42933124E 00-0.42921978E 00-0.42908049E 00-0.42890877E 00-0.42869804E 00
0002100-0.42843163E 00-0.42810565E 00-0.42770416E 00-0.42721200E 00-0.42661333E 00
0002200-0.42588955E 00-0.42502111E 00-0.42398673E 00-0.42276424E 00-0.42133141E 00
0002300-0.41966456E 00-0.41774142E 00-0.41553974E 00-0.41303939E 00-0.41022217E 00
0002400-0.40707242E 00-0.40357971E 00-0.39973116E 00-0.39580405E 00-0.39035749E 00
0002500-0.38942015E 00-0.39035749E 00-0.39580405E 00-0.39973116E 00-0.40357971E 00
EOF
```

```
q
redit pote4
LOADING POTE4
REVERED
EDIT
p99
        TOP RECORD
0000100 0.2691295?E-01 0.2691?9?3E-01 0.2691?955E-01 0.2691?461E-01 0.2691?997E-01
0000200 0.2691A641E-01 0.2691?525E-01 0.2692?9?3E-01 0.2692?704E-01 0.2692?932E-01
0000300 0.2692?59?E-01 0.2691?845E-01 0.2691?224E-01 0.2691?383E-01 0.2690?191E-01
0000400 0.2690?4?3E-01 0.2690?563E-01 0.2690?817E-01 0.2691?551E-01 0.2691?991E-01
0000500 0.2692?954E-01 0.2692?973E-01 0.2692?631E-01 0.2692?603E-01 0.2692?666E-01
0000600 0.2691?374E-01 0.2690?9?7E-01 0.2690?871E-01 0.2690?931E-01 0.2690?523E-01
0000700 0.2690?4?0E-01 0.2690?697E-01 0.2691?155E-01 0.2692?911E-01 0.2693?383E-01
0000800 0.2694?9?8E-01 0.2694?293E-01 0.2693?412E-01 0.2692?584E-01 0.2690?961E-01
0000900 0.2688?789E-01 0.2686?79?E-01 0.2685?936E-01 0.2686?9?0E-01 0.2687?747E-01
0001?00 0.2692?617E-01 0.2691?862E-01 0.2691?659E-01 0.2689??41E-01 0.2691??3?E-01
0001100 0.2665?134E-01 0.2640?3?0E-01 0.2604?282E-01 0.2557?1?4E-01 0.2560?178E-01
0001200 0.2435?7?2E-01 0.2366?566E-01 0.2?9??9??E-01 0.2?411?53E-01 0.2?9??66E-01
0001300 0.2?851137E-01 0.2?9??66E-01 0.2?411?53E-01 0.2?9??9??E-01 0.2366?566E-01
EOF
q
redit pote5
LOADING POTE5
REVERED
EDIT
p99
        TOP RECORD
0000100-0.42978168E 00-0.42977804E 00-0.42976260E 00-0.42976158E 00-0.42975530E 00
0000200-0.42976040E 00-0.42975742E 00-0.42975378E 00-0.42974880E 00-0.42975634E 00
0000300-0.42975795E 00-0.42975754E 00-0.42976975E 00-0.42977883E 00-0.42977708E 00
0000400-0.42978048E 00-0.42977881E 00-0.42977536E 00-0.42976808E 00-0.42975873E 00
0000500-0.42974037E 00-0.42974687E 00-0.42975414E 00-0.42975491E 00-0.42977130E 00
0000600-0.42977738E 00-0.42978507E 00-0.42979078E 00-0.42979383E 00-0.42979145E 00
0000700-0.42978442E 00-0.42977309E 00-0.42976120E 00-0.42975062E 00-0.42974579E 00
0000800-0.42974794E 00-0.42975032E 00-0.42977852E 00-0.42980230E 00-0.42982453E 00
0000900-0.42983918E 00-0.42983812E 00-0.42981523E 00-0.42976302E 00-0.42967430E 00
0001000-0.42954029E 00-0.42934418E 00-0.42905490E 00-0.42862284E 00-0.42786339E 00
0001100-0.42695248E 00-0.42541623E 00-0.42312711E 00-0.41980714E 00-0.41513550E 00
0001200-0.40876824E 00-0.40036684E 00-0.38958801E 00-0.37724626E 00-0.35796390E 00
0001300-0.35423921E 00-0.35796390E 00-0.37724626E 00-0.38958801E 00-0.40036684E 00
EOF
q
-
```

AL NL a=0.5

DENS.

VEFF

```
q
redit note4
LOADING NOTE4
RETRIEVED
EDIT
p99
        TOP RECORD
0000100 0.2691?0?57E-01 0.?691099?E-01 0.?691?C?55E-01 0.?691?4?61E-01 0.?691?00?7E-01
0000200 0.?691?4?41E-01 0.?691?525E-01 0.?692?0?9?E-01 0.?692?17?4E-01 0.?692?0?2?E-01
0000300 0.?692?5?45E-01 0.?691?845E-01 0.?691?4?24E-01 0.?691?3?3?E-01 0.?690?1?15E-01
0000400 0.?690?4?3?E-01 0.?690?5?63E-01 0.?690?81?7E-01 0.?691?5?1?E-01 0.?691?88?1E-01
0000500 0.?692?1?54E-01 0.?692?5?73E-01 0.?692?6?31E-01 0.?692?6?3?E-01 0.?692?666?E-01
0000600 0.?691?3?74E-01 0.?690?8?07E-01 0.?690?8?71E-01 0.?689?8?31E-01 0.?689?5?3?E-01
0000700 0.?689?8?5?E-01 0.?690?6?7?E-01 0.?691?1?5?E-01 0.?693?7?11E-01 0.?693?33?3E-01
0000800 0.?694?8?8?E-01 0.?694?2?3?E-01 0.?693?4?1?E-01 0.?692?4?84E-01 0.?690?5?61E-01
0000900 0.?688?7?9?E-01 0.?686?7?8?E-01 0.?685?33?6E-01 0.?686?4?0?E-01 0.?687?74?E-01
0001?00 0.?682?3?17E-01 0.?691?862E-01 0.?691?059E-01 0.?689?0?41E-01 0.?681?3?3?E-01
0001100 0.?665?134E-01 0.?640?3?9?E-01 0.?604?7?3?E-01 0.?557?184E-01 0.?5?041?8?E-01
0001?00 0.24352?2?E-01 0.?3663566E-01 0.?3?93?9?9E-01 0.?241?2?7?E-01 0.?19?7?66E-01
0001300 0.?1851137E-01 0.?19?7?66E-01 0.?241?2?7?E-01 0.?3?93?9?9E-01 0.?3663566E-01
EOF
q
redit note5
LOADING NOTE5
RETRIEVED
EDIT
p99
        TOP RECORD
0000100-0.42?78?68E 00-0.42?7?8?4E 00-0.42?76?69E 00-0.42?76?58E 00-0.42?755?0E 00
0000?00-0.42?76?4?E 00-0.42?75?42E 00-0.42?75?7?E 00-0.42?74?89E 00-0.42?756?4E 00
0000300-0.42?757?5E 00-0.42?75?54E 00-0.42?76?7?E 00-0.42?7?83E 00-0.42?7??8E 00
0000400-0.42?78?48E 00-0.42?7?83E 00-0.42?775?6E 00-0.42?76?8?E 00-0.42?7??3E 00
0000500-0.42?74?37E 00-0.42?746?7E 00-0.42?754?4E 00-0.42?754?1E 00-0.42?71?2E 00
0000600-0.42?77?8E 00-0.42?78?7E 00-0.42?79?7?E 00-0.42?79?83E 00-0.42?79?45E 00
0000700-0.42?78?42E 00-0.42?77?9E 00-0.42?76?2?E 00-0.42?75?62E 00-0.42?745?0E 00
0000800-0.42?74?94E 00-0.42?75?32E 00-0.42?77?5?E 00-0.42?8?2?E 00-0.42?6?453E 00
0000900-0.42?83?19E 00-0.42?83?12E 00-0.42?81?3?E 00-0.42?76?2E 00-0.42?67?3?E 00
0001000-0.42?54?2?E 00-0.42?34?18E 00-0.42?15?54E 00-0.42?6?284E 00-0.42?6?39E 00
0001100-0.42?5?48E 00-0.42?541?3E 00-0.42?12?11E 00-0.41?8?714E 00-0.41?13?5?E 00
0001?00-0.4?876?24E 00-0.4?36?84E 00-0.38?5?81E 00-0.37?24?5E 00-0.357?63?E 00
0001300-0.354?59?1E 00-0.357?63?8E 00-0.37?24?5E 00-0.38?59?81E 00-0.4?36?84E 00
EOF
q
-
```

AL NL a=0.5
DENS.

VEFF

AL NL a=0.75

DENS

```
0000100 0.2691279005-01 0.2691094005-01 0.2690951505-01 0.2690944605-01 0.2690779805-01
0000200 0.2690765605-01 0.2690330075-01 0.2690033785-01 0.2691020185-01 0.2691190705-01
0000300 0.2691393525-01 0.2691641165-01 0.2691584085-01 0.2692066025-01 0.2692263905-01
0000400 0.2692433175-01 0.2692559075-01 0.2692636175-01 0.2692652555-01 0.2692606755-01
0000500 0.2692501325-01 0.2692332005-01 0.2692211725-01 0.2691957555-01 0.2691566665-01
0000600 0.2691261175-01 0.2690955525-01 0.2690665155-01 0.2690412175-01 0.2690208035-01
0000700 0.2690096755-01 0.2690001325-01 0.2690014205-01 0.2690113755-01 0.2690295905-01
0000800 0.2690555335-01 0.2690987855-01 0.2691255505-01 0.2691567255-01 0.2692009075-01
0000900 0.2692505085-01 0.2693288575-01 0.2693921205-01 0.2693461655-01 0.2693618155-01
0001000 0.2693667655-01 0.2693600275-01 0.2693416255-01 0.2693117805-01 0.2692719555-01
0001100 0.2692233085-01 0.2691693575-01 0.2691099075-01 0.2690551275-01 0.2689956155-01
0001200 0.2689466205-01 0.2689006545-01 0.2688793155-01 0.2688670085-01 0.2688712355-01
0001300 0.2689002765-01 0.2689031585-01 0.2689086605-01 0.2690560455-01 0.2691367355-01
0001400 0.2692224085-01 0.2693151095-01 0.2694049455-01 0.2694864655-01 0.2695553055-01
0001500 0.2696046405-01 0.2696354635-01 0.2696387975-01 0.2696140155-01 0.2695602655-01
0001600 0.2694779115-01 0.2693606675-01 0.2693239025-01 0.2690914655-01 0.2689341155-01
0001700 0.2687749175-01 0.2686223455-01 0.2684861455-01 0.2683746895-01 0.2682961555-01
0001800 0.2682571115-01 0.2682616985-01 0.2683117285-01 0.2684047895-01 0.2685351755-01
0001900 0.2686923785-01 0.2688631755-01 0.2690233485-01 0.2691519355-01 0.2692189095-01
0002000 0.2691286665-01 0.2690256765-01 0.2686029905-01 0.2681460255-01 0.2673458755-01
0002100 0.2662520875-01 0.2648131115-01 0.2630403005-01 0.2608823455-01 0.2582314505-01
0002200 0.2553389025-01 0.2519665755-01 0.2481896015-01 0.2440784555-01 0.2396496855-01
0002300 0.2349623375-01 0.2301907775-01 0.2251559885-01 0.2202047855-01 0.2153648155-01
0002400 0.2107534055-01 0.2064907055-01 0.2027284055-01 0.1990587405-01 0.1957212105-01
0002500 0.1957481375-01 0.1953531655-01 0.1957481375-01 0.1972121075-01 0.1990587405-01
EOF
```

VEFF

```
0000100-0.4297864485 00-0.4297737355 00-0.4297764335 00-0.4297691655 00-0.4297621015 00
0000200-0.4297649035 00-0.4297559085 00-0.4297573335 00-0.4297492555 00-0.4297523555 00
0000300-0.4297553335 00-0.4297474525 00-0.4297512285 00-0.4297433555 00-0.4297465155 00
0000400-0.4297402555 00-0.4297400185 00-0.4297426085 00-0.4297464555 00-0.4297403185 00
0000500-0.4297473985 00-0.4297540855 00-0.4297487155 00-0.4297543855 00-0.4297595055 00
0000600-0.4297656005 00-0.4297707155 00-0.4297762555 00-0.4297698155 00-0.4297759555 00
0000700-0.4297770035 00-0.4297766155 00-0.4297776855 00-0.4297766755 00-0.4297733155 00
0000800-0.4297590985 00-0.4297654655 00-0.4297619355 00-0.4297589755 00-0.4297555755 00
0000900-0.4297527755 00-0.4297490555 00-0.4297472855 00-0.4297561055 00-0.4297577155 00
0001000-0.4297559095 00-0.4297611155 00-0.4297663655 00-0.4297835855 00-0.4297839155 00
0001100-0.4297936655 00-0.4297985455 00-0.4298003155 00-0.4298007665 00-0.4298011065 00
0001200-0.4298013685 00-0.4298014705 00-0.4298138655 00-0.4298115455 00-0.4298071955 00
0001300-0.4298001115 00-0.4297936655 00-0.4297852555 00-0.4297767735 00-0.4297680955 00
0001400-0.4297589325 00-0.4297521755 00-0.4297465155 00-0.4297437755 00-0.4297425755 00
0001500-0.4297444255 00-0.4297503655 00-0.4297577755 00-0.4297683855 00-0.4297808455 00
0001600-0.4297955335 00-0.4298000005 00-0.4298023885 00-0.4298360355 00-0.4298453355 00
0001700-0.4298050045 00-0.4298501005 00-0.4298425355 00-0.4298291155 00-0.4298046255 00
0001800-0.4297713005 00-0.4297277855 00-0.4296726055 00-0.4296049555 00-0.4295246065 00
0001900-0.4294265555 00-0.4293125355 00-0.4291756755 00-0.4290134355 00-0.4288169755 00
0002000-0.4285573875 00-0.4283885225 00-0.4279288995 00-0.4274823755 00-0.4269265555 00
0002100-0.4263341055 00-0.4253733255 00-0.4243077205 00-0.4229933305 00-0.4213852355 00
0002200-0.4194231155 00-0.4170748005 00-0.4142517755 00-0.4109156155 00-0.4069868905 00
0002300-0.4024067555 00-0.3971114855 00-0.3910415455 00-0.3841409755 00-0.3763509225 00
0002400-0.3676547455 00-0.3579006855 00-0.3473449955 00-0.3357006355 00-0.3252363855 00
0002500-0.3184605255 00-0.3175717655 00-0.3184605855 00-0.3252363855 00-0.3357006355 00
EOF
```

AL NL a=1.0
DENS

VEFF

```
redit potel0
LOADING POTE10
REKEYED
EDIT
p99
```

AL NL a=1.5
DENS.

```
        TOP RECORD
0000100 0.26916310E-01 0.26919626E-01 0.26922271E-01 0.26923537E-01 0.26922904E-01
0000200 0.26920266E-01 0.26915945E-01 0.26910573E-01 0.26905127E-01 0.26900765E-01
0000300 0.26898347E-01 0.26899451E-01 0.26901180E-01 0.26906090E-01 0.26912313E-01
0000400 0.26918605E-01 0.26923671E-01 0.26926506E-01 0.26926469E-01 0.26923597E-01
0000500 0.26918568E-01 0.26912529E-01 0.26906956E-01 0.26903372E-01 0.26902970E-01
0000600 0.26906211E-01 0.26912928E-01 0.26922103E-01 0.26932050E-01 0.26940826E-01
0000700 0.26946548E-01 0.26947867E-01 0.26944216E-01 0.26936091E-01 0.26924094E-01
0000800 0.26913114E-01 0.26903037E-01 0.26897050E-01 0.26896715E-01 0.26902508E-01
0000900 0.26913490E-01 0.26927352E-01 0.26941027E-01 0.26951097E-01 0.26954539E-01
0001000 0.26949577E-01 0.26936013E-01 0.26915617E-01 0.26891943E-01 0.26869681E-01
0001100 0.26853759E-01 0.26848324E-01 0.26855625E-01 0.26875425E-01 0.26904419E-01
0001200 0.26936870E-01 0.26965410E-01 0.26982449E-01 0.26982021E-01 0.26961282E-01
0001300 0.26921880E-01 0.26870191E-01 0.26815800E-01 0.26774514E-01 0.26755583E-01
0001400 0.26768006E-01 0.26811823E-01 0.26875846E-01 0.26935533E-01 0.26952986E-01
0001500 0.26879255E-01 0.26609135E-01 0.26238635E-01 0.25573783E-01 0.24640221E-01
0001600 0.23441266E-01 0.22013009E-01 0.20424869E-01 0.18775046E-01 0.17181858E-01
0001700 0.15773591E-01 0.14677763E-01 0.13988215E-01 0.13756499E-01 0.13988215E-01
EOF
q
```

```
redit potel1
LOADING POTE11
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.42978466E 00-0.42976254E 00-0.42974389E 00-0.42972571E 00-0.42972243E 00
0000200-0.42971426E 00-0.42972201E 00-0.42972749E 00-0.42972428E 00-0.42973125E 00
0000300-0.42973393E 00-0.42973369E 00-0.42973042E 00-0.42972422E 00-0.42971551E 00
0000400-0.42972153E 00-0.42971897E 00-0.42972088E 00-0.42973816E 00-0.42974830E 00
0000500-0.42977512E 00-0.42980266E 00-0.42981756E 00-0.42983788E 00-0.42985308E 00
0000600-0.42985779E 00-0.42985857E 00-0.42985004E 00-0.42985088E 00-0.42984176E 00
0000700-0.42983729E 00-0.42984903E 00-0.42985296E 00-0.42987382E 00-0.42988545E 00
0000800-0.42990255E 00-0.42991251E 00-0.42991507E 00-0.42992200E 00-0.42986679E 00
0000900-0.42983854E 00-0.42979693E 00-0.42975521E 00-0.42972130E 00-0.42969412E 00
0001000-0.42969525E 00-0.42969495E 00-0.42970538E 00-0.42971915E 00-0.42972881E 00
0001100-0.42972785E 00-0.42970926E 00-0.42967391E 00-0.42962444E 00-0.42956977E 00
0001200-0.42951608E 00-0.42947924E 00-0.42946690E 00-0.42948556E 00-0.42953461E 00
0001300-0.42960787E 00-0.42969096E 00-0.42976612E 00-0.42981380E 00-0.42981064E 00
0001400-0.42973596E 00-0.42956835E 00-0.42928106E 00-0.42882943E 00-0.42813545E 00
0001500-0.42706025E 00-0.42537570E 00-0.42274344E 00-0.41869026E 00-0.41260719E 00
0001600-0.40376312E 00-0.39134187E 00-0.37450099E 00-0.35245109E 00-0.32455683E 00
0001700-0.29026747E 00-0.25982475E 00-0.23948509E 00-0.23662096E 00-0.23948509E 00
EOF
q
```

```
redit potel2
LOADING POTE12
READY
EDIT
p99
      TOP RECORD
0000100 0.26912950E-01 0.26903402E-01 0.26895709E-01 0.26891705E-01 0.26892547E-01
0000200 0.26898373E-01 0.26908245E-01 0.26920289E-01 0.26932042E-01 0.26940946E-01
0000300 0.26944912E-01 0.26942439E-01 0.26933968E-01 0.26920781E-01 0.26905447E-01
0000400 0.26891325E-01 0.26881602E-01 0.26878879E-01 0.26884370E-01 0.26897606E-01
0000500 0.26916277E-01 0.26936725E-01 0.26954446E-01 0.26965145E-01 0.26965644E-01
0000600 0.26954740E-01 0.26933704E-01 0.26906285E-01 0.26878107E-01 0.26855547E-01
0000700 0.26844561E-01 0.26849154E-01 0.26870229E-01 0.26905108E-01 0.26947405E-01
0000800 0.26988231E-01 0.27017653E-01 0.27026933E-01 0.27010698E-01 0.26968800E-01
0000900 0.26907187E-01 0.26837561E-01 0.26775550E-01 0.26737340E-01 0.26735514E-01
0001000 0.26774090E-01 0.26844308E-01 0.26921432E-01 0.26964009E-01 0.26915874E-01
0001100 0.26711471E-01 0.26284337E-01 0.25577694E-01 0.24556138E-01 0.23215838E-01
0001200 0.21501205E-01 0.19755796E-01 0.17816525E-01 0.15002102E-01 0.14148716E-01
0001300 0.12685370E-01 0.11602927E-01 0.10942794E-01 0.10723203E-01 0.10942794E-01
EOF
e
redit potel3
LOADING POTE13
READY
EDIT
p99
      TOP RECORD
0000100-0.42978472E 00-0.42980200E 00-0.42980397E 00-0.42980897E 00-0.42980570E 00
0000200-0.42980629E 00-0.42979050E 00-0.42977077E 00-0.42975003E 00-0.42974895E 00
0000300-0.42974144E 00-0.42974442E 00-0.42976552E 00-0.42979163E 00-0.42980462E 00
0000400-0.42982870E 00-0.42984104E 00-0.42983961E 00-0.42982411E 00-0.42979807E 00
0000500-0.42976463E 00-0.42973125E 00-0.42971528E 00-0.42970449E 00-0.42972022E 00
0000600-0.42973435E 00-0.42976713E 00-0.42980534E 00-0.42984110E 00-0.42986369E 00
0000700-0.42986655E 00-0.42984659E 00-0.42980587E 00-0.42975146E 00-0.42969662E 00
0000800-0.42965388E 00-0.42963767E 00-0.42965502E 00-0.42970794E 00-0.42978811E 00
0000900-0.42988187E 00-0.42996740E 00-0.43002057E 00-0.43001366E 00-0.42992151E 00
0001000-0.42971057E 00-0.42938185E 00-0.42886615E 00-0.42809892E 00-0.42694253E 00
0001100-0.42515357E 00-0.42230827E 00-0.41812569E 00-0.41165394E 00-0.40212870E 00
0001200-0.38856791E 00-0.36902764E 00-0.34519678E 00-0.31352025E 00-0.27418679E 00
0001300-0.23648721E 00-0.21086651E 00-0.19391042E 00-0.19132918E 00-0.19391042E 00
EOF
e
```

AL NL a=2.0
DENS.

VEFF

```
redit pote2
LOADING POTE2
REREYED
EDIT
p99
      TOP RECORD
0000100 0.26903413E-01 0.26908234E-01 0.26914600E-01 0.26921321E-01 0.26926912E-01
0000200 0.26930168E-01 0.26930209E-01 0.26926057E-01 0.26920944E-01 0.26913352E-01
0000300 0.26905816E-01 0.26899967E-01 0.26897207E-01 0.26898310E-01 0.26903234E-01
0000400 0.26911147E-01 0.26920512E-01 0.26929274E-01 0.26935499E-01 0.26937671E-01
0000500 0.26935045E-01 0.26927911E-01 0.26917525E-01 0.26906002E-01 0.26895743E-01
0000600 0.26889104E-01 0.26887786E-01 0.26892304E-01 0.26902288E-01 0.26915684E-01
0000700 0.26929814E-01 0.26941579E-01 0.26948243E-01 0.26948008E-01 0.26940331E-01
0000800 0.26926436E-01 0.26908953E-01 0.26891522E-01 0.26878107E-01 0.26872035E-01
0000900 0.26875418E-01 0.26888348E-01 0.26907763E-01 0.26932754E-01 0.26955258E-01
0001000 0.26971057E-01 0.26975937E-01 0.26967663E-01 0.26946794E-01 0.26916828E-01
0001100 0.26893695E-01 0.26854713E-01 0.26837062E-01 0.26836202E-01 0.26854355E-01
0001200 0.26889566E-01 0.26935626E-01 0.26982933E-01 0.27020220E-01 0.27036864E-01
0001300 0.27025603E-01 0.26984714E-01 0.26919376E-01 0.26841704E-01 0.26768867E-01
0001400 0.26710768E-01 0.26710175E-01 0.26747264E-01 0.26824415E-01 0.26917297E-01
0001500 0.26982363E-01 0.26958682E-01 0.26773416E-01 0.26351130E-01 0.25625795E-01
0001600 0.24554018E-01 0.23126926E-01 0.21379022E-01 0.19384090E-01 0.17258495E-01
0001700 0.15137065E-01 0.13160501E-01 0.11453763E-01 0.10098509E-01 0.91280937E-02
0001800 0.85479170E-02 0.83562545E-02 0.85479170E-02 0.91280937E-02 0.10098509E-01
EOF
q
redit pote3
LOADING POTE3
REREYED
EDIT
p99
      TOP RECORD
0000100-0.42978466E 00-0.42978722E 00-0.42977870E 00-0.42976958E 00-0.42976487E 00
0000200-0.42976820E 00-0.42976671E 00-0.42977803E 00-0.42979538E 00-0.42980218E 00
0000300-0.42981869E 00-0.42982024E 00-0.42983454E 00-0.42983091E 00-0.42982233E 00
0000400-0.42980886E 00-0.42980373E 00-0.42978019E 00-0.42977929E 00-0.42978275E 00
0000500-0.42978020E 00-0.42979181E 00-0.42980772E 00-0.42981869E 00-0.42983222E 00
0000600-0.42983860E 00-0.42984045E 00-0.42982876E 00-0.42980701E 00-0.42979294E 00
0000700-0.42976898E 00-0.42974865E 00-0.42974508E 00-0.42974728E 00-0.42976375E 00
0000800-0.42978770E 00-0.42982078E 00-0.42985117E 00-0.42987150E 00-0.42986906E 00
0000900-0.42985904E 00-0.42984486E 00-0.42980951E 00-0.42977542E 00-0.42974514E 00
0001000-0.42972791E 00-0.42973745E 00-0.42975694E 00-0.42979300E 00-0.42983884E 00
0001100-0.42988467E 00-0.42991853E 00-0.42992967E 00-0.42991257E 00-0.42986691E 00
0001200-0.42980003E 00-0.42972344E 00-0.42965419E 00-0.42960626E 00-0.42959446E 00
0001300-0.42962259E 00-0.42968935E 00-0.42978197E 00-0.42988127E 00-0.42996335E 00
0001400-0.42999888E 00-0.42996174E 00-0.42982119E 00-0.42954826E 00-0.42909747E 00
0001500-0.42839104E 00-0.42726192E 00-0.42551976E 00-0.42271292E 00-0.41829568E 00
0001600-0.41151398E 00-0.40143350E 00-0.38697636E 00-0.36699057E 00-0.34036040E 00
0001700-0.32608481E 00-0.26449734E 00-0.22399700E 00-0.19278520E 00-0.17156702E 00
0001800-0.15772343E 00-0.15553957E 00-0.15772343E 00-0.17156702E 00-0.19278520E 00
0001900//BIN=26003    , FSRPARTS,BSN=3581, DSNAME=SNEDF
EOF
```

```
redit pote4
LOADING POTE4
REREVED
EDIT
p99
      TOP RECORD
0000100 0.269062335E-01 0.269131515E-01 0.269210495E-01 0.269291605E-01 0.269329995E-01
0000200 0.269341175E-01 0.269313835E-01 0.269250245E-01 0.269163365E-01 0.269070495E-01
0000300 0.268991075E-01 0.268963765E-01 0.268940225E-01 0.268903545E-01 0.268866955E-01
0000400 0.269174395E-01 0.269283095E-01 0.269369595E-01 0.26941352E-01 0.269402605E-01
0000500 0.269336705E-01 0.269226595E-01 0.269093195E-01 0.268965405E-01 0.268972395E-01
0000600 0.268936435E-01 0.268766965E-01 0.268569015E-01 0.268114035E-01 0.268281165E-01
0000700 0.268430885E-01 0.268532605E-01 0.268551595E-01 0.26843672E-01 0.268342405E-01
0000800 0.268144445E-01 0.268033705E-01 0.267955785E-01 0.267653485E-01 0.26865624E-01
0000900 0.268771955E-01 0.268084335E-01 0.268254005E-01 0.268524755E-01 0.268734645E-01
0001000 0.268920745E-01 0.268776175E-01 0.268571885E-01 0.268348045E-01 0.268367025E-01
0001100 0.268511155E-01 0.268266545E-01 0.268204255E-01 0.268361805E-01 0.268730965E-01
0001200 0.268751055E-01 0.268023375E-01 0.267831665E-01 0.267602785E-01 0.270583375E-01
0001300 0.270217435E-01 0.269540965E-01 0.268667965E-01 0.267703035E-01 0.267000255E-01
0001400 0.266512845E-01 0.267033505E-01 0.267737405E-01 0.268713405E-01 0.269524645E-01
0001500 0.269552045E-01 0.268021305E-01 0.264102565E-01 0.257047085E-01 0.246325175E-01
0001600 0.231764685E-01 0.213644685E-01 0.192717395E-01 0.170162975E-01 0.147339065E-01
0001700 0.125775375E-01 0.106768205E-01 0.911361725E-02 0.781460655E-02 0.707564135E-02
0001800 0.658123575E-02 0.641875345E-02 0.650123575E-02 0.707564135E-02 0.781460655E-02
EOF
q
redit pote5
LOADING POTE5
REREVED
EDIT
p99
      TOP RECORD
0000100-0.429783235 00-0.429767495 00-0.429757135 00-0.429755045 00-0.429750565 00
0000200-0.429759505 00-0.429760645 00-0.429773155 00-0.429790175 00-0.429802665 00
0000300-0.429811365 00-0.429813055 00-0.429807965 00-0.429797235 00-0.429790545 00
0000400-0.429772445 00-0.429759335 00-0.429744665 00-0.429753185 00-0.429759475 00
0000500-0.429770895 00-0.429793115 00-0.429812915 00-0.429819055 00-0.429803615 00
0000600-0.429833705 00-0.429823715 00-0.429816135 00-0.429789845 00-0.429765345 00
0000700-0.429753065 00-0.429740315 00-0.429735065 00-0.429756105 00-0.429784365 00
0000800-0.429804565 00-0.429835025 00-0.429855115 00-0.429861615 00-0.429850765 00
0000900-0.429826145 00-0.429797285 00-0.429744435 00-0.429713755 00-0.429695435 00
0001000-0.429702165 00-0.429713415 00-0.429745915 00-0.429791335 00-0.429833035 00
0001100-0.429857705 00-0.429856775 00-0.429850285 00-0.429855705 00-0.429905645 00
0001200-0.429746375 00-0.429694265 00-0.429667125 00-0.429674575 00-0.429721255 00
0001300-0.429801645 00-0.429880035 00-0.429904585 00-0.429857115 00-0.429858065 00
0001400-0.429870845 00-0.429767375 00-0.429643575 00-0.429800375 00-0.429139575 00
0001500-0.427007145 00-0.425277205 00-0.422557505 00-0.419287205 00-0.411715755 00
0001600-0.401824475 00-0.377440885 00-0.347309215 00-0.314065725 00-0.280456325 00
0001700-0.250963015 00-0.219378225 00-0.190375705 00-0.164100185 00-0.141205565 00
0001800-0.124823655 00-0.112224515 00-0.124823655 00-0.135205565 00-0.154100185 00
EOF
q
-
```

VEFF

AL NL a=3.0 DENS.

```
redit note6
LOADING NOTE6
RETRIEVED
EDIT
p99
        TOP RECORD
0000100 0.269963915E-01 0.268990979E-01 0.269066911E-01 0.269158922E-01 0.269248915E-01
0000200 0.269315932E-01 0.269253549E-01 0.269343189E-01 0.269283727E-01 0.269195405E-01
0000300 0.269086402E-01 0.268992284E-01 0.269007965E-01 0.268972009E-01 0.268904990E-01
0000400 0.268982890E-01 0.269008217E-01 0.269228075E-01 0.269344528E-01 0.269421566E-01
0000500 0.269440111E-01 0.269303299E-01 0.269287378E-01 0.269142995E-01 0.268990365E-01
0000600 0.268863258E-01 0.268791957E-01 0.268796505E-01 0.268981473E-01 0.269034329E-01
0000700 0.269225178E-01 0.269415558E-01 0.269563535E-01 0.269633965E-01 0.269606045E-01
0000800 0.269479648E-01 0.269276208E-01 0.269036378E-01 0.268811068E-01 0.268652285E-01
0000900 0.268601935E-01 0.268680305E-01 0.268979725E-01 0.269165008E-01 0.269479045E-01
0001000 0.269752075E-01 0.269017855E-01 0.269027205E-01 0.269762545E-01 0.269445855E-01
0001100 0.269030675E-01 0.268606545E-01 0.268269705E-01 0.268107915E-01 0.268178695E-01
0001200 0.268401545E-01 0.269900345E-01 0.269606325E-01 0.270176465E-01 0.270564005E-01
0001300 0.270642015E-01 0.270365705E-01 0.269728385E-01 0.268842245E-01 0.267890925E-01
0001400 0.267104895E-01 0.266708145E-01 0.266051525E-01 0.265543775E-01 0.264602225E-01
0001500 0.259601645E-01 0.260899405E-01 0.268671595E-01 0.265022895E-01 0.258115085E-01
0001600 0.247331825E-01 0.232420955E-01 0.213648045E-01 0.191737045E-01 0.167891275E-01
0001700 0.143591485E-01 0.120324605E-01 0.994408505E-02 0.817213055E-02 0.673735005E-02
0001800 0.562572115E-02 0.480762875E-02 0.425089525E-02 0.392846765E-02 0.382320635E-02
EOF
q
redit note7
LOADING NOTE7
RETRIEVED
EDIT
p99
        TOP RECORD
0000100-0.429784665E 00-0.429783825E 00-0.429767675E 00-0.429751105E 00-0.429731315E 00
0000200-0.429728335E 00-0.429717305E 00-0.429722135E 00-0.429736855E 00-0.429746095E 00
0000300-0.429763015E 00-0.429780195E 00-0.429790855E 00-0.429794615E 00-0.429784605E 00
0000400-0.429767075E 00-0.429751755E 00-0.429725235E 00-0.429701275E 00-0.429697395E 00
0000500-0.429603345E 00-0.429710575E 00-0.429736735E 00-0.429756645E 00-0.429785015E 00
0000600-0.429808485E 00-0.429819525E 00-0.429817805E 00-0.429803135E 00-0.429790445E 00
0000700-0.429750145E 00-0.429728385E 00-0.429715045E 00-0.429707535E 00-0.429723805E 00
0000800-0.429746935E 00-0.429784925E 00-0.429833835E 00-0.429873115E 00-0.429886765E 00
0000900-0.429891235E 00-0.429882415E 00-0.429841465E 00-0.429790325E 00-0.429737455E 00
0001000-0.429694055E 00-0.429683155E 00-0.429684345E 00-0.429715395E 00-0.429768385E 00
0001100-0.429832585E 00-0.429893855E 00-0.429936055E 00-0.429948515E 00-0.429923425E 00
0001200-0.429863935E 00-0.429779355E 00-0.429688105E 00-0.429609895E 00-0.429564655E 00
0001300-0.429565675E 00-0.429617465E 00-0.429712475E 00-0.429834075E 00-0.429956615E 00
0001400-0.430046505E 00-0.430067545E 00-0.429983085E 00-0.429755995E 00-0.429340795E 00
0001500-0.428666735E 00-0.427602415E 00-0.425008215E 00-0.423197695E 00-0.418887975E 00
0001600-0.412179415E 00-0.402048355E 00-0.387279605E 00-0.366531615E 00-0.338414855E 00
0001700-0.301884505E 00-0.255052325E 00-0.209349025E 00-0.170789005E 00-0.139581385E 00
0001800-0.115332645E 00-0.974839735E-01-0.856341725E-01-0.792440905E-01-0.769455435E-01
EOF
q
-
```

```
redit pote9
LOADING POTE9
REVISED
EDIT
p99
        TOP RECORD
0000100 0.26008752E-01 0.26012083E-01 0.26026707E-01 0.26038442E-01 0.26045736E-01
0000200 0.26046954E-01 0.26041728E-01 0.26031129E-01 0.26017275E-01 0.26003030E-01
0000300 0.25991480E-01 0.25985188E-01 0.25985647E-01 0.25993001E-01 0.26005308E-01
0000400 0.26021675E-01 0.26037030E-01 0.26048507E-01 0.26053656E-01 0.26050844E-01
0000500 0.26040424E-01 0.26024275E-01 0.26005712E-01 0.25988717E-01 0.25977154E-01
0000600 0.25973872E-01 0.25979066E-01 0.25994651E-01 0.26015122E-01 0.26037153E-01
0000700 0.26055891E-01 0.26066852E-01 0.26067172E-01 0.26055017E-01 0.26034701E-01
0000800 0.26007850E-01 0.25980693E-01 0.25950380E-01 0.25940125E-01 0.25953044E-01
0000900 0.25971316E-01 0.26000021E-01 0.26036010E-01 0.26068941E-01 0.26091063E-01
0001000 0.26098825E-01 0.26096454E-01 0.26055804E-01 0.26012432E-01 0.25984031E-01
0001100 0.25824008E-01 0.25800245E-01 0.25800008E-01 0.25820709E-01 0.25850510E-01
0001200 0.25946664E-01 0.27013253E-01 0.27064353E-01 0.27085561E-01 0.27067676E-01
0001300 0.27009696E-01 0.26920352E-01 0.26817407E-01 0.26734756E-01 0.26667103E-01
0001400 0.26663080E-01 0.26717842E-01 0.26815543E-01 0.26920352E-01 0.26966055E-01
0001500 0.26870824E-01 0.26541296E-01 0.25308044E-01 0.24841964E-01 0.23370670E-01
0001600 0.21400846E-01 0.16272840E-01 0.16034955E-01 0.14326554E-01 0.11305551E-01
0001700 0.87108707E-02 0.75259406E-02 0.62720068E-02 0.50324500E-02 0.40725700E-02
0001800 0.33523175E-02 0.28342572E-02 0.24871409E-02 0.22880050E-02 0.22233529E-02
EOF
e
redit pote9
LOADING POTE9
REVISED
EDIT
p99
        TOP RECORD
0000100-0.42977571E 00-0.42982727E 00-0.42986290E 00-0.42988044E 00-0.42988355E 00
0000200-0.42988198E 00-0.42986667E 00-0.42984462E 00-0.42982221E 00-0.42980450E 00
0000300-0.42979638E 00-0.42979518E 00-0.42979755E 00-0.42980497E 00-0.42981563E 00
0000400-0.42982166E 00-0.42982993E 00-0.42983011E 00-0.42982953E 00-0.42982068E 00
0000500-0.42980712E 00-0.42981143E 00-0.42981405E 00-0.42981300E 00-0.42981079E 00
0000600-0.42980174E 00-0.42981350E 00-0.42982540E 00-0.42983504E 00-0.42984373E 00
0000700-0.42984144E 00-0.42983503E 00-0.42982706E 00-0.42982763E 00-0.42982014E 00
0000800-0.42982252E 00-0.42982364E 00-0.42984021E 00-0.42983984E 00-0.42981547E 00
0000900-0.42982560E 00-0.42982225E 00-0.42981908E 00-0.42981900E 00-0.42981520E 00
0001000-0.42981961E 00-0.42981767E 00-0.42981730E 00-0.42981903E 00-0.42981820E 00
0001100-0.42982088E 00-0.42983040E 00-0.42983321E 00-0.42983201E 00-0.42983757E 00
0001200-0.42984560E 00-0.42985070E 00-0.42984114E 00-0.42983134E 00-0.42982478E 00
0001300-0.42982726E 00-0.42981775E 00-0.42981559E 00-0.42981772E 00-0.42982203E 00
0001400-0.42983534E 00-0.42984364E 00-0.42983311E 00-0.42982185E 00-0.42982703E 00
0001500-0.42982400E 00-0.42980733E 00-0.41888677E 00-0.41844636E 00-0.40269840E 00
0001600-0.38837826E 00-0.36801652E 00-0.34033083E 00-0.30766636E 00-0.25674372E 00
0001700-0.20861030E 00-0.16220532E 00-0.13476036E 00-0.10710663E 00-0.85010505E-01
0001800-0.67208340E-01-0.55640900E-01-0.47507434E-01-0.42801243E-01-0.41822627E-01
EOF
```

AL NL a=5.0
DENS.

VEFF

```
redit potel0
LOADING POTEL0
RETRIEVED
EDIT
p99
        TOP RECORD
0000100 0.269370235-01 0.269118215-01 0.268915185-01 0.268800745-01 0.268700655-01
0000200 0.268874355-01 0.269020765-01 0.269187655-01 0.269332005-01 0.269424435-01
0000300 0.269446345-01 0.269402455-01 0.269313405-01 0.269209505-01 0.269123465-01
0000400 0.269090625-01 0.269006285-01 0.268915425-01 0.268824615-01 0.268936895-01
0000500 0.269399595-01 0.269408385-01 0.269353505-01 0.269242085-01 0.269098175-01
0000600 0.268956655-01 0.268855245-01 0.268623215-01 0.268875005-01 0.269008545-01
0000700 0.269195185-01 0.269332955-01 0.269553625-01 0.269632755-01 0.269601465-01
0000800 0.269455695-01 0.269218655-01 0.268937955-01 0.268676035-01 0.268496875-01
0000900 0.268451095-01 0.268563075-01 0.268821575-01 0.269180545-01 0.269564435-01
0001000 0.269886075-01 0.270062615-01 0.270023555-01 0.269790235-01 0.269379395-01
0001100 0.268960055-01 0.268354695-01 0.267985085-01 0.267858325-01 0.268031025-01
0001200 0.268498555-01 0.269184635-01 0.269951345-01 0.270622735-01 0.271032735-01
0001300 0.271017255-01 0.270555235-01 0.269679025-01 0.268555025-01 0.267425485-01
0001400 0.266567845-01 0.266219455-01 0.266501235-01 0.267337045-01 0.268399795-01
0001500 0.269097025-01 0.268603125-01 0.265951165-01 0.260172675-01 0.250471945-01
0001600 0.236404075-01 0.218023595-01 0.195944125-01 0.171306285-01 0.145672035-01
0001700 0.120523425-01 0.974977025-02 0.774610045-02 0.606817015-02 0.470205775-02
0001800 0.361303065-02 0.275870305-02 0.209665285-02 0.158844825-02 0.120121785-02
0001900 0.907904095-03 0.686819675-03 0.520031095-03 0.397056575-03 0.305131085-03
0002000 0.237561215-03 0.188607395-03 0.154421555-03 0.131829215-03 0.119000025-03
0002100 0.114841795-03 0.119000025-03 0.131829215-03 0.154421555-03 0.188607395-03
EOF
q
redit potell
LOADING POTEL1
RETRIEVED
EDIT
p99
        TOP RECORD
0000100-0.429783765 00-0.429795135 00-0.429794735 00-0.429790025 00-0.429782155 00
0000200-0.429783705 00-0.429794365 00-0.429776405 00-0.429782995 00-0.429789365 00
0000300-0.429797935 00-0.429805405 00-0.429809755 00-0.429805585 00-0.429794375 00
0000400-0.429735375 00-0.429763565 00-0.429739245 00-0.429727265 00-0.429711825 00
0000500-0.429715345 00-0.429727975 00-0.429744125 00-0.429753545 00-0.429771545 00
0000600-0.429781735 00-0.429795035 00-0.429782335 00-0.429756765 00-0.429723085 00
0000700-0.429699305 00-0.429667355 00-0.429647035 00-0.429650315 00-0.429666345 00
0000800-0.429694885 00-0.429720945 00-0.429759445 00-0.429787225 00-0.429790445 00
0000900-0.429790745 00-0.429761955 00-0.429719275 00-0.429678325 00-0.429632255 00
0001000-0.429614605 00-0.429605255 00-0.429627605 00-0.429673195 00-0.429735485 00
0001100-0.429801055 00-0.429856365 00-0.429888255 00-0.429885565 00-0.429858155 00
0001200-0.429802365 00-0.429735905 00-0.429677845 00-0.429646435 00-0.429654665 00
0001300-0.429704735 00-0.429790385 00-0.429892965 00-0.429988445 00-0.430042455 00
0001400-0.430021415 00-0.429890515 00-0.429615445 00-0.429155415 00-0.429451545 00
0001500-0.427395055 00-0.425786675 00-0.423290735 00-0.419382515 00-0.413310355 00
0001600-0.404071515 00-0.390418355 00-0.370896645 00-0.343924225 00-0.307015875 00
0001700-0.261271185 00-0.213034635 00-0.172310835 00-0.137783545 00-0.108515625 00
0001800-0.835923555-01-0.622846155-01-0.439792165-01-0.298123965-01-0.144897855-01
0001900-0.258132515-02 0.780474395-02 0.168797925-01 0.248151875-01 0.317883905-01
0002000 0.378290435-01 0.431345485-01 0.476971685-01 0.513097305-01 0.539324135-01
0002100 0.548165705-01 0.539324135-01 0.513097305-01 0.476971685-01 0.431345485-01
EOF
q
```

AL NL a=10.0
DENS.

VEFF

AL NL a=15.0
DENS.

VEFF

```
redit pote2
LOADING POTE2
REVERED
EDIT
p20
        TOP RECORD
0000100 0.25876228E-01 0.25876200E-01 0.25876353E-01 0.25876640E-01 0.25877081E-01
0000200 0.25877643E-01 0.25878333E-01 0.25879122E-01 0.25879964E-01 0.25880855E-01
0000300 0.25881704E-01 0.25882572E-01 0.25883339E-01 0.25883901E-01 0.25884088E-01
0000400 0.25884822E-01 0.25884947E-01 0.25884874E-01 0.25884505E-01 0.25884120E-01
0000500 0.25883447E-01 0.25882628E-01 0.25881667E-01 0.25880634E-01 0.25879566E-01
0000600 0.25879545E-01 0.25877569E-01 0.25876738E-01 0.25876075E-01 0.25875643E-01
0000700 0.25875475E-01 0.25875591E-01 0.25876034E-01 0.25876731E-01 0.25877703E-01
0000800 0.25878928E-01 0.25880285E-01 0.25881771E-01 0.25883276E-01 0.25884748E-01
0000900 0.25886074E-01 0.25887221E-01 0.25888093E-01 0.25888504E-01 0.25888760E-01
0001000 0.25888536E-01 0.25887805E-01 0.25886860E-01 0.25885474E-01 0.25883805E-01
0001100 0.25881890E-01 0.25879834E-01 0.25877750E-01 0.25875709E-01 0.25874045E-01
0001200 0.25872603E-01 0.25871616E-01 0.25871105E-01 0.25871176E-01 0.25871962E-01
0001300 0.25873132E-01 0.25874961E-01 0.25877282E-01 0.25880005E-01 0.25882997E-01
0001400 0.25886111E-01 0.25890166E-01 0.25894715E-01 0.25899348E-01 0.25903156E-01
0001500 0.25907160E-01 0.25907283E-01 0.25906400E-01 0.25904470E-01 0.25901520E-01
0001600 0.25897553E-01 0.25892728E-01 0.25887210E-01 0.25881240E-01 0.25875037E-01
0001700 0.25868983E-01 0.25863340E-01 0.25858407E-01 0.25854730E-01 0.25852324E-01
0001800 0.25851519E-01 0.25852469E-01 0.25854155E-01 0.25856514E-01 0.25859336E-01
0001900 0.25862183E-01 0.25865333E-01 0.25868665E-01 0.25872632E-01 0.25876420E-01
0002000 0.25880815E-01 0.25885481E-01 0.25890115E-01 0.25893939E-01 0.25896786E-01
0002100 0.25898134E-01 0.25896447E-01 0.25892714E-01 0.25886070E-01 0.25879663E-01
0002200 0.25873697E-01 0.25868938E-01 0.25865793E-01 0.25864470E-01 0.25864867E-01
0002300 0.25866315E-01 0.25869471E-01 0.25873930E-01 0.25879411E-01 0.25885303E-01
0002400 0.25890918E-01 0.25895618E-01 0.25899644E-01 0.25902733E-01 0.25904632E-01
0002500 0.25905213E-01 0.25904632E-01 0.25902733E-01 0.25899644E-01 0.25895618E-01
EOF
e
redit pote3
LOADING POTE3
REVERED
EDIT
p20
        TOP RECORD
0000100-0.41869354E 00-0.41869885E 00-0.41870272E 00-0.41871351E 00-0.41871363E 00
0000200-0.41871768E 00-0.41872329E 00-0.41872489E 00-0.41872346E 00-0.41871893E 00
0000300-0.41871774E 00-0.41872150E 00-0.41871375E 00-0.41871041E 00-0.41871315E 00
0000400-0.41871411E 00-0.41871858E 00-0.41871029E 00-0.41870896E 00-0.41871750E 00
0000500-0.41871363E 00-0.41871640E 00-0.41871023E 00-0.41871375E 00-0.41872007E 00
0000600-0.41872185E 00-0.41872382E 00-0.41872637E 00-0.41872107E 00-0.41871089E 00
0000700-0.41870787E 00-0.41870600E 00-0.41870517E 00-0.41870522E 00-0.41870630E 00
0000800-0.41870748E 00-0.41870928E 00-0.41871172E 00-0.41871011E 00-0.41871303E 00
0000900-0.41871607E 00-0.41871876E 00-0.41872036E 00-0.41871721E 00-0.41872531E 00
0001000-0.41872513E 00-0.41872728E 00-0.41873258E 00-0.41873717E 00-0.41874224E 00
0001100-0.41874063E 00-0.41873437E 00-0.41873115E 00-0.41872907E 00-0.41872570E 00
0001200-0.41872263E 00-0.41871505E 00-0.41871625E 00-0.41871333E 00-0.41871107E 00
0001300-0.41870868E 00-0.41870707E 00-0.41870613E 00-0.41870546E 00-0.41870576E 00
0001400-0.41870683E 00-0.41870832E 00-0.41871047E 00-0.41871309E 00-0.41871613E 00
0001500-0.41871858E 00-0.41872138E 00-0.41872394E 00-0.41872448E 00-0.41872430E 00
0001600-0.41872275E 00-0.41871999E 00-0.41871327E 00-0.41870552E 00-0.41869420E 00
0001700-0.41869126E 00-0.41866577E 00-0.41864788E 00-0.41862768E 00-0.41860616E 00
0001800-0.41858351E 00-0.41855985E 00-0.41853571E 00-0.41851181E 00-0.41848719E 00
0001900-0.41846204E 00-0.41843462E 00-0.41840571E 00-0.41837156E 00-0.41833073E 00
0002000-0.41827697E 00-0.41820800E 00-0.41811705E 00-0.41800575E 00-0.41788513E 00
0002100-0.41776243E 00-0.41765107E 00-0.41760077E 00-0.41765636E 00-0.41800120E 00
0002200-0.41871432E 00-0.41947520E 00-0.41946115E 00-0.41924861E 00-0.41881405E 00
0002300-0.40913286E 00-0.40718204E 00-0.40493870E 00-0.40238285E 00-0.39949667E 00
0002400-0.39626622E 00-0.39268106E 00-0.38873394E 00-0.38468677E 00-0.38117215E 00
0002500-0.37716471E 00-0.37017215E 00-0.38468677E 00-0.38873394E 00-0.39268106E 00
EOF
```

AL LDA a=0.25
DENS.

VEFF

```
q
redit pote4
LOADING POTE4                AL+ LDA a=0.5
READY
EDIT                         DENS.
p99
        TOP RECORD
0000100 0.25877744E-01 0.25876749E-01 0.25877073E-01 0.25878742E-01 0.25881443E-01
0000200 0.25884651E-01 0.25887635E-01 0.25889301E-01 0.25890362E-01 0.25889311E-01
0000300 0.25886551E-01 0.25882579E-01 0.25878150E-01 0.25874112E-01 0.25871333E-01
0000400 0.25870539E-01 0.25872059E-01 0.25875777E-01 0.25881071E-01 0.25886934E-01
0000500 0.25892127E-01 0.25895443E-01 0.25895098E-01 0.25893249E-01 0.25887496E-01
0000600 0.25879595E-01 0.25871143E-01 0.25863856E-01 0.25859632E-01 0.25859758E-01
0000700 0.25864795E-01 0.25874231E-01 0.25886558E-01 0.25899306E-01 0.25909547E-01
0000800 0.25914416E-01 0.25911704E-01 0.25905018E-01 0.25891931E-01 0.25858432E-01
0000900 0.25834393E-01 0.25815040E-01 0.25805429E-01 0.25809072E-01 0.25826622E-01
0001000 0.25854450E-01 0.25883935E-01 0.25901102E-01 0.25887321E-01 0.25820410E-01
0001100 0.25478039E-01 0.25439040E-01 0.25092170E-01 0.24630722E-01 0.24054802E-01
0001200 0.23413060E-01 0.22734545E-01 0.22067016E-01 0.21489248E-01 0.21078039E-01
0001300 0.20932663E-01 0.21078039E-01 0.21489248E-01 0.22067016E-01 0.22734545E-01
EOF
q
redit pote5
LOADING POTE5                VEFF
READY
EDIT
p99
        TOP RECORD
0000100-0.41768013E 00-0.41868509E 00-0.41867316E 00-0.41867572E 00-0.41867234E 00
0000200-0.41868371E 00-0.41868591E 00-0.41868436E 00-0.41868371E 00-0.41868604E 00
0000300-0.41868277E 00-0.41868388E 00-0.41868241E 00-0.41868031E 00-0.41867888E 00
0000400-0.41868234E 00-0.41868350E 00-0.41868365E 00-0.41868103E 00-0.41867883E 00
0000500-0.41868102E 00-0.41868608E 00-0.41870564E 00-0.41871172E 00-0.41871732E 00
0000600-0.41871524E 00-0.41870880E 00-0.41868015E 00-0.41868806E 00-0.41867673E 00
0000700-0.41866741E 00-0.41868201E 00-0.41866491E 00-0.41867214E 00-0.41868587E 00
0000800-0.41870133E 00-0.41871670E 00-0.41872405E 00-0.41872060E 00-0.41868783E 00
0000900-0.41865340E 00-0.41869247E 00-0.41871604E 00-0.41872054E 00-0.41873687E 00
0001000-0.41874150E 00-0.41873242E 00-0.41873960E 00-0.41872777E 00-0.41872130E 00
0001100-0.41850179E 00-0.41852201E 00-0.41873257E 00-0.40302713E 00-0.40531517E 00
0001200-0.39888588E 00-0.39030266E 00-0.37021760E 00-0.36630338E 00-0.36659307E 00
0001300-0.36362290E 00-0.36659307E 00-0.36630338E 00-0.37021760E 00-0.39030266E 00
EOF
q
```

```
redit note6
LOADING NOTE6
RENEWED
EDIT
p20
       TOP RECORD
0000100 0.25974209E-01 0.25873190E-01 0.25872622E-01 0.25872558E-01 0.25872964E-01
0000200 0.25873011E-01 0.25875323E-01 0.25877200E-01 0.25879420E-01 0.25881909E-01
0000300 0.25884517E-01 0.25887121E-01 0.25889579E-01 0.25891747E-01 0.25893502E-01
0000400 0.25894731E-01 0.25895335E-01 0.25895290E-01 0.25894571E-01 0.25893159E-01
0000500 0.25891050E-01 0.25888477E-01 0.25885437E-01 0.25882084E-01 0.25878616E-01
0000600 0.25875200E-01 0.25872018E-01 0.25869217E-01 0.25867030E-01 0.25865532E-01
0000700 0.25864847E-01 0.25865003E-01 0.25866251E-01 0.25868308E-01 0.25871105E-01
0000800 0.25874795E-01 0.25878058E-01 0.25883455E-01 0.25888074E-01 0.25892582E-01
0000900 0.25896735E-01 0.25900278E-01 0.25902983E-01 0.25904652E-01 0.25905173E-01
0001000 0.25904421E-01 0.25902364E-01 0.25899064E-01 0.25894664E-01 0.25889281E-01
0001100 0.25883172E-01 0.25876641E-01 0.25870036E-01 0.25863696E-01 0.25857096E-01
0001200 0.25853273E-01 0.25849864E-01 0.25848016E-01 0.25847960E-01 0.25849778E-01
0001300 0.25853518E-01 0.25859058E-01 0.25866255E-01 0.25874801E-01 0.25884274E-01
0001400 0.25894236E-01 0.25904145E-01 0.25913432E-01 0.25921407E-01 0.25927804E-01
0001500 0.25931824E-01 0.25933117E-01 0.25931373E-01 0.25926426E-01 0.25918208E-01
0001600 0.25906906E-01 0.25892872E-01 0.25876567E-01 0.25858680E-01 0.25840078E-01
0001700 0.25821575E-01 0.25804486E-01 0.25789409E-01 0.25777768E-01 0.25770128E-01
0001800 0.25767300E-01 0.25769278E-01 0.25777716E-01 0.25790896E-01 0.25808703E-01
0001900 0.25830968E-01 0.25853366E-01 0.25876550E-01 0.25897067E-01 0.25911830E-01
0002000 0.25917381E-01 0.25909038E-01 0.25895441E-01 0.25839716E-01 0.25768578E-01
0002100 0.25668025E-01 0.25534377E-01 0.25364447E-01 0.25155693E-01 0.24906464E-01
0002200 0.24616074E-01 0.24285011E-01 0.23915004E-01 0.23509115E-01 0.23071785E-01
0002300 0.22603917E-01 0.22127725E-01 0.21636608E-01 0.21145571E-01 0.20665154E-01
0002400 0.20207111E-01 0.19784000E-01 0.19409020E-01 0.19096062E-01 0.18859450E-01
0002500 0.18712517E-01 0.18663049E-01 0.18712517E-01 0.18859450E-01 0.19096062E-01
EOF
e
redit note7
LOADING NOTE7
RENEWED
EDIT
p20
       TOP RECORD
0000100-0.41869438E 00-0.41869198E 00-0.41869849E 00-0.41869217E 00-0.41869074E 00
0000200-0.41868740E 00-0.41868287E 00-0.41868240E 00-0.41868144E 00-0.41868448E 00
0000300-0.41869134E 00-0.41868883E 00-0.41869622E 00-0.41869330E 00-0.41869533E 00
0000400-0.41870284E 00-0.41869038E 00-0.41869980E 00-0.41870350E 00-0.41869986E 00
0000500-0.41870451E 00-0.41870701E 00-0.41870165E 00-0.41870469E 00-0.41870308E 00
0000600-0.41870224E 00-0.41870010E 00-0.41870004E 00-0.41869205E 00-0.41869074E 00
0000700-0.41868860E 00-0.41868669E 00-0.41868562E 00-0.41868323E 00-0.41868109E 00
0000800-0.41868109E 00-0.41868275E 00-0.41868067E 00-0.41868466E 00-0.41868788E 00
0000900-0.41869205E 00-0.41869730E 00-0.41869043E 00-0.41870952E 00-0.41871750E 00
0001000-0.41871744E 00-0.41872329E 00-0.41873014E 00-0.41873562E 00-0.41873616E 00
0001100-0.41873276E 00-0.41872001E 00-0.41872448E 00-0.41871774E 00-0.41871023E 00
0001200-0.41870207E 00-0.41869366E 00-0.41868436E 00-0.41867590E 00-0.41866803E 00
0001300-0.41866082E 00-0.41865510E 00-0.41865134E 00-0.41864985E 00-0.41865128E 00
0001400-0.41865420E 00-0.41866046E 00-0.41866940E 00-0.41868031E 00-0.41869169E 00
0001500-0.41870409E 00-0.41871708E 00-0.41872978E 00-0.41873996E 00-0.41874641E 00
0001600-0.41874886E 00-0.41874677E 00-0.41873747E 00-0.41872108E 00-0.41869766E 00
0001700-0.41866601E 00-0.41862714E 00-0.41858059E 00-0.41852832E 00-0.41847044E 00
0001800-0.41840792E 00-0.41834277E 00-0.41827505E 00-0.41820782E 00-0.41813982E 00
0001900-0.41807026E 00-0.41799909E 00-0.41792178E 00-0.41783470E 00-0.41772220E 00
0002000-0.41759735E 00-0.41742486E 00-0.41719615E 00-0.41688985E 00-0.41648138E 00
0002100-0.41594172E 00-0.41523510E 00-0.41432261E 00-0.41315788E 00-0.41169119E 00
0002200-0.40986657E 00-0.40762413E 00-0.40489966E 00-0.40162629E 00-0.39773500E 00
0002300-0.39315766E 00-0.38782567E 00-0.38167387E 00-0.37464303E 00-0.36668283E 00
0002400-0.35775244E 00-0.34781319E 00-0.33624069E 00-0.32483912E 00-0.31306034E 00
0002500-0.30509912E 00-0.30507797E 00-0.30509912E 00-0.31306034E 00-0.32483912E 00
```

AL+ LDA a=0.75
DENS.

VEFF

```
redit note$
LOADING NOTE$
REKEYED
EDIT
p$$
        TOP RECORD
0000100 0.25873102E-01 0.25860946E-01 0.25863960E-01 0.25870867E-01 0.25875310E-01
0000200 0.25881480E-01 0.25880018E-01 0.25803521E-01 0.25806665E-01 0.25806542E-01
0000300 0.25892805E-01 0.25885099E-01 0.25877282E-01 0.25863345E-01 0.25861092E-01
0000400 0.25857220E-01 0.25857022E-01 0.25863398E-01 0.25872027E-01 0.25884740E-01
0000500 0.25896579E-01 0.25905702E-01 0.25910091E-01 0.25900315E-01 0.25890766E-01
0000600 0.25885291E-01 0.25868371E-01 0.25852943E-01 0.25840152E-01 0.25835808E-01
0000700 0.25841307E-01 0.25856458E-01 0.25870270E-01 0.25905684E-01 0.25930025E-01
0000800 0.25946293E-01 0.25949220E-01 0.25935654E-01 0.25905520E-01 0.25852563E-01
0000900 0.25814031E-01 0.25760737E-01 0.25740353E-01 0.25734870E-01 0.25757831E-01
0001000 0.25806561E-01 0.25868206E-01 0.25923602E-01 0.25923153E-01 0.25873389E-01
0001100 0.25886031E-01 0.25338847E-01 0.24708557E-01 0.24051744E-01 0.23106378E-01
0001200 0.21896400E-01 0.20783474E-01 0.19540191E-01 0.18390786E-01 0.17449067E-01
0001300 0.16018825E-01 0.16602777E-01 0.15013825E-01 0.17449067E-01 0.18390786E-01
EOF
e
redit note$
LOADING NOTE$
REKEYED
EDIT
p$$
        TOP RECORD
0000100-0.41869368E 00-0.41868812E 00-0.41867054E 00-0.41866267E 00-0.41865647E 00
0000200-0.41865987E 00-0.41865801E 00-0.41865671E 00-0.41866201E 00-0.41867113E 00
0000300-0.41866045E 00-0.41866457E 00-0.41867161E 00-0.41867203E 00-0.41865635E 00
0000400-0.41865474E 00-0.41864717E 00-0.41864443E 00-0.41864586E 00-0.41864520E 00
0000500-0.41865116E 00-0.41866014E 00-0.41867805E 00-0.41868371E 00-0.41870204E 00
0000600-0.41870120E 00-0.41868743E 00-0.41868764E 00-0.41867303E 00-0.41865772E 00
0000700-0.41864377E 00-0.41863555E 00-0.41863745E 00-0.41865015E 00-0.41867465E 00
0000800-0.41870469E 00-0.41873521E 00-0.41875547E 00-0.41875577E 00-0.41872525E 00
0000900-0.41865015E 00-0.41855752E 00-0.41842550E 00-0.41837637E 00-0.41812241E 00
0001000-0.41787200E 00-0.41781038E 00-0.41762608E 00-0.41731573E 00-0.41674787E 00
0001100-0.41570252E 00-0.41396301E 00-0.41082542E 00-0.40606457E 00-0.39005368E 00
0001200-0.38832111E 00-0.37409487E 00-0.35620252E 00-0.33374435E 00-0.30621321E 00
0001300-0.27857409E 00-0.27653024E 00-0.27857409E 00-0.30621321E 00-0.33374435E 00
EOF
e
-
```

AL LDA a=1.0
DENS.

VEFF

```
redit potel0
LOADING POTEL0
READY
EDIT
p99
        TOP RECORD
0000100 0.2587210?E-01 0.25?611145E-01 0.25853664E-01 0.25851458E-01 0.25?55165E-01
0000200 0.258640?6E-01 0.25?763?0E-01 0.25?09542E-01 0.25?005?7E-01 0.25?06?13E-01
0000300 0.25?066?0E-01 0.25?06?62E-01 0.25?06301E-01 0.25?06?64E-01 0.25?527?5E-01
0000400 0.25330522E-01 0.25?33?16E-01 0.25?25?72E-01 0.25?47?00E-01 0.25?67?2?E-01
0000500 0.25?01?21E-01 0.25?141?3E-01 0.25?315?7E-01 0.25?30?25E-01 0.25?33?2?3-01
0000600 0.25?15?05E-01 0.25?27594E-01 0.25?546?8E-01 0.25?235?4E-01 0.25?015?2E-01
0000700 0.25?047?7E-01 0.25?06?55E-01 0.25?37?49E-01 0.25?21?61E-01 0.25?31?24E-01
0000800 0.25?5?90?E-01 0.26?0431?E-01 0.26?07?41E-01 0.25?7?46?E-01 0.25?21?60E-01
0000900 0.25841?74E-01 0.25?551?7E-01 0.25?79450E-01 0.25?37?10E-01 0.25?32?00E-01
0001000 0.25?32?2?E-01 0.25?74?43E-01 0.25?3?64?E-01 0.25?56?22E-01 0.25?66?50E-01
0001100 0.25?15?62E-01 0.254?31?E-01 0.247???20E-01 0.22?16425E-01 0.225162?6E-01
0001200 0.2?0?1?42E-01 0.1?1?4?52E-01 0.171?1?4?E-01 0.152?5?53E-01 0.13?03??2E-01
0001300 0.1?01??12E-01 0.1?3?7?9?E-01 0.1?2?3?43E-01 0.1?041?42E-01 0.1?2?3?43E-01
EOF
a
redit potell
LOADING POTELL
READY
EDIT                    VEFF
p99
        TOP RECORD
0000100-0.41?69?73E 00-0.41?66?23E 00-0.41?62?22E 00-0.41?6?13?E 00-0.41?5??3?E 00
0000200-0.41?5??3?E 00-0.41?5?7?9E 00-0.41?5?1?E 00-0.41?5?7?3E 00-0.41?61?45E 00
0000300-0.41?63?6?E 00-0.41?63?7?E 00-0.41?653?1E 00-0.41?66?6?E 00-0.41?65575E 00
0000400-0.41?65??3E 00-0.41?6?1?E 00-0.41?63?4?E 00-0.41?63?00E 00-0.41?63??5E 00
0000500-0.41?62?5?E 00-0.41?635?E 00-0.41?655?E 00-0.41?6?7?E 00-0.41?71?2E 00
0000600-0.41?72?36E 00-0.41?73?4E 00-0.41?72?0E 00-0.41?6?3?E 00-0.41?64?2E 00
0000700-0.41?62?2E 00-0.41?5??5E 00-0.41?56?3E 00-0.41?55?5E 00-0.41?57?4E 00
0000800-0.41?62?3E 00-0.41?6?4E 00-0.41?75?5E 00-0.41?81?4E 00-0.41?63?3E 00
0000900-0.41?6?1?E 00-0.41?6?5E 00-0.41?53?3E 00-0.41?3?7E 00-0.41?45?E 00
0001000-0.41?76?1E 00-0.41?47?E 00-0.41?15?7E 00-0.41?4?6E 00-0.41?5??4E 00
0001100-0.41?5?5?E 00-0.41?3?5E 00-0.4??5?6E 00-0.41?3?7E 00-0.3?5?6?E 00
0001200-0.3?5?6?E 00-0.3?4?1?E 00-0.3?6?3E 00-0.3?7?11E 00-0.3?67?6E 00
0001300-0.3?4?5?E 00-0.1?7?7?E 00-0.17?5?E 00-0.17??5?E 00-0.17??5?E 00
EOF
a
```

```
q
redit potel2
LOADING POTEL2
READYED
EDIT
p99
        TOP RECORD
0000100 0.25875565E-01 0.25885787E-01 0.25895014E-01 0.25901347E-01 0.25903564E-01
0000200 0.25901217E-01 0.25894757E-01 0.25885522E-01 0.25875472E-01 0.25865015E-01
0000300 0.25861513E-01 0.25860376E-01 0.25865339E-01 0.25874145E-01 0.25885623E-01
0000400 0.25897406E-01 0.25906947E-01 0.25912002E-01 0.25911186E-01 0.25904242E-01
0000500 0.25892254E-01 0.25877409E-01 0.25862686E-01 0.25851235E-01 0.25845665E-01
0000600 0.25847632E-01 0.25857106E-01 0.25872536E-01 0.25890072E-01 0.25903675E-01
0000700 0.25921706E-01 0.25926888E-01 0.25922507E-01 0.25908791E-01 0.25897059E-01
0000800 0.25863042E-01 0.25841724E-01 0.25826283E-01 0.25821447E-01 0.25828203E-01
0000900 0.25848813E-01 0.25877044E-01 0.25908324E-01 0.25936193E-01 0.25953079E-01
0001000 0.25956515E-01 0.25942013E-01 0.25911838E-01 0.25871154E-01 0.25837059E-01
0001100 0.25791794E-01 0.25771726E-01 0.25774291E-01 0.25801743E-01 0.25851034E-01
0001200 0.25913700E-01 0.25976071E-01 0.26026115E-01 0.26047286E-01 0.26030665E-01
0001300 0.25974236E-01 0.25893591E-01 0.25773031E-01 0.25667217E-01 0.25588386E-01
0001400 0.25550723E-01 0.25504484E-01 0.25620544E-01 0.25225600E-01 0.25053414E-01
0001500 0.26014302E-01 0.25921606E-01 0.25911617E-01 0.24944447E-01 0.23825408E-01
0001600 0.22514883E-01 0.20739418E-01 0.18674660E-01 0.16438220E-01 0.14174201E-01
0001700 0.12032453E-01 0.10145102E-01 0.85033506E-02 0.74035712E-02 0.65713330E-02
0001800 0.60810670E-02 0.59188023E-02 0.60810670E-02 0.65713330E-02 0.74035712E-02
EOF
q
redit potel3
LOADING POTEL3
READYED
EDIT
p99
        TOP RECORD
0000100-0.41868839E 00-0.41871613E 00-0.41874318E 00-0.41875631E 00-0.41876202E 00
0000200-0.41877073E 00-0.41877747E 00-0.41877043E 00-0.41876680E 00-0.41876345E 00
0000300-0.41875297E 00-0.41874337E 00-0.41873533E 00-0.41872958E 00-0.41872132E 00
0000400-0.41872466E 00-0.41871923E 00-0.41871911E 00-0.41872085E 00-0.41872053E 00
0000500-0.41873628E 00-0.41873670E 00-0.41873652E 00-0.41872191E 00-0.41871333E 00
0000600-0.41870570E 00-0.41870632E 00-0.41870284E 00-0.41869724E 00-0.41870236E 00
0000700-0.41871661E 00-0.41872191E 00-0.41872770E 00-0.41873814E 00-0.41874051E 00
0000800-0.41872036E 00-0.41871780E 00-0.41870242E 00-0.41868359E 00-0.41866523E 00
0000900-0.41864854E 00-0.41864324E 00-0.41864530E 00-0.41867018E 00-0.41868085E 00
0001000-0.41871774E 00-0.41873640E 00-0.41874623E 00-0.41874260E 00-0.41872403E 00
0001100-0.41869366E 00-0.41865546E 00-0.41861662E 00-0.41859448E 00-0.41860156E 00
0001200-0.41861546E 00-0.41866511E 00-0.41873380E 00-0.41880635E 00-0.41884169E 00
0001300-0.41887432E 00-0.41883277E 00-0.41869301E 00-0.41848326E 00-0.41830880E 00
0001400-0.41788833E 00-0.41753770E 00-0.41730076E 00-0.41703063E 00-0.41671500E 00
0001500-0.41620785E 00-0.41523063E 00-0.41330082E 00-0.41005087E 00-0.40433003E 00
0001600-0.39539022E 00-0.38169826E 00-0.36200860E 00-0.33403145E 00-0.30878204E 00
0001700-0.25314724E 00-0.20761210E 00-0.17104685E 00-0.14204237E 00-0.12222837E 00
0001800-0.11041337E 00-0.10791240E 00-0.11041337E 00-0.12222837E 00-0.14204237E 00
EOF
q
```

```
redit pote20
LOADING POTE20   Al LDA  a=5.0
REKEYED
EDIT             DENS.
p99
        TOP RECORD
0000100 0.25878567E-01 0.25891971E-01 0.25903478E-01 0.25910731E-01 0.25912166E-01
0000200 0.25907520E-01 0.25897678E-01 0.25884707E-01 0.25871433E-01 0.25860835E-01
0000300 0.25855452E-01 0.25856815E-01 0.25864992E-01 0.25878664E-01 0.25895193E-01
0000400 0.25911152E-01 0.25923099E-01 0.25928214E-01 0.25924880E-01 0.25913287E-01
0000500 0.25895391E-01 0.25874574E-01 0.25855042E-01 0.25840964E-01 0.25835641E-01
0000600 0.25840644E-01 0.25855470E-01 0.25877442E-01 0.25902260E-01 0.25924619E-01
0000700 0.25939405E-01 0.25942892E-01 0.25933471E-01 0.25912181E-01 0.25882740E-01
0000800 0.25850952E-01 0.25823541E-01 0.25806744E-01 0.25805075E-01 0.25820006E-01
0000900 0.25849648E-01 0.25888614E-01 0.25929090E-01 0.25962200E-01 0.25979962E-01
0001000 0.25976960E-01 0.25951952E-01 0.25908362E-01 0.25854200E-01 0.25800545E-01
0001100 0.25759600E-01 0.25742032E-01 0.25754437E-01 0.25797341E-01 0.25864471E-01
0001200 0.25943138E-01 0.26016396E-01 0.26066095E-01 0.26076999E-01 0.26040543E-01
0001300 0.25957871E-01 0.25840968E-01 0.25711786E-01 0.25598478E-01 0.25529638E-01
0001400 0.25526948E-01 0.25597356E-01 0.25726542E-01 0.25874939E-01 0.25977582E-01
0001500 0.25949009E-01 0.25692906E-01 0.25116369E-01 0.24146646E-01 0.22747643E-01
0001600 0.20932768E-01 0.18769879E-01 0.16375907E-01 0.13900939E-01 0.11504337E-01
0001700 0.93275346E-02 0.74563511E-02 0.59138201E-02 0.46842471E-02 0.37332345E-02
0001800 0.30210461E-02 0.25098461E-02 0.21680235E-02 0.19723144E-02 0.19087025E-02
EOF
q
redit pote21
LOADING POTE21
REKEYED          VEFF
EDIT
p99
        TOP RECORD
0000100-0.41867054E 00-0.41869301E 00-0.41871971E 00-0.41874379E 00-0.41875559E 00
0000200-0.41877371E 00-0.41879010E 00-0.41879350E 00-0.41880178E 00-0.41880196E 00
0000300-0.41879529E 00-0.41879785E 00-0.41878849E 00-0.41878080E 00-0.41877824E 00
0000400-0.41876692E 00-0.41877240E 00-0.41877675E 00-0.41877389E 00-0.41877615E 00
0000500-0.41877270E 00-0.41877103E 00-0.41876376E 00-0.41875339E 00-0.41873872E 00
0000600-0.41872388E 00-0.41871256E 00-0.41869527E 00-0.41869229E 00-0.41869617E 00
0000700-0.41869813E 00-0.41870254E 00-0.41871762E 00-0.41871929E 00-0.41871846E 00
0000800-0.41870916E 00-0.41869426E 00-0.41867739E 00-0.41865993E 00-0.41863084E 00
0000900-0.41862375E 00-0.41862094E 00-0.41863054E 00-0.41865087E 00-0.41867626E 00
0001000-0.41870552E 00-0.41872710E 00-0.41873372E 00-0.41872501E 00-0.41869879E 00
0001100-0.41865808E 00-0.41861033E 00-0.41856742E 00-0.41853946E 00-0.41853786E 00
0001200-0.41856670E 00-0.41862506E 00-0.41870266E 00-0.41878229E 00-0.41883898E 00
0001300-0.41884917E 00-0.41878796E 00-0.41864502E 00-0.41842073E 00-0.41813451E 00
0001400-0.41781300E 00-0.41748023E 00-0.41713691E 00-0.41673368E 00-0.41614175E 00
0001500-0.41512138E 00-0.41328216E 00-0.41004717E 00-0.40461254E 00-0.39592963E 00
0001600-0.38270652E 00-0.36344761E 00-0.33653313E 00-0.30033135E 00-0.25333160E 00
0001700-0.20457238E 00-0.16332537E 00-0.12858003E 00-0.99493146E-01-0.74951053E-01
0001800-0.55222806E-01-0.39980281E-01-0.29052254E-01-0.22143506E-01-0.20363085E-01
EOF
q
```

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.25862034E-01 0.25877625E-01 0.25895026E-01 0.25910705E-01 0.25921781E-01
0000200 0.25925737E-01 0.25921717E-01 0.25913415E-01 0.25904031E-01 0.25895870E-01
0000300 0.25859709E-01 0.25849242E-01 0.25846600E-01 0.25853967E-01 0.25867056E-01
0000400 0.25886193E-01 0.25906418E-01 0.25923386E-01 0.25933117E-01 0.25932042E-01
0000500 0.25922511E-01 0.25903113E-01 0.25879407E-01 0.25853235E-01 0.25832947E-01
0000600 0.25821995E-01 0.25823250E-01 0.25837030E-01 0.25861073E-01 0.25890768E-01
0000700 0.25920011E-01 0.25942396E-01 0.25952660E-01 0.25947813E-01 0.25927901E-01
0000800 0.25896214E-01 0.25858853E-01 0.25823552E-01 0.25798195E-01 0.25788851E-01
0000900 0.25798898E-01 0.25827533E-01 0.25869039E-01 0.25917802E-01 0.25961027E-01
0001000 0.25990655E-01 0.25996130E-01 0.25977161E-01 0.25934719E-01 0.25876179E-01
0001100 0.25813102E-01 0.25759518E-01 0.25728218E-01 0.25728591E-01 0.25763821E-01
0001200 0.25829494E-01 0.25913708E-01 0.25998872E-01 0.26064910E-01 0.26093531E-01
0001300 0.26072534E-01 0.25999710E-01 0.25884386E-01 0.25747363E-01 0.25617484E-01
0001400 0.25525972E-01 0.25498662E-01 0.25547713E-01 0.25664076E-01 0.25812674E-01
0001500 0.25931239E-01 0.25934566E-01 0.25723856E-01 0.25201082E-01 0.24286300E-01
0001600 0.22935200E-01 0.21153133E-01 0.19001581E-01 0.16593955E-01 0.14080256E-01
0001700 0.11623148E-01 0.93694590E-02 0.74105039E-02 0.57732537E-02 0.44440255E-02
0001800 0.33883739E-02 0.25640933E-02 0.19289709E-02 0.14447235E-02 0.10786231E-02
0001900 0.80376887E-03 0.59864367E-03 0.44639152E-03 0.33401581E-03 0.25163288E-03
0002000 0.19182169E-03 0.14098613E-03 0.11943899E-03 0.10007943E-03 0.89160647E-04
0002100 0.85634427E-04 0.89160647E-04 0.10007943E-03 0.11943899E-03 0.14098613E-03
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.41869259E 00-0.41872185E 00-0.41874236E 00-0.41875809E 00-0.41876966E 00
0000200-0.41877252E 00-0.41877550E 00-0.41877538E 00-0.41876239E 00-0.41875893E 00
0000300-0.41874415E 00-0.41872680E 00-0.41871715E 00-0.41870296E 00-0.41868889E 00
0000400-0.41868198E 00-0.41866899E 00-0.41867125E 00-0.41867697E 00-0.41867208E 00
0000500-0.41868091E 00-0.41867644E 00-0.41867965E 00-0.41866958E 00-0.41865712E 00
0000600-0.41864347E 00-0.41863179E 00-0.41862428E 00-0.41861212E 00-0.41861629E 00
0000700-0.41863099E 00-0.41863739E 00-0.41864640E 00-0.41866732E 00-0.41867369E 00
0000800-0.41867548E 00-0.41866994E 00-0.41865997E 00-0.41864049E 00-0.41862226E 00
0000900-0.41859698E 00-0.41858995E 00-0.41858751E 00-0.41861147E 00-0.41863471E 00
0001000-0.41866446E 00-0.41869718E 00-0.41872263E 00-0.41873413E 00-0.41872853E 00
0001100-0.41870302E 00-0.41866207E 00-0.41861266E 00-0.41856682E 00-0.41853565E 00
0001200-0.41852960E 00-0.41855341E 00-0.41860574E 00-0.41867691E 00-0.41874921E 00
0001300-0.41879952E 00-0.41880476E 00-0.41874170E 00-0.41860199E 00-0.41838479E 00
0001400-0.41811031E 00-0.41780430E 00-0.41748989E 00-0.41716641E 00-0.41678405E 00
0001500-0.41621524E 00-0.41522485E 00-0.41343433E 00-0.41028393E 00-0.40499526E 00
0001600-0.39654869E 00-0.38960034E 00-0.36490947E 00-0.33860337E 00-0.30306745E 00
0001700-0.25663787E 00-0.20827389E 00-0.16718894E 00-0.13223368E 00-0.10238498E 00
0001800-0.76764166E-01-0.54640070E-01-0.35408981E-01-0.18585101E-01-0.37790874E-02
0001900 0.93220323E-02 0.20058349E-01 0.31316735E-01 0.40532134E-01 0.48725620E-01
0002000 0.55831578E-01 0.61935879E-01 0.66927254E-01 0.70673823E-01 0.73032200E-01
0002100 0.73812902E-01 0.73032200E-01 0.70673823E-01 0.66927254E-01 0.61935879E-01
EOF
q
```

At LDA a=10.0 DENS.

VEFF

C-3

```
redit pote4
LOADING POTE4
REVIVED
EDIT
p99
        TOP RECORD
0000100 0.25860474E-01 0.25876694E-01 0.25894616E-01 0.25911022E-01 0.25922619E-01
0000200 0.25927044E-01 0.25923319E-01 0.25912143E-01 0.25895692E-01 0.25877371E-01
0000300 0.25861062E-01 0.25850315E-01 0.25847659E-01 0.25853928E-01 0.25868151E-01
0000400 0.25887513E-01 0.25903053E-01 0.25925312E-01 0.25935307E-01 0.25935356E-01
0000500 0.25924354E-01 0.25905322E-01 0.25880359E-01 0.25854886E-01 0.25834244E-01
0000600 0.25823072E-01 0.25824215E-01 0.25838006E-01 0.25862202E-01 0.25892168E-01
0000700 0.25921702E-01 0.25944524E-01 0.25955014E-01 0.25950234E-01 0.25930088E-01
0000800 0.25897954E-01 0.25859941E-01 0.25823876E-01 0.25797714E-01 0.25787812E-01
0000900 0.25797486E-01 0.25826048E-01 0.25868658E-01 0.25917005E-01 0.25960825E-01
0001000 0.25999117E-01 0.25997147E-01 0.25978446E-01 0.25935993E-01 0.25877137E-01
0001100 0.25813565E-01 0.25759153E-01 0.25727104E-01 0.25726918E-01 0.25761873E-01
0001200 0.25827698E-01 0.25912505E-01 0.25998604E-01 0.26065793E-01 0.26095562E-01
0001300 0.26075535E-01 0.26003134E-01 0.25887650E-01 0.25749773E-01 0.25618453E-01
0001400 0.25525063E-01 0.25495756E-01 0.25543012E-01 0.25658149E-01 0.25806352E-01
0001500 0.25925517E-01 0.25930531E-01 0.25722336E-01 0.25202632E-01 0.24291020E-01
0001600 0.22942910E-01 0.21163054E-01 0.19013129E-01 0.16606476E-01 0.14093224E-01
0001700 0.11636037E-01 0.93815662E-02 0.74209347E-02 0.57813413E-02 0.44494048E-02
0001800 0.33909348E-02 0.25639222E-02 0.19262589E-02 0.14397064E-02 0.10715292E-02
0001900 0.79477788E-03 0.58786455E-03 0.43383776E-03 0.31958529E-03 0.23508118E-03
0002000 0.17272751E-03 0.12680753E-03 0.93044160E-04 0.68212470E-04 0.50069459E-04
0002100 0.36747748E-04 0.26998736E-04 0.19875370E-04 0.14683238E-04 0.10914515E-04
0002200 0.81994576E-05 0.62709914E-05 0.49390019E-05 0.40722380E-05 0.35844960E-05
0002300 0.34271434E-05 0.35844960E-05 0.40722380E-05 0.49390019E-05 0.62709914E-05
EOF
q
redit pote5
LOADING POTE5
REVIVED
EDIT
p99
        TOP RECORD
0000100-0.41860313E 00-0.41872925E 00-0.41875833E 00-0.41877705E 00-0.41879106E 00
0000200-0.41879779E 00-0.41880715E 00-0.41880780E 00-0.41879779E 00-0.41879541E 00
0000300-0.41878289E 00-0.41876668E 00-0.41875625E 00-0.41874403E 00-0.41873151E 00
0000400-0.41872722E 00-0.41871589E 00-0.41871506E 00-0.41872358E 00-0.41871959E 00
0000500-0.41872662E 00-0.41872382E 00-0.41872746E 00-0.41871011E 00-0.41869712E 00
0000600-0.41868297E 00-0.41867197E 00-0.41865973E 00-0.41864300E 00-0.41864264E 00
0000700-0.41865414E 00-0.41866273E 00-0.41867310E 00-0.41869575E 00-0.41870385E 00
0000800-0.41870451E 00-0.41870010E 00-0.41868824E 00-0.41866755E 00-0.41864717E 00
0000900-0.41862094E 00-0.41861296E 00-0.41861105E 00-0.41863292E 00-0.41865426E 00
0001000-0.41868860E 00-0.41872030E 00-0.41874433E 00-0.41875392E 00-0.41874576E 00
0001100-0.41871715E 00-0.41867191E 00-0.41861808E 00-0.41856885E 00-0.41853565E 00
0001200-0.41852957E 00-0.41855448E 00-0.41861051E 00-0.41868609E 00-0.41876340E 00
0001300-0.41881776E 00-0.41882497E 00-0.41876018E 00-0.41861337E 00-0.41838539E 00
0001400-0.41800654E 00-0.41777533E 00-0.41744769E 00-0.41711575E 00-0.41673267E 00
0001500-0.41617197E 00-0.41519904E 00-0.41343266E 00-0.41030884E 00-0.40504187E 00
0001600-0.39660418E 00-0.38372397E 00-0.36492056E 00-0.33857554E 00-0.30303794E 00
0001700-0.25674397E 00-0.20858669E 00-0.16752704E 00-0.13274485E 00-0.10293442E 00
0001800-0.77328563E-01-0.55198904E-01-0.35942886E-01-0.19071989E-01-0.41902363E-02
0001900 0.90209922E-02 0.20818211E-01 0.31407561E-01 0.40954869E-01 0.49599446E-01
0002000 0.57432212E-01 0.64555764E-01 0.71035087E-01 0.76924086E-01 0.82267463E-01
0002100 0.87100089E-01 0.91576159E-01 0.95754325E-01 0.99611700E-01 0.10311425E 00
0002200 0.10620821E 00 0.10913974E 00 0.11205482E 00 0.11374694E 00 0.11480522E 00
0002300 0.11519516E 00 0.11480522E 00 0.11374694E 00 0.11205482E 00 0.10913974E 00
EOF
q
```

VEFF

AL+ LDA a=15.0
DENS.

redit note6
LOADING NOTE6
READY
EDIT
p99

Alt NL a=0.25
DENS.

TOP RECORD
0000100 0.25876491E-01 0.25876269E-01 0.25876187E-01 0.25876287E-01 0.25876522E-01
0000200 0.25876058E-01 0.25877550E-01 0.25878269E-01 0.25879107E-01 0.25880042E-01
0000300 0.25881048E-01 0.25882032E-01 0.25883019E-01 0.25883928E-01 0.25884703E-01
0000400 0.25885347E-01 0.25885794E-01 0.25886040E-01 0.25886059E-01 0.25885855E-01
0000500 0.25885433E-01 0.25884829E-01 0.25884070E-01 0.25883172E-01 0.25882240E-01
0000600 0.25881272E-01 0.25880337E-01 0.25879434E-01 0.25878768E-01 0.25878198E-01
0000700 0.25877852E-01 0.25877737E-01 0.25877852E-01 0.25878195E-01 0.25878791E-01
0000800 0.25879513E-01 0.25880430E-01 0.25881420E-01 0.25882460E-01 0.25883447E-01
0000900 0.25884380E-01 0.25885139E-01 0.25885656E-01 0.25885925E-01 0.25885876E-01
0001000 0.25885515E-01 0.25884803E-01 0.25883783E-01 0.25882479E-01 0.25880910E-01
0001100 0.25879163E-01 0.25877327E-01 0.25875490E-01 0.25873747E-01 0.25872204E-01
0001200 0.25870953E-01 0.25870092E-01 0.25869664E-01 0.25869727E-01 0.25870323E-01
0001300 0.25871441E-01 0.25873076E-01 0.25875144E-01 0.25877561E-01 0.25880236E-01
0001400 0.25883015E-01 0.25885787E-01 0.25888372E-01 0.25890626E-01 0.25892373E-01
0001500 0.25893524E-01 0.25893923E-01 0.25893535E-01 0.25892273E-01 0.25890175E-01
0001600 0.25887273E-01 0.25883649E-01 0.25879484E-01 0.25874946E-01 0.25870264E-01
0001700 0.25865709E-01 0.25861520E-01 0.25857974E-01 0.25855318E-01 0.25853787E-01
0001800 0.25853489E-01 0.25854528E-01 0.25856897E-01 0.25860462E-01 0.25864951E-01
0001900 0.25869999E-01 0.25875028E-01 0.25879364E-01 0.25882158E-01 0.25882419E-01
0002000 0.25879063E-01 0.25870841E-01 0.25856405E-01 0.25834657E-01 0.25804047E-01
0002100 0.25763385E-01 0.25711466E-01 0.25647301E-01 0.25570057E-01 0.25479190E-01
0002200 0.25374409E-01 0.25256105E-01 0.25124639E-01 0.24981050E-01 0.24826963E-01
0002300 0.24664417E-01 0.24496000E-01 0.24324860E-01 0.24154671E-01 0.23989622E-01
0002400 0.23834392E-01 0.23694173E-01 0.23574494E-01 0.23481302E-01 0.23420755E-01
0002500 0.23390990E-01 0.23420755E-01 0.23481302E-01 0.23574494E-01 0.23694173E-01
EOF
q
redit note7
LOADING NOTE7
READY
EDIT
p99

VEFF

TOP RECORD
0000100-0.41869324E 00-0.41867912E 00-0.41867948E 00-0.41868442E 00-0.41867900E 00
0000200-0.41868532E 00-0.41868460E 00-0.41868842E 00-0.41868389E 00-0.41868925E 00
0000300-0.41868716E 00-0.41869682E 00-0.41869527E 00-0.41870689E 00-0.41870707E 00
0000400-0.41870904E 00-0.41872233E 00-0.41872346E 00-0.41872603E 00-0.41873515E 00
0000500-0.41873246E 00-0.41873127E 00-0.41873026E 00-0.41872752E 00-0.41873652E 00
0000600-0.41873521E 00-0.41873348E 00-0.41873169E 00-0.41872889E 00-0.41872525E 00
0000700-0.41872251E 00-0.41871917E 00-0.41871501E 00-0.41871309E 00-0.41870993E 00
0000800-0.41870725E 00-0.41870403E 00-0.41870070E 00-0.41868758E 00-0.41868877E 00
0000900-0.41869074E 00-0.41869253E 00-0.41869384E 00-0.41869466E 00-0.41868633E 00
0001000-0.41869199E 00-0.41868830E 00-0.41869456E 00-0.41870081E 00-0.41869771E 00
0001100-0.41869749E 00-0.41869658E 00-0.41869581E 00-0.41869649E 00-0.41869569E 00
0001200-0.41869497E 00-0.41869396E 00-0.41869307E 00-0.41869158E 00-0.41868949E 00
0001300-0.41868758E 00-0.41868460E 00-0.41868228E 00-0.41867959E 00-0.41867715E 00
0001400-0.41867501E 00-0.41867369E 00-0.41867292E 00-0.41867286E 00-0.41867375E 00
0001500-0.41867560E 00-0.41867864E 00-0.41868258E 00-0.41868746E 00-0.41869354E 00
0001600-0.41869986E 00-0.41870463E 00-0.41871083E 00-0.41871619E 00-0.41871959E 00
0001700-0.41872209E 00-0.41872305E 00-0.41872108E 00-0.41871661E 00-0.41870910E 00
0001800-0.41869849E 00-0.41868418E 00-0.41866547E 00-0.41864240E 00-0.41861397E 00
0001900-0.41857904E 00-0.41853803E 00-0.41848773E 00-0.41842616E 00-0.41835219E 00
0002000-0.41826135E 00-0.41814953E 00-0.41801125E 00-0.41784000E 00-0.41762732E 00
0002100-0.41736478E 00-0.41704047E 00-0.41664225E 00-0.41615564E 00-0.41556489E 00
0002200-0.41485262E 00-0.41400057E 00-0.41298777E 00-0.41179419E 00-0.41039783E 00
0002300-0.40877724E 00-0.40691102E 00-0.40477884E 00-0.40236151E 00-0.39964163E 00
0002400-0.39660531E 00-0.39324319E 00-0.38954163E 00-0.38577044E 00-0.38053781E 00
0002500-0.37964255E 00-0.38053781E 00-0.38577044E 00-0.38954163E 00-0.39324319E 00
EOF

```
EDIT NOTES
LOADING NOTES   ALT NL a=0.5
REVISED
EDIT            DENS.
200
        TOP RECORD
0000100 0.25876172E-01 0.25875434E-01 0.25875822E-01 0.25877371E-01 0.25879860E-01
0000200 0.25892307E-01 0.25885612E-01 0.25887600E-01 0.25888585E-01 0.25888011E-01
0000300 0.25886029E-01 0.25883948E-01 0.25879476E-01 0.25876228E-01 0.25874019E-01
0000400 0.25873449E-01 0.25874796E-01 0.25877012E-01 0.25882315E-01 0.25887124E-01
0000500 0.25891369E-01 0.25893042E-01 0.25894146E-01 0.25891569E-01 0.25886461E-01
0000600 0.25879603E-01 0.25872320E-01 0.25866121E-01 0.25862530E-01 0.25862671E-01
0000700 0.25866870E-01 0.25875003E-01 0.25885403E-01 0.25896370E-01 0.25905203E-01
0000800 0.25909403E-01 0.25907785E-01 0.25899164E-01 0.25884463E-01 0.25866035E-01
0000900 0.25847465E-01 0.25832940E-01 0.25826422E-01 0.25830343E-01 0.25844473E-01
0001000 0.25864906E-01 0.25862788E-01 0.25855276E-01 0.25855068E-01 0.25772303E-01
0001100 0.25616910E-01 0.25370955E-01 0.25022916E-01 0.24570212E-01 0.24022356E-01
0001200 0.23403004E-01 0.22750698E-01 0.22119274E-01 0.21570984E-01 0.21123351E-01
0001300 0.21045275E-01 0.21123517E-01 0.21570984E-01 0.22119274E-01 0.22750698E-01
EOF
0
EDIT NOTES
LOADING NOTES
REVISED         VEFF
EDIT
200
        TOP RECORD
0000100-0.41868115E 00-0.41869505E 00-0.41868963E 00-0.41868593E 00-0.41869740E 00
0000200-0.41868502E 00-0.41868776E 00-0.41868258E 00-0.41868705E 00-0.41868545E 00
0000300-0.41868891E 00-0.41870117E 00-0.41871715E 00-0.41872346E 00-0.41872174E 00
0000400-0.41872297E 00-0.41871933E 00-0.41871739E 00-0.41871993E 00-0.41869697E 00
0000500-0.41869467E 00-0.41869539E 00-0.41869396E 00-0.41869628E 00-0.41870034E 00
0000600-0.41870672E 00-0.41871315E 00-0.41871607E 00-0.41871554E 00-0.41871305E 00
0000700-0.41868896E 00-0.41868663E 00-0.41867322E 00-0.41866261E 00-0.41865820E 00
0000800-0.41866150E 00-0.41867303E 00-0.41868378E 00-0.41871685E 00-0.41872711E 00
0000900-0.41874097E 00-0.41874641E 00-0.41872221E 00-0.41866945E 00-0.41858019E 00
0001000-0.41844933E 00-0.41835622E 00-0.41707215E 00-0.41754501E 00-0.41689372E 00
0001100-0.41590373E 00-0.41477572E 00-0.41211065E 00-0.40885235E 00-0.40429366E 00
0001200-0.39999096E 00-0.39063096E 00-0.37950351E 00-0.36757356E 00-0.34999567E 00
0001300-0.34551936E 00-0.34598567E 00-0.36757356E 00-0.37950361E 00-0.39099096E 00
EOF
0
```

```
redit potel0
LOADING POTEL0                AL+ NL a=0.75
REKEYED
EDIT                          DENS
p99
        TOP RECORD
0000100 0.25875504E-01 0.25874577E-01 0.25873955E-01 0.25873698E-01 0.25873926E-01
0000200 0.25874563E-01 0.25875635E-01 0.25877073E-01 0.25878835E-01 0.25880791E-01
0000300 0.25882889E-01 0.25884964E-01 0.25886953E-01 0.25888707E-01 0.25890104E-01
0000400 0.25891111E-01 0.25891624E-01 0.25891580E-01 0.25890961E-01 0.25889792E-01
0000500 0.25888089E-01 0.25885925E-01 0.25883414E-01 0.25880657E-01 0.25877702E-01
0000600 0.25874957E-01 0.25872331E-01 0.25870018E-01 0.25868177E-01 0.25866915E-01
0000700 0.25866367E-01 0.25866557E-01 0.25867525E-01 0.25869228E-01 0.25871631E-01
0000800 0.25874589E-01 0.25878042E-01 0.25881756E-01 0.25885586E-01 0.25889326E-01
0000900 0.25892731E-01 0.25895610E-01 0.25897812E-01 0.25899164E-01 0.25899503E-01
0001000 0.25898822E-01 0.25897086E-01 0.25894892E-01 0.25890570E-01 0.25886070E-01
0001100 0.25880081E-01 0.25875553E-01 0.25870085E-01 0.25864862E-01 0.25860170E-01
0001200 0.25856365E-01 0.25853626E-01 0.25852248E-01 0.25852323E-01 0.25854018E-01
0001300 0.25857250E-01 0.25862053E-01 0.25868181E-01 0.25875427E-01 0.25883455E-01
0001400 0.25891803E-01 0.25900260E-01 0.25908109E-01 0.25914963E-01 0.25920358E-01
0001500 0.25923882E-01 0.25925193E-01 0.25924034E-01 0.25920268E-01 0.25913913E-01
0001600 0.25905091E-01 0.25894105E-01 0.25881406E-01 0.25867570E-01 0.25853243E-01
0001700 0.25839228E-01 0.25826342E-01 0.25815390E-01 0.25807113E-01 0.25802210E-01
0001800 0.25801141E-01 0.25804192E-01 0.25811322E-01 0.25822241E-01 0.25836151E-01
0001900 0.25851976E-01 0.25868140E-01 0.25882643E-01 0.25893029E-01 0.25896479E-01
0002000 0.25889829E-01 0.25869608E-01 0.25832154E-01 0.25773760E-01 0.25690679E-01
0002100 0.25579434E-01 0.25436811E-01 0.25260091E-01 0.25047209E-01 0.24796858E-01
0002200 0.24509650E-01 0.24183314E-01 0.23822628E-01 0.23429640E-01 0.23008671E-01
0002300 0.22565275E-01 0.22106212E-01 0.21639466E-01 0.21174084E-01 0.20720090E-01
0002400 0.20288300E-01 0.19890402E-01 0.19538652E-01 0.19245952E-01 0.19025590E-01
0002500 0.18888783E-01 0.18842760E-01 0.18888783E-01 0.19025590E-01 0.19245952E-01
EOF
q
redit potell
LOADING POTEL1
REKEYED
EDIT                          VEFF
p99
        TOP RECORD
0000100-0.41869336E 00-0.41869523E 00-0.41869885E 00-0.41869003E 00-0.41869283E 00
0000200-0.41868290E 00-0.41868353E 00-0.41867495E 00-0.41867721E 00-0.41868893E 00
0000300-0.41867209E 00-0.41866386E 00-0.41866708E 00-0.41866076E 00-0.41865519E 00
0000400-0.41865987E 00-0.41865718E 00-0.41865557E 00-0.41866642E 00-0.41866553E 00
0000500-0.41866559E 00-0.41866535E 00-0.41866887E 00-0.41868347E 00-0.41868782E 00
0000600-0.41869229E 00-0.41869730E 00-0.41869760E 00-0.41869742E 00-0.41869831E 00
0000700-0.41869986E 00-0.41870052E 00-0.41869634E 00-0.41869223E 00-0.41868913E 00
0000800-0.41868645E 00-0.41868454E 00-0.41867220E 00-0.41867107E 00-0.41866881E 00
0000900-0.41866590E 00-0.41866440E 00-0.41865838E 00-0.41866297E 00-0.41866606E 00
0001000-0.41866481E 00-0.41867363E 00-0.41868722E 00-0.41868627E 00-0.41869158E 00
0001100-0.41869682E 00-0.41870248E 00-0.41870928E 00-0.41871327E 00-0.41871691E 00
0001200-0.41871947E 00-0.41872013E 00-0.41871870E 00-0.41871560E 00-0.41871083E 00
0001300-0.41870373E 00-0.41869551E 00-0.41868573E 00-0.41867620E 00-0.41866636E 00
0001400-0.41865671E 00-0.41864926E 00-0.41864413E 00-0.41864091E 00-0.41864073E 00
0001500-0.41864365E 00-0.41865003E 00-0.41865951E 00-0.41867298E 00-0.41868877E 00
0001600-0.41870546E 00-0.41872418E 00-0.41874230E 00-0.41875893E 00-0.41877371E 00
0001700-0.41878504E 00-0.41879082E 00-0.41879040E 00-0.41878271E 00-0.41876662E 00
0001800-0.41874021E 00-0.41870296E 00-0.41865498E 00-0.41859251E 00-0.41851628E 00
0001900-0.41842246E 00-0.41830993E 00-0.41817325E 00-0.41800958E 00-0.41780919E 00
0002000-0.41756552E 00-0.41726661E 00-0.41689670E 00-0.41643751E 00-0.41586846E 00
0002100-0.41516215E 00-0.41428757E 00-0.41321093E 00-0.41189098E 00-0.41028321E 00
0002200-0.40833855E 00-0.40600586E 00-0.40322840E 00-0.39994830E 00-0.39610666E 00
0002300-0.39164370E 00-0.38650233E 00-0.38062692E 00-0.37396455E 00-0.36647111E 00
0002400-0.35810649E 00-0.34883761E 00-0.33864939E 00-0.32751209E 00-0.31784302E 00
0002500-0.31136686E 00-0.31053269E 00-0.31136686E 00-0.31784302E 00-0.32751209E 00
EOF
```

```
:.vi
$edit potel2
LOADING POTE12
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.25873449E-01 0.25870800E-01 0.25870308E-01 0.25872171E-01 0.25876146E-01
0000200 0.25881581E-01 0.25887378E-01 0.25892328E-01 0.25895320E-01 0.25895540E-01
0000300 0.25892768E-01 0.25887381E-01 0.25880378E-01 0.25873117E-01 0.25867205E-01
0000400 0.25864091E-01 0.25864661E-01 0.25869101E-01 0.25876973E-01 0.25886681E-01
0000500 0.25896337E-01 0.25903746E-01 0.25907069E-01 0.25905029E-01 0.25897425E-01
0000600 0.25885329E-01 0.25870871E-01 0.25856927E-01 0.25846642E-01 0.25842745E-01
0000700 0.25846891E-01 0.25859106E-01 0.25877897E-01 0.25899645E-01 0.25919836E-01
0000800 0.25933530E-01 0.25936540E-01 0.25926378E-01 0.25903199E-01 0.25870156E-01
0000900 0.25833294E-01 0.25800601E-01 0.25780417E-01 0.25779299E-01 0.25799681E-01
0001000 0.25837507E-01 0.25880609E-01 0.25907848E-01 0.25889866E-01 0.25791202E-01
0001100 0.25574122E-01 0.25203772E-01 0.24654336E-01 0.23915093E-01 0.22995539E-01
0001200 0.21928683E-01 0.20771459E-01 0.19602239E-01 0.18516365E-01 0.17620601E-01
0001300 0.17025873E-01 0.16822603E-01 0.17025873E-01 0.17620601E-01 0.18516365E-01
EOF
$
redit potel3
LOADING POTE13
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.41869366E 00-0.41870329E 00-0.41870105E 00-0.41869589E 00-0.41868615E 00
0000200-0.41867810E 00-0.41866964E 00-0.41865839E 00-0.41865063E 00-0.41866755E 00
0000300-0.41866088E 00-0.41867858E 00-0.41869861E 00-0.41870815E 00-0.41871005E 00
0000400-0.41872540E 00-0.41872101E 00-0.41871417E 00-0.41870153E 00-0.41867912E 00
0000500-0.41866750E 00-0.41865093E 00-0.41865832E 00-0.41866010E 00-0.41866904E 00
0000600-0.41868508E 00-0.41870326E 00-0.41871715E 00-0.41872424E 00-0.41872042E 00
0000700-0.41870546E 00-0.41868043E 00-0.41865033E 00-0.41862106E 00-0.41860020E 00
0000800-0.41859347E 00-0.41860521E 00-0.41863570E 00-0.41867988E 00-0.41872042E 00
0000900-0.41877401E 00-0.41879922E 00-0.41879278E 00-0.41874633E 00-0.41863132E 00
0001000-0.41844852E 00-0.41817254E 00-0.41776070E 00-0.41714079E 00-0.41618896E 00
0001100-0.41471517E 00-0.41244591E 00-0.40991291E 00-0.40306112E 00-0.39675510E 00
0001200-0.38681215E 00-0.37354445E 00-0.35641277E 00-0.33408472E 00-0.30960727E 00
0001300-0.28591041E 00-0.28273082E 00-0.28591041E 00-0.30960727E 00-0.33408472E 00
EOF
$
```

AL NL a=1.0
DENS.

VEFF

```
redit pote2
LOADING POTE2
RETRIEVED
EDIT
p99
        TOP RECORD
0000100 0.25869180E-01 0.25861699E-01 0.25857380E-01 0.25857437E-01 0.25862221E-01
0000200 0.25871128E-01 0.25882591E-01 0.25894485E-01 0.25904428E-01 0.25910206E-01
0000300 0.25910337E-01 0.25904536E-01 0.25893688E-01 0.25879797E-01 0.25865726E-01
0000400 0.25854543E-01 0.25849011E-01 0.25850790E-01 0.25860138E-01 0.25875658E-01
0000500 0.25894478E-01 0.25912747E-01 0.25926244E-01 0.25931429E-01 0.25926229E-01
0000600 0.25910627E-01 0.25896803E-01 0.25859337E-01 0.25833596E-01 0.25815606E-01
0000700 0.25810245E-01 0.25820225E-01 0.25845133E-01 0.25881175E-01 0.25921509E-01
0000800 0.25957342E-01 0.25979657E-01 0.25981214E-01 0.25958408E-01 0.25912736E-01
0000900 0.25851361E-01 0.25786355E-01 0.25732756E-01 0.25705203E-01 0.25714032E-01
0001000 0.25760859E-01 0.25834836E-01 0.25910176E-01 0.25945801E-01 0.25888033E-01
0001100 0.25675006E-01 0.25245536E-01 0.24548523E-01 0.23553565E-01 0.22260007E-01
0001200 0.20702679E-01 0.18952224E-01 0.17109532E-01 0.15205021E-01 0.13635583E-01
0001300 0.12251392E-01 0.11227351E-01 0.10602638E-01 0.10304752E-01 0.10602638E-01
EOF
q
redit pote3
LOADING POTE3
RETRIEVED
EDIT
p99
        TOP RECORD
0000100-0.41860360E 00-0.41871023E 00-0.41872954E 00-0.41873521E 00-0.41873197E 00
0000200-0.41872323E 00-0.41871083E 00-0.41868704E 00-0.41868252E 00-0.41868764E 00
0000300-0.41868734E 00-0.41868961E 00-0.41872847E 00-0.41875285E 00-0.41877288E 00
0000400-0.41878825E 00-0.41879302E 00-0.41878271E 00-0.41876334E 00-0.41872406E 00
0000500-0.41869307E 00-0.41865939E 00-0.41864711E 00-0.41863549E 00-0.41863918E 00
0000600-0.41866630E 00-0.41868718E 00-0.41872925E 00-0.41875434E 00-0.41876394E 00
0000700-0.41875243E 00-0.41871804E 00-0.41866618E 00-0.41860479E 00-0.41854841E 00
0000800-0.41850024E 00-0.41849053E 00-0.41852555E 00-0.41858603E 00-0.41867202E 00
0000900-0.41877132E 00-0.41885841E 00-0.41891265E 00-0.41890693E 00-0.41881990E 00
0001000-0.41862744E 00-0.41830519E 00-0.41791211E 00-0.41797290E 00-0.41584535E 00
0001100-0.41419792E 00-0.41146619E 00-0.40724909E 00-0.40086579E 00-0.39148815E 00
0001200-0.37820917E 00-0.36091945E 00-0.33595026E 00-0.30524117E 00-0.26718968E 00
0001300-0.23092155E 00-0.20606166E 00-0.18966490E 00-0.18177734E 00-0.18966490E 00
EOF
q
```

AL+ NL a=2.0
DENS.

VEFF

```
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
```

Alt NL a=3.0 DENS.

```
      TOP RECORD
0000100 0.25878575E-01 0.25886111E-01 0.25892753E-01 0.25897074E-01 0.25898017E-01
0000200 0.25895178E-01 0.25889046E-01 0.25880679E-01 0.25871754E-01 0.25864091E-01
0000300 0.25859367E-01 0.25858741E-01 0.25862575E-01 0.25870215E-01 0.25880270E-01
0000400 0.25890734E-01 0.25899403E-01 0.25904398E-01 0.25904465E-01 0.25899336E-01
0000500 0.25889874E-01 0.25877897E-01 0.25865875E-01 0.25856413E-01 0.25851827E-01
0000600 0.25853425E-01 0.25861334E-01 0.25874287E-01 0.25889866E-01 0.25904972E-01
0000700 0.25916319E-01 0.25921198E-01 0.25918100E-01 0.25907189E-01 0.25893253E-01
0000800 0.25870558E-01 0.25852177E-01 0.25839295E-01 0.25835142E-01 0.25841366E-01
0000900 0.25857408E-01 0.25880609E-01 0.25906391E-01 0.25929213E-01 0.25943626E-01
0001000 0.25945544E-01 0.25933143E-01 0.25907651E-01 0.25873311E-01 0.25836755E-01
0001100 0.25805804E-01 0.25788262E-01 0.25789230E-01 0.25810819E-01 0.25850400E-01
0001200 0.25901161E-01 0.25952712E-01 0.25993101E-01 0.26011209E-01 0.25999311E-01
0001300 0.25956096E-01 0.25888346E-01 0.25806520E-01 0.25729381E-01 0.25676575E-01
0001400 0.25654635E-01 0.25701478E-01 0.25781110E-01 0.25879711E-01 0.25954096E-01
0001500 0.25943343E-01 0.25774326E-01 0.25370724E-01 0.24664890E-01 0.23611113E-01
0001600 0.22197433E-01 0.20453781E-01 0.18453222E-01 0.16305350E-01 0.14142293E-01
0001700 0.12100417E-01 0.10301165E-01 0.88206530E-02 0.76840296E-02 0.68870500E-02
0001800 0.64184479E-02 0.62640943E-02 0.64184479E-02 0.68870500E-02 0.76840296E-02
EOF
q
```

```
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
```

VEFF

```
      TOP RECORD
0000100-0.41860301E 00-0.41868550E 00-0.41867632E 00-0.41867274E 00-0.41867453E 00
0000200-0.41866904E 00-0.41867870E 00-0.41869247E 00-0.41869682E 00-0.41871107E 00
0000300-0.41871011E 00-0.41870475E 00-0.41870559E 00-0.41869140E 00-0.41867894E 00
0000400-0.41866732E 00-0.41865176E 00-0.41865218E 00-0.41866404E 00-0.41867101E 00
0000500-0.41869849E 00-0.41872195E 00-0.41874027E 00-0.41876012E 00-0.41876894E 00
0000600-0.41876698E 00-0.41875499E 00-0.41873807E 00-0.41870707E 00-0.41868960E 00
0000700-0.41868412E 00-0.41867965E 00-0.41868406E 00-0.41871554E 00-0.41874468E 00
0000800-0.41877562E 00-0.41880184E 00-0.41881734E 00-0.41881686E 00-0.41880101E 00
0000900-0.41876042E 00-0.41872340E 00-0.41867005E 00-0.41864324E 00-0.41861028E 00
0001000-0.41861743E 00-0.41864115E 00-0.41867590E 00-0.41871828E 00-0.41875094E 00
0001100-0.41878582E 00-0.41879022E 00-0.41876435E 00-0.41871053E 00-0.41863602E 00
0001200-0.41855812E 00-0.41849160E 00-0.41845483E 00-0.41845948E 00-0.41851056E 00
0001300-0.41860217E 00-0.41872107E 00-0.41884559E 00-0.41894633E 00-0.41899085E 00
0001400-0.41895068E 00-0.41879619E 00-0.41840756E 00-0.41801673E 00-0.41722383E 00
0001500-0.41615529E 00-0.41442776E 00-0.41160298E 00-0.40740901E 00-0.40082407E 00
0001600-0.39099300E 00-0.37680495E 00-0.35704815E 00-0.33050019E 00-0.29611737E 00
0001700-0.25294298E 00-0.21003300E 00-0.17631704E 00-0.15104753E 00-0.13307229E 00
0001800-0.12301993E 00-0.12118661E 00-0.12301993E 00-0.13307229E 00-0.15104753E 00
EOF
q
```

```
redit pote6
LOADING POTE6
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.25880627E-01 0.25891166E-01 0.25900029E-01 0.25905229E-01 0.25905456E-01
0000200 0.25900446E-01 0.25890972E-01 0.25878776E-01 0.25865259E-01 0.25856070E-01
0000300 0.25850337E-01 0.25850613E-01 0.25856946E-01 0.25868297E-01 0.25882509E-01
0000400 0.25896695E-01 0.25907896E-01 0.25913641E-01 0.25912367E-01 0.25904156E-01
0000500 0.25890440E-01 0.25873974E-01 0.25858197E-01 0.25846660E-01 0.25842201E-01
0000600 0.25846265E-01 0.25858562E-01 0.25877036E-01 0.25898147E-01 0.25917511E-01
0000700 0.25930855E-01 0.25934953E-01 0.25928371E-01 0.25911804E-01 0.25888249E-01
0000800 0.25862336E-01 0.25839634E-01 0.25825344E-01 0.25823217E-01 0.25834642E-01
0000900 0.25858149E-01 0.25889393E-01 0.25922023E-01 0.25948711E-01 0.25962844E-01
0001000 0.25959954E-01 0.25938913E-01 0.25902543E-01 0.25857415E-01 0.25812663E-01
0001100 0.25778331E-01 0.25763232E-01 0.25772732E-01 0.25807235E-01 0.25861587E-01
0001200 0.25925361E-01 0.25986652E-01 0.26024867E-01 0.26033871E-01 0.26005290E-01
0001300 0.25940865E-01 0.25851216E-01 0.25754832E-01 0.25674764E-01 0.25633398E-01
0001400 0.25645979E-01 0.25714036E-01 0.25819674E-01 0.25922626E-01 0.25960539E-01
0001500 0.25853775E-01 0.25514867E-01 0.24861544E-01 0.23832109E-01 0.22400118E-01
0001600 0.20585164E-01 0.18456414E-01 0.16126443E-01 0.13735928E-01 0.11431824E-01
0001700 0.93432851E-02 0.75478293E-02 0.60654357E-02 0.48808642E-02 0.39618015E-02
0001800 0.32709695E-02 0.27731815E-02 0.24391860E-02 0.22474513E-02 0.21850574E-02
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.41869116E 00-0.41868198E 00-0.41867793E 00-0.41867590E 00-0.41866761E 00
0000200-0.41867483E 00-0.41868597E 00-0.41868764E 00-0.41870183E 00-0.41870433E 00
0000300-0.41869897E 00-0.41870475E 00-0.41869223E 00-0.41867822E 00-0.41866308E 00
0000400-0.41863680E 00-0.41863400E 00-0.41864163E 00-0.41864747E 00-0.41867143E 00
0000500-0.41869521E 00-0.41873533E 00-0.41875798E 00-0.41877413E 00-0.41877735E 00
0000600-0.41877097E 00-0.41875333E 00-0.41871404E 00-0.41869223E 00-0.41867065E 00
0000700-0.41865045E 00-0.41864729E 00-0.41867280E 00-0.41870141E 00-0.41874224E 00
0000800-0.41878396E 00-0.41881394E 00-0.41883159E 00-0.41882282E 00-0.41878253E 00
0000900-0.41873658E 00-0.41867107E 00-0.41861868E 00-0.41857314E 00-0.41854560E 00
0001000-0.41855502E 00-0.41858417E 00-0.41863215E 00-0.41868901E 00-0.41873920E 00
0001100-0.41876829E 00-0.41876459E 00-0.41872448E 00-0.41865128E 00-0.41855800E 00
0001200-0.41846472E 00-0.41839325E 00-0.41836411E 00-0.41838872E 00-0.41846907E 00
0001300-0.41859776E 00-0.41875243E 00-0.41890574E 00-0.41901881E 00-0.41905463E 00
0001400-0.41897333E 00-0.41873699E 00-0.41830462E 00-0.41761166E 00-0.41653943E 00
0001500-0.41487324E 00-0.41225344E 00-0.40813428E 00-0.40174991E 00-0.39210981E 00
0001600-0.37801385E 00-0.35810930E 00-0.33098137E 00-0.29529864E 00-0.24978721E 00
0001700-0.20314604E 00-0.16402465E 00-0.13140136E 00-0.10465872E 00-0.83226502E-01
0001800-0.66741109E-01-0.54809820E-01-0.47062423E-01-0.42431314E-01-0.41562166E-01
EOF
q
```

AL+ NL a=5.0 DENS.

VEFF

```
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
```

Alt NL a=10.0 DENS.

```
        TOP RECORD
0000100 0.25865432E-01 0.25876511E-01 0.25889453E-01 0.25901485E-01 0.25909852E-01
0000200 0.25912440E-01 0.25908392E-01 0.25899091E-01 0.25883280E-01 0.25866814E-01
0000300 0.25851960E-01 0.25841862E-01 0.25838833E-01 0.25843717E-01 0.25855865E-01
0000400 0.25872087E-01 0.25891781E-01 0.25908370E-01 0.25919188E-01 0.25921714E-01
0000500 0.25915150E-01 0.25900505E-01 0.25880635E-01 0.25859583E-01 0.25841955E-01
0000600 0.25831833E-01 0.25831874E-01 0.25842771E-01 0.25862876E-01 0.25888521E-01
0000700 0.25914568E-01 0.25935493E-01 0.25946569E-01 0.25944030E-01 0.25930144E-01
0000800 0.25904696E-01 0.25873501E-01 0.25843024E-01 0.25819987E-01 0.25809259E-01
0000900 0.25816020E-01 0.25837980E-01 0.25872137E-01 0.25911767E-01 0.25948390E-01
0001000 0.25973454E-01 0.25980346E-01 0.25965832E-01 0.25931146E-01 0.25882177E-01
0001100 0.25828490E-01 0.25781713E-01 0.25752950E-01 0.25750440E-01 0.25777213E-01
0001200 0.25830105E-01 0.25899507E-01 0.25970958E-01 0.26027814E-01 0.26054863E-01
0001300 0.26041988E-01 0.25987305E-01 0.25898773E-01 0.25793754E-01 0.25696158E-01
0001400 0.25631201E-01 0.25613821E-01 0.25666207E-01 0.25761306E-01 0.25868621E-01
0001500 0.25928523E-01 0.25861371E-01 0.25576383E-01 0.24984892E-01 0.24016500E-01
0001600 0.22634972E-01 0.20850707E-01 0.18725947E-01 0.16370106E-01 0.13924927E-01
0001700 0.11542037E-01 0.93572102E-02 0.74542910E-02 0.58577470E-02 0.45547187E-02
0001800 0.35130742E-02 0.26933826E-02 0.20560967E-02 0.15652205E-02 0.11898465E-02
0001900 0.90444623E-03 0.68849139E-03 0.52580121E-03 0.40381867E-03 0.31292369E-03
0002000 0.24583959E-03 0.19713987E-03 0.16285988E-03 0.14019928E-03 0.12730421E-03
0002100 0.12312019E-03 0.12730421E-03 0.14019928E-03 0.16285988E-03 0.19713987E-03
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.41869348E 00-0.41868508E 00-0.41866416E 00-0.41864395E 00-0.41862571E 00
0000200-0.41859758E 00-0.41859049E 00-0.41858941E 00-0.41858655E 00-0.41860312E 00
0000300-0.41861105E 00-0.41861939E 00-0.41863298E 00-0.41863000E 00-0.41861957E 00
0000400-0.41860527E 00-0.41857868E 00-0.41856557E 00-0.41856259E 00-0.41856050E 00
0000500-0.41858393E 00-0.41860944E 00-0.41865414E 00-0.41868663E 00-0.41871810E 00
0000600-0.41873664E 00-0.41874123E 00-0.41873336E 00-0.41870213E 00-0.41867322E 00
0000700-0.41865021E 00-0.41861916E 00-0.41861057E 00-0.41862816E 00-0.41865671E 00
0000800-0.41870064E 00-0.41875225E 00-0.41879916E 00-0.41883153E 00-0.41884106E 00
0000900-0.41881227E 00-0.41877282E 00-0.41870648E 00-0.41864735E 00-0.41858816E 00
0001000-0.41854841E 00-0.41854596E 00-0.41856813E 00-0.41861755E 00-0.41868454E 00
0001100-0.41875255E 00-0.41880482E 00-0.41882515E 00-0.41880476E 00-0.41874170E 00
0001200-0.41864723E 00-0.41854012E 00-0.41844457E 00-0.41839503E 00-0.41837817E 00
0001300-0.41843283E 00-0.41854644E 00-0.41870010E 00-0.41886723E 00-0.41900957E 00
0001400-0.41908455E 00-0.41904616E 00-0.41884965E 00-0.41844845E 00-0.41777909E 00
0001500-0.41673172E 00-0.41510874E 00-0.41257381E 00-0.40860814E 00-0.40247160E 00
0001600-0.39319038E 00-0.37956923E 00-0.36023939E 00-0.33374351E 00-0.29867566E 00
0001700-0.25365329E 00-0.20725274E 00-0.16796935E 00-0.13457388E 00-0.10619754E 00
0001800-0.82018614E-01-0.61344087E-01-0.43597504E-01-0.28306045E-01-0.15086506E-01
0001900-0.36259938E-02 0.63271970E-02 0.14977705E-01 0.22493567E-01 0.29019643E-01
0002000 0.34675252E-01 0.39576236E-01 0.43771889E-01 0.47171034E-01 0.49503684E-01
0002100 0.50313290E-01 0.49503684E-01 0.47171034E-01 0.43771889E-01 0.39576236E-01
EOF
q
```

```
redit potel0
LOADING POTE10
RETRIEVED
EDIT
p99
```

AL+ NL a=15.0
DENS.

```
        TOP RECORD
0000100 0.25363899E-01 0.25875714E-01 0.25869615E-01 0.25902711E-01 0.25912140E-01
0000200 0.25915623E-01 0.25912195E-01 0.25902200E-01 0.25887430E-01 0.25870711E-01
0000300 0.25855403E-01 0.25845010E-01 0.25841676E-01 0.25846478E-01 0.25858708E-01
0000400 0.25876127E-01 0.25895240E-01 0.25912158E-01 0.25923114E-01 0.25925517E-01
0000500 0.25914689E-01 0.25903001E-01 0.25892017E-01 0.25859680E-01 0.25840778E-01
0000600 0.25829513E-01 0.25829730E-01 0.25839155E-01 0.25859144E-01 0.25884960E-01
0000700 0.25911316E-01 0.25932517E-01 0.25943618E-01 0.25941636E-01 0.25926076E-01
0000800 0.25899407E-01 0.25866710E-01 0.25834646E-01 0.25810242E-01 0.25799267E-01
0000900 0.25805030E-01 0.25827471E-01 0.25862302E-01 0.25904194E-01 0.25942877E-01
0001000 0.25970053E-01 0.25978911E-01 0.25965501E-01 0.25931604E-01 0.25882725E-01
0001100 0.25839674E-01 0.25791348E-01 0.25752280E-01 0.25750097E-01 0.25777951E-01
0001200 0.25832983E-01 0.25905486E-01 0.25980726E-01 0.26041601E-01 0.26072290E-01
0001300 0.26062075E-01 0.26008546E-01 0.25919333E-01 0.25811713E-01 0.25709759E-01
0001400 0.25639319E-01 0.25621004E-01 0.25662906E-01 0.25753863E-01 0.25859091E-01
0001500 0.25919504E-01 0.25855627E-01 0.25576387E-01 0.24992589E-01 0.24032820E-01
0001600 0.22659667E-01 0.20882316E-01 0.18762022E-01 0.16407602E-01 0.13960741E-01
0001700 0.11573597E-01 0.93828291E-02 0.74731484E-02 0.58697052E-02 0.45600384E-02
0001800 0.35122668E-02 0.26870880E-02 0.20440767E-02 0.15498970E-02 0.11708622E-02
0001900 0.88222604E-03 0.66332193E-03 0.49781450E-03 0.37297024E-03 0.27896743E-03
0002000 0.20829155E-03 0.15522444E-03 0.11543636E-03 0.85656182E-04 0.63415868E-04
0002100 0.46858448E-04 0.34576937E-04 0.25511064E-04 0.18857725E-04 0.14010164E-04
0002200 0.10513025E-04 0.80293448E-05 0.63152866E-05 0.52005962E-05 0.45736606E-05
0002300 0.43714672E-05 0.45736606E-05 0.52005962E-05 0.63152866E-05 0.80293448E-05
EOF
q
redit potell
LOADING POTE11
RETRIEVED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.41860342E 00-0.41868603E 00-0.41866875E 00-0.41865391E 00-0.41864318E 00
0000200-0.41862702E 00-0.41862845E 00-0.41864020E 00-0.41864711E 00-0.41867005E 00
0000300-0.41868144E 00-0.41869044E 00-0.41870099E 00-0.41869551E 00-0.41868180E 00
0000400-0.41866022E 00-0.41862851E 00-0.41861212E 00-0.41860574E 00-0.41860163E 00
0000500-0.41862309E 00-0.41864121E 00-0.41868204E 00-0.41870987E 00-0.41872984E 00
0000600-0.41874295E 00-0.41873717E 00-0.41871887E 00-0.41867471E 00-0.41863841E 00
0000700-0.41860306E 00-0.41857237E 00-0.41855580E 00-0.41857558E 00-0.41860300E 00
0000800-0.41864192E 00-0.41869026E 00-0.41873521E 00-0.41876411E 00-0.41877276E 00
0000900-0.41874659E 00-0.41870952E 00-0.41864711E 00-0.41859448E 00-0.41854072E 00
0001000-0.41851109E 00-0.41851372E 00-0.41854405E 00-0.41860056E 00-0.41867495E 00
0001100-0.41875035E 00-0.41881049E 00-0.41884035E 00-0.41883308E 00-0.41878700E 00
0001200-0.41871381E 00-0.41863054E 00-0.41856086E 00-0.41852629E 00-0.41854101E 00
0001300-0.41861099E 00-0.41873032E 00-0.41887796E 00-0.41902958E 00-0.41914254E 00
0001400-0.41918188E 00-0.41910368E 00-0.41896759E 00-0.41843092E 00-0.41773367E 00
0001500-0.41666824E 00-0.41504061E 00-0.41251713E 00-0.40958257E 00-0.40249956E 00
0001600-0.39329481E 00-0.37977046E 00-0.36054862E 00-0.33415842E 00-0.29917371E 00
0001700-0.25419921E 00-0.20782620E 00-0.16057833E 00-0.13522887E 00-0.10689157E 00
0001800-0.82736194E-01-0.62061414E-01-0.44278871E-01-0.28005034E-01-0.15541349E-01
0001900-0.38551392E-02 0.64364858E-02 0.15581075E-01 0.23804624E-01 0.31327348E-01
0002000 0.38370166E-01 0.45170017E-01 0.51973328E-01 0.59021648E-01 0.66502512E-01
0002100 0.74476004E-01 0.82800746E-01 0.91066062E-01 0.98682165E-01 0.10511845E 00
0002200 0.11015171E 00 0.11380452E 00 0.11670226E 00 0.11858702E 00 0.11973262E 00
0002300 0.12012446E 00 0.11973262E 00 0.11858702E 00 0.11670226E 00 0.11380452E 00
EOF
q
```

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
```

ZN LDA a=0.25 DENS.

```
        TOP RECORD
0000100 0.19620318E-01 0.19621130E-01 0.19621875E-01 0.19622527E-01 0.19623104E-01
0000200 0.19623522E-01 0.19623797E-01 0.19623935E-01 0.19623902E-01 0.19623715E-01
0000300 0.19623376E-01 0.19622922E-01 0.19622363E-01 0.19621722E-01 0.19621015E-01
0000400 0.19620296E-01 0.19619573E-01 0.19618910E-01 0.19618329E-01 0.19617870E-01
0000500 0.19617554E-01 0.19617412E-01 0.19617442E-01 0.19617654E-01 0.19618038E-01
0000600 0.19618601E-01 0.19619327E-01 0.19620169E-01 0.19621100E-01 0.19622102E-01
0000700 0.19623104E-01 0.19624107E-01 0.19625023E-01 0.19625857E-01 0.19626517E-01
0000800 0.19626956E-01 0.19627195E-01 0.19627154E-01 0.19626874E-01 0.19626327E-01
0000900 0.19625526E-01 0.19624505E-01 0.19623265E-01 0.19621901E-01 0.19620456E-01
0001000 0.19618995E-01 0.19617550E-01 0.19616209E-01 0.19615043E-01 0.19614112E-01
0001100 0.19613452E-01 0.19613113E-01 0.19613162E-01 0.19613571E-01 0.19614395E-01
0001200 0.19615568E-01 0.19617081E-01 0.19618902E-01 0.19620944E-01 0.19623138E-01
0001300 0.19625396E-01 0.19627582E-01 0.19629620E-01 0.19631408E-01 0.19632842E-01
0001400 0.19633789E-01 0.19634206E-01 0.19634012E-01 0.19633181E-01 0.19631688E-01
0001500 0.19629553E-01 0.19626804E-01 0.19623529E-01 0.19619849E-01 0.19615870E-01
0001600 0.19611765E-01 0.19607738E-01 0.19603938E-01 0.19600600E-01 0.19597903E-01
0001700 0.19596044E-01 0.19595150E-01 0.19595385E-01 0.19596785E-01 0.19599412E-01
0001800 0.19603200E-01 0.19608028E-01 0.19613717E-01 0.19619945E-01 0.19626342E-01
0001900 0.19632477E-01 0.19637726E-01 0.19641493E-01 0.19643053E-01 0.19641627E-01
0002000 0.19636378E-01 0.19626461E-01 0.19611008E-01 0.19589197E-01 0.19560203E-01
0002100 0.19523315E-01 0.19477893E-01 0.19423470E-01 0.19359738E-01 0.19286532E-01
0002200 0.19203991E-01 0.19112427E-01 0.19012496E-01 0.18905099E-01 0.18791486E-01
0002300 0.18673159E-01 0.18552005E-01 0.18430199E-01 0.18310230E-01 0.18194921E-01
0002400 0.18087324E-01 0.17990828E-01 0.17909002E-01 0.17845657E-01 0.17804708E-01
0002500 0.17790701E-01 0.17804708E-01 0.17845657E-01 0.17909002E-01 0.17990828E-01
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812564E 00-0.34813291E 00-0.34814113E 00-0.34814495E 00-0.34814441E 00
0000200-0.34814394E 00-0.34815389E 00-0.34815300E 00-0.34815091E 00-0.34814620E 00
0000300-0.34815174E 00-0.34815031E 00-0.34815186E 00-0.34815031E 00-0.34815103E 00
0000400-0.34814870E 00-0.34815133E 00-0.34814495E 00-0.34814507E 00-0.34814513E 00
0000500-0.34814292E 00-0.34814358E 00-0.34814465E 00-0.34814692E 00-0.34814876E 00
0000600-0.34814399E 00-0.34814662E 00-0.34815007E 00-0.34815079E 00-0.34814107E 00
0000700-0.34814137E 00-0.34814316E 00-0.34814459E 00-0.34814769E 00-0.34814894E 00
0000800-0.34815192E 00-0.34815246E 00-0.34815675E 00-0.34815723E 00-0.34815514E 00
0000900-0.34815347E 00-0.34815222E 00-0.34815037E 00-0.34814829E 00-0.34814882E 00
0001000-0.34814632E 00-0.34814513E 00-0.34814370E 00-0.34814262E 00-0.34814405E 00
0001100-0.34814143E 00-0.34813702E 00-0.34813422E 00-0.34813243E 00-0.34812993E 00
0001200-0.34812838E 00-0.34812713E 00-0.34812623E 00-0.34812558E 00-0.34812605E 00
0001300-0.34812683E 00-0.34812784E 00-0.34812987E 00-0.34813213E 00-0.34813505E 00
0001400-0.34813827E 00-0.34814119E 00-0.34814453E 00-0.34814769E 00-0.34815085E 00
0001500-0.34815240E 00-0.34815365E 00-0.34815401E 00-0.34815258E 00-0.34815013E 00
0001600-0.34814578E 00-0.34814012E 00-0.34813273E 00-0.34812409E 00-0.34811348E 00
0001700-0.34810209E 00-0.34808922E 00-0.34807622E 00-0.34806210E 00-0.34804881E 00
0001800-0.34803528E 00-0.34802294E 00-0.34801102E 00-0.34799957E 00-0.34798831E 00
0001900-0.34797657E 00-0.34796315E 00-0.34794670E 00-0.34792471E 00-0.34789413E 00
0002000-0.34785151E 00-0.34779227E 00-0.34771013E 00-0.34759867E 00-0.34744960E 00
0002100-0.34725469E 00-0.34700310E 00-0.34668297E 00-0.34628177E 00-0.34578538E 00
0002200-0.34517914E 00-0.34444678E 00-0.34357172E 00-0.34253705E 00-0.34132534E 00
0002300-0.33991981E 00-0.33830404E 00-0.33646274E 00-0.33438236E 00-0.33205104E 00
0002400-0.32946032E 00-0.32660472E 00-0.32348299E 00-0.32028902E 00-0.31596708E 00
0002500-0.31517977E 00-0.31596708E 00-0.32028902E 00-0.32348299E 00-0.32660472E 00
EOF
```

```
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
```

ZN LDA a=0.5 DENS.

```
        TOP RECORD
0000100 0.19624937E-01 0.19627079E-01 0.19628558E-01 0.19629136E-01 0.19628581E-01
0000200 0.19626949E-01 0.19624483E-01 0.19621495E-01 0.19618515E-01 0.19616090E-01
0000300 0.19614659E-01 0.19614592E-01 0.19616019E-01 0.19618746E-01 0.19622400E-01
0000400 0.19626383E-01 0.19630000E-01 0.19632492E-01 0.19633330E-01 0.19632101E-01
0000500 0.19628853E-01 0.19623961E-01 0.19618154E-01 0.19612320E-01 0.19607544E-01
0000600 0.19604821E-01 0.19604906E-01 0.19608114E-01 0.19614223E-01 0.19622475E-01
0000700 0.19631572E-01 0.19639920E-01 0.19645784E-01 0.19647624E-01 0.19644432E-01
0000800 0.19635994E-01 0.19622944E-01 0.19607037E-01 0.19590814E-01 0.19577291E-01
0000900 0.19569658E-01 0.19570395E-01 0.19580837E-01 0.19600280E-01 0.19625623E-01
0001000 0.19650906E-01 0.19667413E-01 0.19663967E-01 0.19627698E-01 0.19545320E-01
0001100 0.19404612E-01 0.19196261E-01 0.18915661E-01 0.18564768E-01 0.18153459E-01
0001200 0.17700396E-01 0.17233171E-01 0.16787894E-01 0.16407751E-01 0.16141050E-01
0001300 0.16047154E-01 0.16141050E-01 0.16407751E-01 0.16787894E-01 0.17233171E-01
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34811997E 00-0.34812868E 00-0.34812379E 00-0.34813035E 00-0.34812599E 00
0000200-0.34813267E 00-0.34813547E 00-0.34813458E 00-0.34813142E 00-0.34813243E 00
0000300-0.34812576E 00-0.34812593E 00-0.34812373E 00-0.34812665E 00-0.34811759E 00
0000400-0.34811980E 00-0.34812343E 00-0.34812951E 00-0.34813118E 00-0.34812707E 00
0000500-0.34812689E 00-0.34812719E 00-0.34812981E 00-0.34812719E 00-0.34812427E 00
0000600-0.34811729E 00-0.34811038E 00-0.34810346E 00-0.34809899E 00-0.34809738E 00
0000700-0.34809959E 00-0.34810650E 00-0.34811783E 00-0.34813064E 00-0.34814399E 00
0000800-0.34815365E 00-0.34815687E 00-0.34814954E 00-0.34813094E 00-0.34809935E 00
0000900-0.34805721E 00-0.34800816E 00-0.34795833E 00-0.34791207E 00-0.34787089E 00
0001000-0.34783018E 00-0.34777379E 00-0.34766674E 00-0.34745276E 00-0.34704399E 00
0001100-0.34632027E 00-0.34512043E 00-0.34324682E 00-0.34046555E 00-0.33651841E 00
0001200-0.33113718E 00-0.32406884E 00-0.31509948E 00-0.30478090E 00-0.28924131E 00
0001300-0.28613877E 00-0.28924131E 00-0.30478090E 00-0.31509948E 00-0.32406884E 00
EOF
q
```

```
redit pote6
LOADING POTE6   ZN LDA  a=0.75
REKEYED         DENS.
EDIT
p99
        TOP RECORD
0000100 0.19625846E-01 0.19627914E-01 0.19629873E-01 0.19631624E-01 0.19633088E-01
0000200 0.19634217E-01 0.19634943E-01 0.19635264E-01 0.19635107E-01 0.19634493E-01
0000300 0.19633476E-01 0.19632038E-01 0.19630298E-01 0.19628253E-01 0.19626059E-01
0000400 0.19623790E-01 0.19621532E-01 0.19619420E-01 0.19617528E-01 0.19615997E-01
0000500 0.19614868E-01 0.19614235E-01 0.19614138E-01 0.19614592E-01 0.19615617E-01
0000600 0.19617170E-01 0.19619234E-01 0.19621693E-01 0.19624479E-01 0.19627463E-01
0000700 0.19630540E-01 0.19633520E-01 0.19636337E-01 0.19638769E-01 0.19640747E-01
0000800 0.19642122E-01 0.19642811E-01 0.19642726E-01 0.19641824E-01 0.19640137E-01
0000900 0.19637652E-01 0.19634478E-01 0.19630697E-01 0.19626435E-01 0.19621879E-01
0001000 0.19617204E-01 0.19612614E-01 0.19608308E-01 0.19604500E-01 0.19601386E-01
0001100 0.19599121E-01 0.19597862E-01 0.19597743E-01 0.19598804E-01 0.19601084E-01
0001200 0.19604545E-01 0.19609094E-01 0.19614555E-01 0.19620769E-01 0.19627459E-01
0001300 0.19634355E-01 0.19641157E-01 0.19647505E-01 0.19653112E-01 0.19657601E-01
0001400 0.19660711E-01 0.19662179E-01 0.19661795E-01 0.19659452E-01 0.19655056E-01
0001500 0.19648690E-01 0.19640438E-01 0.19630559E-01 0.19619372E-01 0.19607294E-01
0001600 0.19594781E-01 0.19582432E-01 0.19570783E-01 0.19560494E-01 0.19552130E-01
0001700 0.19546244E-01 0.19543380E-01 0.19543894E-01 0.19548040E-01 0.19555926E-01
0001800 0.19567445E-01 0.19582231E-01 0.19599706E-01 0.19619081E-01 0.19639231E-01
0001900 0.19658789E-01 0.19676123E-01 0.19689374E-01 0.19696459E-01 0.19695144E-01
0002000 0.19683048E-01 0.19657761E-01 0.19616790E-01 0.19557782E-01 0.19478541E-01
0002100 0.19377068E-01 0.19251674E-01 0.19101162E-01 0.18924732E-01 0.18722214E-01
0002200 0.18493995E-01 0.18241264E-01 0.17965816E-01 0.17670333E-01 0.17358117E-01
0002300 0.17033327E-01 0.16700801E-01 0.16366042E-01 0.16035192E-01 0.15714943E-01
0002400 0.15412502E-01 0.15135441E-01 0.14891766E-01 0.14689818E-01 0.14538184E-01
0002500 0.14444217E-01 0.14412623E-01 0.14444217E-01 0.14538184E-01 0.14689818E-01
EOF
q
redit pote7
LOADING POTE7
REKEYED         VEFF
EDIT
p99
        TOP RECORD
0000100-0.34812576E 00-0.34813708E 00-0.34814811E 00-0.34815055E 00-0.34815770E 00
0000200-0.34816819E 00-0.34817231E 00-0.34817141E 00-0.34817630E 00-0.34818292E 00
0000300-0.34818685E 00-0.34818977E 00-0.34819162E 00-0.34819245E 00-0.34819281E 00
0000400-0.34819406E 00-0.34819138E 00-0.34819144E 00-0.34818423E 00-0.34818554E 00
0000500-0.34818071E 00-0.34817815E 00-0.34818107E 00-0.34818119E 00-0.34817404E 00
0000600-0.34817004E 00-0.34817559E 00-0.34817410E 00-0.34816444E 00-0.34816527E 00
0000700-0.34816688E 00-0.34816706E 00-0.34817183E 00-0.34817076E 00-0.34817672E 00
0000800-0.34818047E 00-0.34818476E 00-0.34818411E 00-0.34818417E 00-0.34818304E 00
0000900-0.34818232E 00-0.34818089E 00-0.34817898E 00-0.34817761E 00-0.34817481E 00
0001000-0.34816992E 00-0.34816527E 00-0.34816039E 00-0.34815627E 00-0.34814984E 00
0001100-0.34814221E 00-0.34813523E 00-0.34812856E 00-0.34812129E 00-0.34811521E 00
0001200-0.34811050E 00-0.34810627E 00-0.34810352E 00-0.34810257E 00-0.34810328E 00
0001300-0.34810519E 00-0.34810936E 00-0.34811544E 00-0.34812278E 00-0.34813172E 00
0001400-0.34814095E 00-0.34815127E 00-0.34816116E 00-0.34817106E 00-0.34817922E 00
0001500-0.34818536E 00-0.34818923E 00-0.34818941E 00-0.34818560E 00-0.34817797E 00
0001600-0.34816575E 00-0.34814924E 00-0.34812760E 00-0.34810179E 00-0.34807211E 00
0001700-0.34803933E 00-0.34800464E 00-0.34796816E 00-0.34793264E 00-0.34789723E 00
0001800-0.34786505E 00-0.34783494E 00-0.34780854E 00-0.34778476E 00-0.34776348E 00
0001900-0.34774226E 00-0.34771824E 00-0.34768653E 00-0.34764087E 00-0.34757352E 00
0002000-0.34747374E 00-0.34732747E 00-0.34712070E 00-0.34683251E 00-0.34644300E 00
0002100-0.34592545E 00-0.34525162E 00-0.34438884E 00-0.34330219E 00-0.34195203E 00
0002200-0.34029675E 00-0.33829230E 00-0.33589214E 00-0.33304930E 00-0.32971591E 00
0002300-0.32584494E 00-0.32139140E 00-0.31631339E 00-0.31057215E 00-0.30413747E 00
0002400-0.29698426E 00-0.28909463E 00-0.28045964E 00-0.27108568E 00-0.26274252E 00
0002500-0.25731814E 00-0.25654954E 00-0.25731814E 00-0.26274252E 00-0.27108568E 00
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
```

ZN LDA a=1.0
DENS.

```
        TOP RECORD
0000100 0.19624453E-01 0.19629121E-01 0.19632921E-01 0.19635092E-01 0.19635130E-01
0000200 0.19632906E-01 0.19628581E-01 0.19622833E-01 0.19616548E-01 0.19610833E-01
0000300 0.19606698E-01 0.19605096E-01 0.19606471E-01 0.19610789E-01 0.19617550E-01
0000400 0.19625708E-01 0.19633923E-01 0.19640643E-01 0.19644529E-01 0.19644521E-01
0000500 0.19640282E-01 0.19632146E-01 0.19621182E-01 0.19609082E-01 0.19597966E-01
0000600 0.19589972E-01 0.19586995E-01 0.19590132E-01 0.19599609E-01 0.19614432E-01
0000700 0.19632541E-01 0.19650918E-01 0.19666117E-01 0.19674715E-01 0.19674055E-01
0000800 0.19662723E-01 0.19641094E-01 0.19611564E-01 0.19578397E-01 0.19547332E-01
0000900 0.19524768E-01 0.19516613E-01 0.19526936E-01 0.19556724E-01 0.19602522E-01
0001000 0.19655731E-01 0.19702215E-01 0.19722704E-01 0.19694008E-01 0.19591052E-01
0001100 0.19389618E-01 0.19069664E-01 0.18618841E-01 0.18035814E-01 0.17332815E-01
0001200 0.16537018E-01 0.15690245E-01 0.14847338E-01 0.14073189E-01 0.13439707E-01
0001300 0.13021257E-01 0.12878101E-01 0.13021257E-01 0.13439707E-01 0.14073189E-01
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812564E 00-0.34812838E 00-0.34812003E 00-0.34812361E 00-0.34812009E 00
0000200-0.34812683E 00-0.34812778E 00-0.34812796E 00-0.34812868E 00-0.34813070E 00
0000300-0.34812534E 00-0.34812421E 00-0.34812260E 00-0.34812444E 00-0.34811240E 00
0000400-0.34811562E 00-0.34811604E 00-0.34811896E 00-0.34812331E 00-0.34812260E 00
0000500-0.34812587E 00-0.34812933E 00-0.34813470E 00-0.34813195E 00-0.34813547E 00
0000600-0.34812582E 00-0.34811586E 00-0.34810430E 00-0.34809422E 00-0.34808683E 00
0000700-0.34808493E 00-0.34809065E 00-0.34810483E 00-0.34812564E 00-0.34815109E 00
0000800-0.34817439E 00-0.34819049E 00-0.34819210E 00-0.34817290E 00-0.34812874E 00
0000900-0.34805995E 00-0.34797210E 00-0.34787273E 00-0.34777349E 00-0.34768295E 00
0001000-0.34760320E 00-0.34751993E 00-0.34739161E 00-0.34714043E 00-0.34663868E 00
0001100-0.34569651E 00-0.34405237E 00-0.34136754E 00-0.33722675E 00-0.33115113E 00
0001200-0.32262224E 00-0.31112093E 00-0.29617572E 00-0.27742374E 00-0.25522536E 00
0001300-0.23462331E 00-0.23160708E 00-0.23462331E 00-0.25522536E 00-0.27742374E 00
EOF
q
```

```
redit potel0
LOADING POTEl0
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.19616533E-01 0.19613635E-01 0.19612029E-01 0.19612096E-01 0.19613944E-01
0000200 0.19617315E-01 0.19621711E-01 0.19626435E-01 0.19630697E-01 0.19633740E-01
0000300 0.19634921E-01 0.19633945E-01 0.19630898E-01 0.19626215E-01 0.19620638E-01
0000400 0.19615054E-01 0.19610532E-01 0.19607909E-01 0.19607767E-01 0.19610267E-01
0000500 0.19615158E-01 0.19621659E-01 0.19628711E-01 0.19635074E-01 0.19639507E-01
0000600 0.19641064E-01 0.19639246E-01 0.19634143E-01 0.19626331E-01 0.19617014E-01
0000700 0.19607760E-01 0.19600164E-01 0.19595802E-01 0.19595642E-01 0.19600049E-01
0000800 0.19608617E-01 0.19620139E-01 0.19632760E-01 0.19644231E-01 0.19652370E-01
0000900 0.19655339E-01 0.19652143E-01 0.19642714E-01 0.19628216E-01 0.19610759E-01
0001000 0.19593347E-01 0.19579176E-01 0.19571315E-01 0.19571971E-01 0.19582089E-01
0001100 0.19600954E-01 0.19626133E-01 0.19653708E-01 0.19678712E-01 0.19695994E-01
0001200 0.19701034E-01 0.19690942E-01 0.19665234E-01 0.19626293E-01 0.19579433E-01
0001300 0.19532442E-01 0.19494522E-01 0.19474842E-01 0.19480597E-01 0.19514997E-01
0001400 0.19575521E-01 0.19652512E-01 0.19728441E-01 0.19778285E-01 0.19770972E-01
0001500 0.19672070E-01 0.19447546E-01 0.19068275E-01 0.18515088E-01 0.17783087E-01
0001600 0.16885173E-01 0.15853446E-01 0.14738165E-01 0.13604425E-01 0.12527145E-01
0001700 0.11585619E-01 0.10857116E-01 0.10399271E-01 0.10245122E-01 0.10399271E-01
EOF
q
redit potel1
LOADING POTEl1
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.34812564E 00-0.34811980E 00-0.34812337E 00-0.34811336E 00-0.34811807E 00
0000200-0.34812087E 00-0.34812123E 00-0.34811068E 00-0.34811288E 00-0.34812653E 00
0000300-0.34812838E 00-0.34812480E 00-0.34812319E 00-0.34812891E 00-0.34813237E 00
0000400-0.34812212E 00-0.34811884E 00-0.34811473E 00-0.34811157E 00-0.34810483E 00
0000500-0.34810036E 00-0.34809369E 00-0.34810114E 00-0.34809822E 00-0.34810162E 00
0000600-0.34809655E 00-0.34810054E 00-0.34810370E 00-0.34810448E 00-0.34810120E 00
0000700-0.34809035E 00-0.34807813E 00-0.34807545E 00-0.34806031E 00-0.34805721E 00
0000800-0.34804881E 00-0.34805244E 00-0.34805977E 00-0.34807056E 00-0.34808570E 00
0000900-0.34809285E 00-0.34810311E 00-0.34811056E 00-0.34811264E 00-0.34810865E 00
0001000-0.34809792E 00-0.34808177E 00-0.34806317E 00-0.34804493E 00-0.34803319E 00
0001100-0.34802979E 00-0.34803909E 00-0.34806228E 00-0.34809804E 00-0.34814078E 00
0001200-0.34818441E 00-0.34821880E 00-0.34823465E 00-0.34822267E 00-0.34817743E 00
0001300-0.34809750E 00-0.34798974E 00-0.34786701E 00-0.34774780E 00-0.34765232E 00
0001400-0.34759426E 00-0.34757596E 00-0.34757566E 00-0.34753698E 00-0.34735465E 00
0001500-0.34686214E 00-0.34581596E 00-0.34388357E 00-0.34064019E 00-0.33556771E 00
0001600-0.32807136E 00-0.31750691E 00-0.30322498E 00-0.28462791E 00-0.26123267E 00
0001700-0.23318708E 00-0.20825315E 00-0.19121987E 00-0.18849307E 00-0.19121987E 00
EOF
q
```

ZN LDA a=1.5 DENS.

VEFF

```
redit potel2
LOADING POTE12
REKEYED
EDIT
p99
```

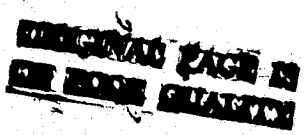
ZN LDA a=2.0 DENS.

```
        TOP RECORD
0000100 0.19616701E-01 0.19626047E-01 0.19635182E-01 0.19642483E-01 0.19646499E-01
0000200 0.19646309E-01 0.19641615E-01 0.19632898E-01 0.19621488E-01 0.19609228E-01
0000300 0.19598279E-01 0.19590702E-01 0.19588172E-01 0.19591551E-01 0.19600712E-01
0000400 0.19614514E-01 0.19630842E-01 0.19646954E-01 0.19659892E-01 0.19666962E-01
0000500 0.19666418E-01 0.19657567E-01 0.19641254E-01 0.19619703E-01 0.19596323E-01
0000600 0.19575275E-01 0.19560657E-01 0.19555971E-01 0.19563183E-01 0.19582387E-01
0000700 0.19611411E-01 0.19646015E-01 0.19680332E-01 0.19707806E-01 0.19722119E-01
0000800 0.19718606E-01 0.19695152E-01 0.19653168E-01 0.19597720E-01 0.19537374E-01
0000900 0.19483048E-01 0.19446481E-01 0.19437917E-01 0.19463699E-01 0.19523911E-01
0001000 0.19610379E-01 0.19705385E-01 0.19781798E-01 0.19804165E-01 0.19731697E-01
0001100 0.19522291E-01 0.19137971E-01 0.18550839E-01 0.17748822E-01 0.16740240E-01
0001200 0.15556257E-01 0.14250077E-01 0.12893047E-01 0.11567876E-01 0.10360878E-01
0001300 0.93541145E-02 0.86085312E-02 0.81531182E-02 0.80012530E-02 0.81531182E-02
EOF
q
redit potel3
LOADING POTE13
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812576E 00-0.34812015E 00-0.34810805E 00-0.34810817E 00-0.34810632E 00
0000200-0.34811538E 00-0.34811950E 00-0.34812337E 00-0.34812611E 00-0.34813064E 00
0000300-0.34812796E 00-0.34812897E 00-0.34812516E 00-0.34812480E 00-0.34811145E 00
0000400-0.34810913E 00-0.34810704E 00-0.34810817E 00-0.34811121E 00-0.34811169E 0(
0000500-0.34811789E 00-0.34812576E 00-0.34813792E 00-0.34814179E 00-0.34814531E 00
0000600-0.34813595E 00-0.34812105E 00-0.34810036E 00-0.34807777E 00-0.34805620E 00
0000700-0.34804046E 00-0.34803557E 00-0.34804589E 00-0.34807110E 00-0.34810990E 00
0000800-0.34815669E 00-0.34820211E 00-0.34823477E 00-0.34824282E 00-0.34821504E 00
0000900-0.34814566E 00-0.34803551E 00-0.34789461E 00-0.34773767E 00-0.34758186E 00
0001000-0.34744036E 00-0.34730852E 00-0.34715199E 00-0.34688938E 00-0.34637403E 00
0001100-0.34537500E 00-0.34355336E 00-0.34044850E 00-0.33546513E 00-0.32788014E 00
0001200-0.31686181E 00-0.30151677E 00-0.28095663E 00-0.25438219E 00-0.22118187E 00
0001300-0.18805856E 00-0.16553348E 00-0.15063775E 00-0.14799178E 00-0.15063775E 00
EOF
q
```

```
redit pote14
LOADING POTE14   ZN LDA  a=2.5
REKEYED          DENS.
EDIT
p99
        TOP RECORD
0000100 0.19622348E-01 0.19616295E-01 0.19610655E-01 0.19606486E-01 0.19604601E-01
0000200 0.19605502E-01 0.19609205E-01 0.19615296E-01 0.19622795E-01 0.19630574E-01
0000300 0.19637261E-01 0.19641660E-01 0.19642901E-01 0.19640561E-01 0.19634932E-01
0000400 0.19626811E-01 0.19617513E-01 0.19608635E-01 0.19601759E-01 0.19598231E-01
0000500 0.19598857E-01 0.19603767E-01 0.19612316E-01 0.19623213E-01 0.19634608E-01
0000600 0.19644465E-01 0.19650891E-01 0.19652471E-01 0.19648574E-01 0.19639466E-01
0000700 0.19626386E-01 0.19611411E-01 0.19597072E-01 0.19586015E-01 0.19580442E-01
0000800 0.19581813E-01 0.19590352E-01 0.19605167E-01 0.19624036E-01 0.19643825E-01
0000900 0.19660972E-01 0.19672126E-01 0.19674718E-01 0.19667465E-01 0.19650750E-01
0001000 0.19626774E-01 0.19599229E-01 0.19572929E-01 0.19552913E-01 0.19543674E-01
0001100 0.19548155E-01 0.19567139E-01 0.19598830E-01 0.19638754E-01 0.19680370E-01
0001200 0.19715872E-01 0.19737575E-01 0.19739240E-01 0.19717515E-01 0.19672979E-01
0001300 0.19610710E-01 0.19540034E-01 0.19473508E-01 0.19425124E-01 0.19407704E-01
0001400 0.19430105E-01 0.19494273E-01 0.19592792E-01 0.19707356E-01 0.19808408E-01
0001500 0.19856509E-01 0.19805405E-01 0.19606750E-01 0.19216388E-01 0.18601179E-01
0001600 0.17745692E-01 0.16657494E-01 0.15369609E-01 0.13939209E-01 0.12442641E-01
0001700 0.10966931E-01 0.96001141E-02 0.84206760E-02 0.74815005E-02 0.68062879E-02
0001800 0.64011998E-02 0.62669814E-02 0.64011998E-02 0.68062879E-02 0.74815005E-02
EOF
q
redit pote15
LOADING POTE15
REKEYED          VEFF
EDIT
p99
        TOP RECORD
0000100-0.34812564E 00-0.34812611E 00-0.34812880E 00-0.34813797E 00-0.34813470E 00
0000200-0.34813827E 00-0.34814107E 00-0.34814477E 00-0.34813666E 00-0.34814018E 00
0000300-0.34815317E 00-0.34815747E 00-0.34816021E 00-0.34815693E 00-0.34816283E 00
0000400-0.34816563E 00-0.34815478E 00-0.34815168E 00-0.34814817E 00-0.34814125E 00
0000500-0.34813464E 00-0.34812725E 00-0.34812009E 00-0.34812653E 00-0.34812415E 00
0000600-0.34812963E 00-0.34813076E 00-0.34813941E 00-0.34814823E 00-0.34814942E 00
0000700-0.34814680E 00-0.34813702E 00-0.34812617E 00-0.34811968E 00-0.34810424E 00
0000800-0.34809536E 00-0.34808052E 00-0.34808093E 00-0.34808624E 00-0.34809512E 00
0000900-0.34811080E 00-0.34812170E 00-0.34813893E 00-0.34815425E 00-0.34816289E 00
0001000-0.34816289E 00-0.34815288E 00-0.34813213E 00-0.34810454E 00-0.34807259E 00
0001100-0.34804517E 00-0.34802735E 00-0.34802425E 00-0.34804040E 00-0.34807646E 00
0001200-0.34812784E 00-0.34818792E 00-0.34824467E 00-0.34828466E 00-0.34829336E 00
0001300-0.34826046E 00-0.34817880E 00-0.34805286E 00-0.34789509E 00-0.34772855E 00
0001400-0.34758145E 00-0.34747857E 00-0.34743530E 00-0.34744096E 00-0.34744829E 00
0001500-0.34735286E 00-0.34697819E 00-0.34605384E 00-0.34419632E 00-0.34089583E 00
0001600-0.33551019E 00-0.32727367E 00-0.31532383E 00-0.29874873E 00-0.27664924E 00
0001700-0.24823737E 00-0.21342206E 00-0.17906147E 00-0.15206933E 00-0.13313735E 00
0001800-0.12069595E 00-0.11834872E 00-0.12069595E 00-0.13313735E 00-0.15206933E 00
EOF
```




```
redit potel6
LOADING POTE16
REKEYED
EDIT
p99
```

ZN LDA a=3.0 DENS.

```
        TOP RECORD
0000100 0.19618534E-01 0.19611605E-01 0.19605979E-01 0.19602727E-01 0.19602567E-01
0000200 0.19605722E-01 0.19611813E-01 0.19619927E-01 0.19628808E-01 0.19636884E-01
0000300 0.19642700E-01 0.19645046E-01 0.19643355E-01 0.19637737E-01 0.19628927E-01
0000400 0.19618288E-01 0.19607652E-01 0.19598849E-01 0.19593619E-01 0.19593053E-01
0000500 0.19597553E-01 0.19606650E-01 0.19618981E-01 0.19632544E-01 0.19645050E-01
0000600 0.19654192E-01 0.19658148E-01 0.19655831E-01 0.19647315E-01 0.19633695E-01
0000700 0.19617066E-01 0.19600254E-01 0.19586280E-01 0.19577898E-01 0.19577052E-01
0000800 0.19584440E-01 0.19599415E-01 0.19619849E-01 0.19642428E-01 0.19663226E-01
0000900 0.19678246E-01 0.19684207E-01 0.19679196E-01 0.19663136E-01 0.19637845E-01
0001000 0.19607134E-01 0.19576110E-01 0.19550525E-01 0.19535773E-01 0.19535761E-01
0001100 0.19552212E-01 0.19583963E-01 0.19626889E-01 0.19674223E-01 0.19717526E-01
0001200 0.19747950E-01 0.19757818E-01 0.19742228E-01 0.19700382E-01 0.19636322E-01
0001300 0.19559059E-01 0.19481529E-01 0.19418932E-01 0.19386124E-01 0.19394457E-01
0001400 0.19448601E-01 0.19543640E-01 0.19662924E-01 0.19777559E-01 0.19847203E-01
0001500 0.19822963E-01 0.19652281E-01 0.19285299E-01 0.18682376E-01 0.17821629E-01
0001600 0.16705237E-01 0.15363019E-01 0.13851941E-01 0.12251049E-01 0.10652300E-01
0001700 0.91492124E-02 0.78243539E-02 0.67302771E-02 0.58862492E-02 0.52922592E-02
0001800 0.49406812E-02 0.48247837E-02 0.49406812E-02 0.52922592E-02 0.58862492E-02
EOF
q
redit potel7
LOADING POTE17
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812242E 00-0.34812921E 00-0.34814173E 00-0.34814173E 00-0.34814340E 00
0000200-0.34814662E 00-0.34814906E 00-0.34813893E 00-0.34813988E 00-0.34814388E 00
0000300-0.34814197E 00-0.34813988E 00-0.34813499E 00-0.34813827E 00-0.34813851E 00
0000400-0.34813780E 00-0.34813702E 00-0.34813607E 00-0.34814036E 00-0.34813756E 00
0000500-0.34814024E 00-0.34814078E 00-0.34814638E 00-0.34814030E 00-0.34814268E 00
0000600-0.34814197E 00-0.34815127E 00-0.34815395E 00-0.34815538E 00-0.34815770E 00
0000700-0.34816271E 00-0.34816116E 00-0.34816176E 00-0.34815949E 00-0.34815788E 00
0000800-0.34814459E 00-0.34813875E 00-0.34813535E 00-0.34813249E 00-0.34813243E 00
0000900-0.34813005E 00-0.34813547E 00-0.34814429E 00-0.34815937E 00-0.34816712E 00
0001000-0.34817600E 00-0.34817225E 00-0.34816140E 00-0.34814209E 00-0.34811801E 00
0001100-0.34809250E 00-0.34807134E 00-0.34806097E 00-0.34806782E 00-0.34809315E 00
0001200-0.34813774E 00-0.34819436E 00-0.34825420E 00-0.34830242E 00-0.34832287E 00
0001300-0.34829992E 00-0.34822333E 00-0.34809095E 00-0.34791213E 00-0.34770644E 00
0001400-0.34749973E 00-0.34731686E 00-0.34716767E 00-0.34702975E 00-0.34683263E 00
0001500-0.34643143E 00-0.34558505E 00-0.34392744E 00-0.34094620E 00-0.33596230E 00
0001600-0.32813120E 00-0.31646162E 00-0.29986304E 00-0.27721798E 00-0.24747592E 00
0001700-0.21002781E 00-0.17258364E 00-0.14241326E 00-0.11916411E 00-0.10282660E 00
0001800-0.92197895E-01-0.90035677E-01-0.92197895E-01-0.10282660E 00-0.11916411E 00
EOF
q
```

```
redit pote18
LOADING POTE18
REKEYED
EDIT
p99
```

ZN LDA a=4.0 DENS.

```
        TOP RECORD
0000100 0.19633308E-01 0.19624963E-01 0.19615892E-01 0.19607656E-01 0.19601837E-01
0000200 0.19599542E-01 0.19601382E-01 0.19607231E-01 0.19616317E-01 0.19627213E-01
0000300 0.19638125E-01 0.19647144E-01 0.19652557E-01 0.19653317E-01 0.19649055E-01
0000400 0.19640248E-01 0.19628279E-01 0.19615073E-01 0.19602958E-01 0.19594114E-01
0000500 0.19590277E-01 0.19592423E-01 0.19600429E-01 0.19613203E-01 0.19628625E-01
0000600 0.19644037E-01 0.19656587E-01 0.19663751E-01 0.19663807E-01 0.19656174E-01
0000700 0.19641597E-01 0.19622110E-01 0.19600898E-01 0.19581489E-01 0.19567441E-01
0000800 0.19561633E-01 0.19565634E-01 0.19579403E-01 0.19601159E-01 0.19627418E-01
0000900 0.19653764E-01 0.19675307E-01 0.19687761E-01 0.19688040E-01 0.19675031E-01
0001000 0.19650012E-01 0.19616589E-01 0.19580279E-01 0.19547660E-01 0.19525375E-01
0001100 0.19518767E-01 0.19530874E-01 0.19561589E-01 0.19607238E-01 0.19660875E-01
0001200 0.19713175E-01 0.19753806E-01 0.19773267E-01 0.19764792E-01 0.19725960E-01
0001300 0.19659925E-01 0.19575629E-01 0.19487031E-01 0.19411337E-01 0.19366082E-01
0001400 0.19365698E-01 0.19417688E-01 0.19519202E-01 0.19654483E-01 0.19793693E-01
0001500 0.19893792E-01 0.19901413E-01 0.19758288E-01 0.19408345E-01 0.18806133E-01
0001600 0.17925519E-01 0.16766526E-01 0.15359338E-01 0.13763428E-01 0.12061663E-01
0001700 0.10349642E-01 0.87216757E-02 0.72575323E-02 0.60060620E-02 0.49827024E-02
0001800 0.41816086E-02 0.35864038E-02 0.31781283E-02 0.29403588E-02 0.28624758E-02
EOF
q
redit pote19
LOADING POTE19
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812564E 00-0.34812534E 00-0.34812391E 00-0.34812367E 00-0.34811771E 00
0000200-0.34812176E 00-0.34812367E 00-0.34812737E 00-0.34812093E 00-0.34812808E 00
0000300-0.34814394E 00-0.34815317E 00-0.34815896E 00-0.34816015E 00-0.34817207E 00
0000400-0.34817946E 00-0.34817004E 00-0.34816819E 00-0.34816337E 00-0.34815311E 00
0000500-0.34814304E 00-0.34813160E 00-0.34812361E 00-0.34812659E 00-0.34811938E 00
0000600-0.34812474E 00-0.34811985E 00-0.34812582E 00-0.34813076E 00-0.34813213E 00
0000700-0.34812653E 00-0.34811556E 00-0.34809977E 00-0.34808969E 00-0.34806401E 00
0000800-0.34804767E 00-0.34802365E 00-0.34801507E 00-0.34801519E 00-0.34802443E 00
0000900-0.34803939E 00-0.34805292E 00-0.34807748E 00-0.34810305E 00-0.34812504E 00
0001000-0.34813857E 00-0.34814262E 00-0.34813321E 00-0.34811467E 00-0.34808803E 00
0001100-0.34806240E 00-0.34804261E 00-0.34803671E 00-0.34804946E 00-0.34808296E 00
0001200-0.34813428E 00-0.34819669E 00-0.34825850E 00-0.34830582E 00-0.34832168E 00
0001300-0.34829277E 00-0.34821135E 00-0.34807879E 00-0.34790754E 00-0.34772491E 00
0001400-0.34756333E 00-0.34745669E 00-0.34742939E 00-0.34748000E 00-0.34756893E 00
0001500-0.34759682E 00-0.34738582E 00-0.34665632E 00-0.34500366E 00-0.34187973E 00
0001600-0.33658254E 00-0.32826018E 00-0.31593549E 00-0.29855007E 00-0.27503037E 00
0001700-0.24493545E 00-0.20793402E 00-0.17003024E 00-0.13738656E 00-0.10988057E 00
0001800-0.87613285E-01-0.70357084E-01-0.58127884E-01-0.50260391E-01-0.48465177E-01
EOF
q
```

```
redit pote20
LOADING POTE20
REKEYED
EDIT
p99
```

ZN LDA a=5.0

DENS

```
        TOP RECORD
0000100 0.19616585E-01 0.19605801E-01 0.19597303E-01 0.19592654E-01 0.19592773E-01
0000200 0.19597817E-01 0.19607075E-01 0.19619092E-01 0.19631892E-01 0.19643195E-01
0000300 0.19650977E-01 0.19653723E-01 0.19650713E-01 0.19642260E-01 0.19629601E-01
0000400 0.19614857E-01 0.19600574E-01 0.19589413E-01 0.19583534E-01 0.19584313E-01
0000500 0.19592043E-01 0.19605760E-01 0.19623391E-01 0.19641995E-01 0.19658335E-01
0000600 0.19669339E-01 0.19672737E-01 0.19667450E-01 0.19653905E-01 0.19634016E-01
0000700 0.19610956E-01 0.19588705E-01 0.19571327E-01 0.19562304E-01 0.19563843E-01
0000800 0.19576438E-01 0.19598629E-01 0.19627038E-01 0.19657008E-01 0.19683100E-01
0000900 0.19700252E-01 0.19704595E-01 0.19694209E-01 0.19669726E-01 0.19634411E-01
0001000 0.19593813E-01 0.19554999E-01 0.19525331E-01 0.19511312E-01 0.19517146E-01
0001100 0.19543827E-01 0.19588612E-01 0.19644987E-01 0.19703574E-01 0.19753385E-01
0001200 0.19783679E-01 0.19786067E-01 0.19756269E-01 0.19695591E-01 0.19611496E-01
0001300 0.19517083E-01 0.19429490E-01 0.19367229E-01 0.19346584E-01 0.19377772E-01
0001400 0.19461140E-01 0.19584250E-01 0.19720174E-01 0.19827940E-01 0.19854967E-01
0001500 0.19741967E-01 0.19429877E-01 0.18868323E-01 0.18024541E-01 0.16891167E-01
0001600 0.15491396E-01 0.13879690E-01 0.12136940E-01 0.10360595E-01 0.86510926E-02
0001700 0.70967227E-02 0.57518408E-02 0.46322607E-02 0.37294521E-02 0.30225692E-02
0001800 0.24869214E-02 0.20983263E-02 0.18361874E-02 0.16851551E-02 0.16359009E-02
EOF
q
redit pote21
LOADING POTE21
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34809452E 00-0.34808815E 00-0.34808153E 00-0.34808171E 00-0.34808332E 00
0000200-0.34808618E 00-0.34808731E 00-0.34809691E 00-0.34810925E 00-0.34811825E 00
0000300-0.34811968E 00-0.34812719E 00-0.34813154E 00-0.34813648E 00-0.34813279E 00
0000400-0.34812981E 00-0.34812987E 00-0.34812796E 00-0.34812915E 00-0.34812528E 00
0000500-0.34812558E 00-0.34813029E 00-0.34813344E 00-0.34814095E 00-0.34813899E 00
0000600-0.34814012E 00-0.34814268E 00-0.34814149E 00-0.34813786E 00-0.34813690E 00
0000700-0.34813356E 00-0.34813374E 00-0.34813112E 00-0.34813231E 00-0.34812516E 00
0000800-0.34812117E 00-0.34812027E 00-0.34811807E 00-0.34812081E 00-0.34811431E 00
0000900-0.34811628E 00-0.34812492E 00-0.34812903E 00-0.34813839E 00-0.34815055E 00
0001000-0.34815300E 00-0.34815472E 00-0.34814614E 00-0.34813219E 00-0.34811336E 00
0001100-0.34809285E 00-0.34807575E 00-0.34806854E 00-0.34807545E 00-0.34810054E 00
0001200-0.34814304E 00-0.34819818E 00-0.34825546E 00-0.34830195E 00-0.34832031E 00
0001300-0.34829712E 00-0.34822053E 00-0.34809011E 00-0.34791380E 00-0.34770983E 00
0001400-0.34749806E 00-0.34729093E 00-0.34707713E 00-0.34680200E 00-0.34634280E 00
0001500-0.34548587E 00-0.34389317E 00-0.34107608E 00-0.33636850E 00-0.32891113E 00
0001600-0.31765896E 00-0.30141300E 00-0.27888519E 00-0.24878508E 00-0.20992529E 00
0001700-0.16962218E 00-0.13540924E 00-0.10648686E 00-0.82196474E-01-0.61404586E-01
0001800-0.44733934E-01-0.31891093E-01-0.22655275E-01-0.16835116E-01-0.15331045E-01
EOF
q
```

```
redit pote22
LOADING POTE22
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.19631371E-01 0.19618593E-01 0.19605480E-01 0.19594308E-01 0.19587174E-01
0000200 0.19585550E-01 0.19589990E-01 0.19600026E-01 0.19614201E-01 0.19630216E-01
0000300 0.19645400E-01 0.19656990E-01 0.19662835E-01 0.19661695E-01 0.19653365E-01
0000400 0.19638997E-01 0.19620869E-01 0.19601997E-01 0.19585662E-01 0.19574914E-01
0000500 0.19571938E-01 0.19577663E-01 0.19591536E-01 0.19611493E-01 0.19634314E-01
0000600 0.19656047E-01 0.19672826E-01 0.19681301E-01 0.19679502E-01 0.19667119E-01
0000700 0.19645762E-01 0.19618772E-01 0.19590627E-01 0.19566342E-01 0.19550603E-01
0000800 0.19546777E-01 0.19556459E-01 0.19578766E-01 0.19610584E-01 0.19646771E-01
0000900 0.19681029E-01 0.19706994E-01 0.19719251E-01 0.19714464E-01 0.19692093E-01
0001000 0.19654810E-01 0.19608214E-01 0.19560155E-01 0.19519426E-01 0.19494280E-01
0001100 0.19490905E-01 0.19512050E-01 0.19556101E-01 0.19617058E-01 0.19685041E-01
0001200 0.19747730E-01 0.19792333E-01 0.19807961E-01 0.19787874E-01 0.19731320E-01
0001300 0.19644547E-01 0.19540548E-01 0.19437648E-01 0.19356661E-01 0.19317094E-01
0001400 0.19332826E-01 0.19407772E-01 0.19532338E-01 0.19681338E-01 0.19813880E-01
0001500 0.19875724E-01 0.19804325E-01 0.19536100E-01 0.19015528E-01 0.18204711E-01
0001600 0.17092023E-01 0.15697721E-01 0.14074896E-01 0.12304612E-01 0.10485698E-01
0001700 0.87206475E-02 0.71000271E-02 0.56806393E-02 0.44807903E-02 0.34934797E-02
0001800 0.26979162E-02 0.20674232E-02 0.15743836E-02 0.11930109E-02 0.90067158E-03
0001900 0.67829341E-03 0.51027117E-03 0.38411631E-03 0.29001315E-03 0.22035750E-03
0002000 0.16934775E-03 0.13262669E-03 0.10699201E-03 0.90170390E-04 0.80651080E-04
0002100 0.77571545E-04 0.80651080E-04 0.90170390E-04 0.10699201E-03 0.13262669E-03
EOF
q
redit pote23
LOADING POTE23
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.34812516E 00-0.34812391E 00-0.34813362E 00-0.34812468E 00-0.34812498E 00
0000200-0.34812790E 00-0.34813195E 00-0.34812093E 00-0.34812665E 00-0.34814280E 00
0000300-0.34815186E 00-0.34815890E 00-0.34816360E 00-0.34818017E 00-0.34819114E 00
0000400-0.34818631E 00-0.34818792E 00-0.34818286E 00-0.34817582E 00-0.34816360E 00
0000500-0.34815025E 00-0.34813857E 00-0.34814149E 00-0.34813643E 00-0.34814596E 00
0000600-0.34814799E 00-0.34816277E 00-0.34817821E 00-0.34819174E 00-0.34820205E 00
0000700-0.34820521E 00-0.34819841E 00-0.34819686E 00-0.34817708E 00-0.34816188E 00
0000800-0.34813380E 00-0.34812069E 00-0.34811562E 00-0.34811991E 00-0.34813279E 00
0000900-0.34814519E 00-0.34817201E 00-0.34820205E 00-0.34822875E 00-0.34824556E 00
0001000-0.34824955E 00-0.34823501E 00-0.34820455E 00-0.34815925E 00-0.34810859E 00
0001100-0.34806013E 00-0.34802407E 00-0.34800988E 00-0.34802294E 00-0.34806383E 00
0001200-0.34812909E 00-0.34820771E 00-0.34828585E 00-0.34834361E 00-0.34836257E 00
0001300-0.34832639E 00-0.34822792E 00-0.34807009E 00-0.34787136E 00-0.34766102E 00
0001400-0.34747273E 00-0.34733778E 00-0.34726638E 00-0.34723550E 00-0.34716964E 00
0001500-0.34692138E 00-0.34625071E 00-0.34479725E 00-0.34205866E 00-0.33737087E 00
0001600-0.32990128E 00-0.31866020E 00-0.30253482E 00-0.28034389E 00-0.25090998E 00
0001700-0.21314007E 00-0.17384130E 00-0.13993430E 00-0.11063808E 00-0.85245609E-01
0001800-0.63138068E-01-0.43791465E-01-0.26764449E-01-0.11698436E-01 0.16987547E-02
0001900 0.13661653E-01 0.24374757E-01 0.33978898E-01 0.42574529E-01 0.50224654E-01
0002000 0.56939658E-01 0.62696278E-01 0.67411542E-01 0.70951939E-01 0.73179781E-01
0002100 0.73917627E-01 0.73179781E-01 0.70951939E-01 0.67411542E-01 0.62696278E-01
EOF
q
```

ZN LDA a=10.0 DENS.

VEFF

```
redit pote24
LOADING POTE24
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.19632339E-01 0.19617643E-01 0.19602455E-01 0.19589268E-01 0.19580312E-01
0000200 0.19577164E-01 0.19580439E-01 0.19589711E-01 0.19603491E-01 0.19619498E-01
0000300 0.19634925E-01 0.19646980E-01 0.19653425E-01 0.19652933E-01 0.19645292E-01
0000400 0.19631535E-01 0.19613966E-01 0.19595575E-01 0.19579682E-01 0.19569571E-01
0000500 0.19566804E-01 0.19572981E-01 0.19587338E-01 0.19607805E-01 0.19631170E-01
0000600 0.19653410E-01 0.19670624E-01 0.19679438E-01 0.19677848E-01 0.19665524E-01
0000700 0.19644104E-01 0.19616921E-01 0.19588552E-01 0.19564036E-01 0.19548129E-01
0000800 0.19544315E-01 0.19554134E-01 0.19576777E-01 0.19609079E-01 0.19645896E-01
0000900 0.19680858E-01 0.19707508E-01 0.19720387E-01 0.19716069E-01 0.19693982E-01
0001000 0.19656748E-01 0.19609988E-01 0.19561507E-01 0.19520219E-01 0.19494437E-01
0001100 0.19490402E-01 0.19510977E-01 0.19554675E-01 0.19615505E-01 0.19683640E-01
0001200 0.19746710E-01 0.19791912E-01 0.19808244E-01 0.19788835E-01 0.19732852E-01
0001300 0.19646380E-01 0.19542348E-01 0.19439042E-01 0.19357279E-01 0.19316651E-01
0001400 0.19331191E-01 0.19405004E-01 0.19528717E-01 0.19677322E-01 0.19810155E-01
0001500 0.19873057E-01 0.19803539E-01 0.19537888E-01 0.19020408E-01 0.18212888E-01
0001600 0.17103337E-01 0.15711583E-01 0.14090449E-01 0.12320802E-01 0.10501496E-01
0001700 0.87351874E-02 0.71127154E-02 0.56911558E-02 0.44889748E-02 0.34992932E-02
0001800 0.27013996E-02 0.20686665E-02 0.15735072E-02 0.11901415E-02 0.89592580E-03
0001900 0.67175645E-03 0.50198450E-03 0.37405430E-03 0.27806195E-03 0.20629072E-03
0002000 0.15279213E-03 0.11301752E-03 0.83512088E-04 0.61667088E-04 0.45521898E-04
0002100 0.33609016E-04 0.24834182E-04 0.18384235E-04 0.13657036E-04 0.10208372E-04
0002200 0.77124932E-05 0.59325284E-05 0.46988653E-05 0.38936014E-05 0.34394716E-05
0002300 0.32928010E-05 0.34394716E-05 0.38936014E-05 0.46988653E-05 0.59325284E-05
EOF
q
redit pote25
LOADING POTE25
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.34812540E 00-0.34808493E 00-0.34806365E 00-0.34803617E 00-0.34802192E 00
0000200-0.34801441E 00-0.34801155E 00-0.34799993E 00-0.34800673E 00-0.34802324E 00
0000300-0.34803540E 00-0.34804577E 00-0.34805882E 00-0.34808046E 00-0.34809929E 00
0000400-0.34810239E 00-0.34810758E 00-0.34810907E 00-0.34810734E 00-0.34809965E 00
0000500-0.34809166E 00-0.34808552E 00-0.34809208E 00-0.34808969E 00-0.34810519E 00
0000600-0.34810978E 00-0.34813058E 00-0.34814894E 00-0.34816605E 00-0.34817642E 00
0000700-0.34817922E 00-0.34817654E 00-0.34817278E 00-0.34815222E 00-0.34814113E 00
0000800-0.34811580E 00-0.34810442E 00-0.34810019E 00-0.34810406E 00-0.34811777E 00
0000900-0.34813070E 00-0.34815526E 00-0.34818351E 00-0.34820920E 00-0.34822619E 00
0001000-0.34823185E 00-0.34821904E 00-0.34819108E 00-0.34814823E 00-0.34809995E 00
0001100-0.34805220E 00-0.34801596E 00-0.34799987E 00-0.34800953E 00-0.34804648E 00
0001200-0.34810776E 00-0.34818339E 00-0.34825933E 00-0.34831727E 00-0.34833950E 00
0001300-0.34830880E 00-0.34821695E 00-0.34806681E 00-0.34787387E 00-0.34766740E 00
0001400-0.34748006E 00-0.34734225E 00-0.34726512E 00-0.34722674E 00-0.34715337E 00
0001500-0.34690017E 00-0.34622920E 00-0.34478307E 00-0.34206045E 00-0.33739883E 00
0001600-0.32996464E 00-0.31876510E 00-0.30268258E 00-0.28052866E 00-0.25112152E 00
0001700-0.21336573E 00-0.17408782E 00-0.14022523E 00-0.11099190E 00-0.85672259E-01
0001800-0.63641846E-01-0.44369135E-01-0.27406648E-01-0.12387436E-01 0.99001662E-03
0001900 0.12971945E-01 0.23758821E-01 0.33513851E-01 0.42370211E-01 0.50437871E-01
0002000 0.57804186E-01 0.64544439E-01 0.70721209E-01 0.76384604E-01 0.81577003E-01
0002100 0.86333990E-01 0.90701878E-01 0.94708920E-01 0.98363042E-01 0.10166454E 00
0002200 0.10461116E 00 0.10717762E 00 0.10938346E 00 0.11098289E 00 0.11199051E 00
0002300 0.11233902E 00 0.11199051E 00 0.11098289E 00 0.10938346E 00 0.10717762E 00
EOF
q
```

ZN LDA a=15.0 DENS.

VEFF

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
```

ZN NL a=0.25 DENS.

```
        TOP RECORD
0000100 0.19620989E-01 0.19621558E-01 0.19622102E-01 0.19622561E-01 0.19622926E-01
0000200 0.19623201E-01 0.19623365E-01 0.19623406E-01 0.19623317E-01 0.19623123E-01
0000300 0.19622859E-01 0.19622497E-01 0.19622043E-01 0.19621540E-01 0.19621029E-01
0000400 0.19620501E-01 0.19619994E-01 0.19619543E-01 0.19619174E-01 0.19618921E-01
0000500 0.19618772E-01 0.19618791E-01 0.19618951E-01 0.19619297E-01 0.19619770E-01
0000600 0.19620404E-01 0.19621167E-01 0.19622017E-01 0.19622967E-01 0.19623958E-01
0000700 0.19624952E-01 0.19625925E-01 0.19626822E-01 0.19627593E-01 0.19628230E-01
0000800 0.19628678E-01 0.19628894E-01 0.19628890E-01 0.19628637E-01 0.19628141E-01
0000900 0.19627389E-01 0.19626446E-01 0.19625328E-01 0.19624066E-01 0.19622698E-01
0001000 0.19621324E-01 0.19619983E-01 0.19618720E-01 0.19617606E-01 0.19616690E-01
0001100 0.19616026E-01 0.19615654E-01 0.19615598E-01 0.19615874E-01 0.19616500E-01
0001200 0.19617442E-01 0.19618709E-01 0.19620221E-01 0.19621942E-01 0.19623797E-01
0001300 0.19625701E-01 0.19627575E-01 0.19629307E-01 0.19630823E-01 0.19632023E-01
0001400 0.19632865E-01 0.19633204E-01 0.19633029E-01 0.19632325E-01 0.19631065E-01
0001500 0.19629247E-01 0.19626934E-01 0.19624181E-01 0.19621100E-01 0.19617770E-01
0001600 0.19614380E-01 0.19611083E-01 0.19608002E-01 0.19605320E-01 0.19603234E-01
0001700 0.19601829E-01 0.19601289E-01 0.19601688E-01 0.19603070E-01 0.19605424E-01
0001800 0.19608684E-01 0.19612730E-01 0.19617356E-01 0.19622300E-01 0.19627135E-01
0001900 0.19631416E-01 0.19634660E-01 0.19636236E-01 0.19635476E-01 0.19631639E-01
0002000 0.19624013E-01 0.19611754E-01 0.19594122E-01 0.19570332E-01 0.19539680E-01
0002100 0.19501485E-01 0.19455247E-01 0.19400515E-01 0.19337043E-01 0.19264750E-01
0002200 0.19183777E-01 0.19094490E-01 0.18997472E-01 0.18893667E-01 0.18784225E-01
0002300 0.18670637E-01 0.18554647E-01 0.18438287E-01 0.18323939E-01 0.18214226E-01
0002400 0.18112030E-01 0.18020499E-01 0.17942958E-01 0.17883014E-01 0.17844282E-01
0002500 0.17831016E-01 0.17844282E-01 0.17883014E-01 0.17942958E-01 0.18020499E-01
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812480E 00-0.34812379E 00-0.34812641E 00-0.34812504E 00-0.34811801E 00
0000200-0.34811699E 00-0.34812218E 00-0.34811956E 00-0.34811503E 00-0.34811199E 00
0000300-0.34811854E 00-0.34811735E 00-0.34812230E 00-0.34812278E 00-0.34812880E 00
0000400-0.34812957E 00-0.34813428E 00-0.34813273E 00-0.34813648E 00-0.34813768E 00
0000500-0.34814006E 00-0.34813839E 00-0.34814239E 00-0.34814829E 00-0.34814906E 00
0000600-0.34814513E 00-0.34814590E 00-0.34815204E 00-0.34815162E 00-0.34814554E 00
0000700-0.34814525E 00-0.34815013E 00-0.34814990E 00-0.34815490E 00-0.34815478E 00
0000800-0.34816051E 00-0.34815955E 00-0.34816474E 00-0.34816664E 00-0.34816307E 00
0000900-0.34816116E 00-0.34816080E 00-0.34815997E 00-0.34815907E 00-0.34815890E 00
0001000-0.34815866E 00-0.34815788E 00-0.34815717E 00-0.34815651E 00-0.34815663E 00
0001100-0.34815490E 00-0.34815252E 00-0.34814984E 00-0.34814781E 00-0.34814471E 00
0001200-0.34814167E 00-0.34813923E 00-0.34813595E 00-0.34813327E 00-0.34813124E 00
0001300-0.34812874E 00-0.34812683E 00-0.34812623E 00-0.34812564E 00-0.34812599E 00
0001400-0.34812707E 00-0.34812850E 00-0.34813100E 00-0.34813386E 00-0.34813797E 00
0001500-0.34814143E 00-0.34814519E 00-0.34814912E 00-0.34815270E 00-0.34815538E 00
0001600-0.34815729E 00-0.34815830E 00-0.34815884E 00-0.34815735E 00-0.34815395E 00
0001700-0.34814984E 00-0.34814382E 00-0.34813666E 00-0.34812641E 00-0.34811622E 00
0001800-0.34810311E 00-0.34808922E 00-0.34807271E 00-0.34805411E 00-0.34803182E 00
0001900-0.34800726E 00-0.34797657E 00-0.34793895E 00-0.34789318E 00-0.34783566E 00
0002000-0.34776360E 00-0.34767139E 00-0.34755522E 00-0.34740812E 00-0.34722257E 00
0002100-0.34699231E 00-0.34670645E 00-0.34635460E 00-0.34592634E 00-0.34540814E 00
0002200-0.34478766E 00-0.34405023E 00-0.34318101E 00-0.34216547E 00-0.34098780E 00
0002300-0.33963352E 00-0.33808798E 00-0.33633721E 00-0.33436936E 00-0.33217353E 00
0002400-0.32974118E 00-0.32706773E 00-0.32414591E 00-0.32118225E 00-0.31711197E 00
0002500-0.31640929E 00-0.31711197E 00-0.32118225E 00-0.32414591E 00-0.32706773E 00
```

```
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
```

ZN NL a=0.5

DENS.

```
        TOP RECORD
0000100+0.19623950E-01+0.19625810E-01+0.19627040E-01+0.19627480E-01+0.19626960E-01
0000200+0.19625540E-01+0.19623440E-01+0.19620920E-01+0.19618420E-01+0.19616380E-01
0000300+0.19615210E-01+0.19615200E-01+0.19616420E-01+0.19618760E-01+0.19621880E-01
0000400+0.19625290E-01+0.19628380E-01+0.19630520E-01+0.19631230E-01+0.19630190E-01
0000500+0.19627450E-01+0.19623340E-01+0.19618410E-01+0.19613500E-01+0.19609490E-01
0000600+0.19607210E-01+0.19607290E-01+0.19609980E-01+0.19615110E-01+0.19627050E-01
0000700+0.19629680E-01+0.19636730E-01+0.19641740E-01+0.19643500E-01+0.19641200E-01
0000800+0.19634730E-01+0.19624710E-01+0.19612570E-01+0.19600480E-01+0.19590960E-01
0000900+0.19586410E-01+0.19588690E-01+0.19598440E-01+0.19614550E-01+0.19633690E-01
0001000+0.19650040E-01+0.19655410E-01+0.19639550E-01+0.19590870E-01+0.19497630E-01
0001100+0.19349250E-01+0.19138000E-01+0.18860550E-01+0.18519670E-01+0.18125130E-01
0001200+0.17694710E-01+0.17254110E-01+0.16846470E-01+0.16481440E-01+0.16232880E-01
0001300+0.16145610E-01+0.16232880E-01+0.16481440E-01+0.16836470E-01+0.17254110E-01
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812440E+00-0.34812850E+00-0.34811900E+00-0.34812270E+00-0.34811310E+00
0000200-0.34811970E+00-0.34812490E+00-0.34812960E+00-0.34813350E+00-0.34813380E+00
0000300-0.34813140E+00-0.34813640E+00-0.34812930E+00-0.34812890E+00-0.34811710E+00
0000400-0.34811660E+00-0.34811600E+00-0.34811380E+00-0.34811680E+00-0.34811100E+00
0000500-0.34811400E+00-0.34811950E+00-0.34812570E+00-0.34813120E+00-0.34813550E+00
0000600-0.34813520E+00-0.34813170E+00-0.34812390E+00-0.34811430E+00-0.34810330E+00
0000700-0.34809370E+00-0.34808830E+00-0.34808920E+00-0.34809650E+00-0.34811090E+00
0000800-0.34810380E+00-0.34815490E+00-0.34817830E+00-0.34819880E+00-0.34824110E+00
0000900-0.34821280E+00-0.34820030E+00-0.34817260E+00-0.34812750E+00-0.34805880E+00
0001000-0.34795710E+00-0.34708280E+00-0.34756280E+00-0.34718360E+00-0.34658750E+00
0001100-0.34566730E+00-0.34428390E+00-0.34226780E+00-0.33942180E+00-0.33553170E+00
0001200-0.33037670E+00-0.32374920E+00-0.31544760E+00-0.30616780E+00-0.29178510E+00
0001300-0.28914140E+00-0.29178510E+00-0.30610780E+00-0.31544760E+00-0.32374920E+00
EOF
q
```

```
redit pote6
LOADING POTE6   ZN NL a=0.75
REKEYED
EDIT            DENS.
p99
        TOP RECORD
0000100 0.19624867E-01 0.19626413E-01 0.19627843E-01 0.19629076E-01 0.19630060E-01
0000200 0.19630756E-01 0.19631125E-01 0.19631140E-01 0.19630797E-01 0.19630115E-01
0000300 0.19629061E-01 0.19627720E-01 0.19626122E-01 0.19624330E-01 0.19622430E-01
0000400 0.19620474E-01 0.19618556E-01 0.19616790E-01 0.19615233E-01 0.19613970E-01
0000500 0.19613054E-01 0.19612588E-01 0.19612566E-01 0.19613001E-01 0.19613922E-01
0000600 0.19615274E-01 0.19617058E-01 0.19619189E-01 0.19621581E-01 0.19624125E-01
0000700 0.19626759E-01 0.19629333E-01 0.19631740E-01 0.19633852E-01 0.19635580E-01
0000800 0.19636773E-01 0.19637406E-01 0.19637410E-01 0.19636709E-01 0.19635376E-01
0000900 0.19633379E-01 0.19630805E-01 0.19627713E-01 0.19624267E-01 0.19620575E-01
0001000 0.19616764E-01 0.19613035E-01 0.19609530E-01 0.19606452E-01 0.19603945E-01
0001100 0.19602139E-01 0.19601170E-01 0.19601122E-01 0.19602049E-01 0.19603956E-01
0001200 0.19606829E-01 0.19610584E-01 0.19615080E-01 0.19620184E-01 0.19625686E-01
0001300 0.19631334E-01 0.19636907E-01 0.19642118E-01 0.19646700E-01 0.19650403E-01
0001400 0.19652989E-01 0.19654267E-01 0.19654047E-01 0.19652311E-01 0.19648947E-01
0001500 0.19644070E-01 0.19637741E-01 0.19630201E-01 0.19621730E-01 0.19612651E-01
0001600 0.19603383E-01 0.19594371E-01 0.19586075E-01 0.19579012E-01 0.19573621E-01
0001700 0.19570351E-01 0.19569527E-01 0.19571431E-01 0.19576162E-01 0.19583713E-01
0001800 0.19593887E-01 0.19606266E-01 0.19620247E-01 0.19634973E-01 0.19649383E-01
0001900 0.19662175E-01 0.19671816E-01 0.19676596E-01 0.19674610E-01 0.19663818E-01
0002000 0.19642126E-01 0.19607324E-01 0.19557297E-01 0.19489974E-01 0.19403450E-01
0002100 0.19296039E-01 0.19166391E-01 0.19013532E-01 0.18836927E-01 0.18636551E-01
0002200 0.18412966E-01 0.18167410E-01 0.17901685E-01 0.17618291E-01 0.17320439E-01
0002300 0.17011978E-01 0.16697373E-01 0.16381729E-01 0.16070690E-01 0.15770368E-01
0002400 0.15487351E-01 0.15228603E-01 0.15001412E-01 0.14813427E-01 0.14672540E-01
0002500 0.14585271E-01 0.14555935E-01 0.14585271E-01 0.14672540E-01 0.14813427E-01
EOF
q
redit pote7
LOADING POTE7
REKEYED         VEFF
EDIT
p99
        TOP RECORD
0000100-0.34812498E 00-0.34812778E 00-0.34812289E 00-0.34811455E 00-0.34811324E 00
0000200-0.34811735E 00-0.34811574E 00-0.34810710E 00-0.34810591E 00-0.34811276E 00
0000300-0.34811097E 00-0.34811664E 00-0.34812033E 00-0.34812582E 00-0.34812766E 00
0000400-0.34813291E 00-0.34813321E 00-0.34813845E 00-0.34813893E 00-0.34814149E 00
0000500-0.34814084E 00-0.34814447E 00-0.34815001E 00-0.34815079E 00-0.34814316E 00
0000600-0.34814048E 00-0.34814441E 00-0.34813857E 00-0.34813124E 00-0.34812510E 00
0000700-0.34812558E 00-0.34812504E 00-0.34812516E 00-0.34812260E 00-0.34812880E 00
0000800-0.34812504E 00-0.34812915E 00-0.34812897E 00-0.34812802E 00-0.34812915E 00
0000900-0.34813237E 00-0.34813565E 00-0.34814018E 00-0.34814495E 00-0.34815085E 00
0001000-0.34815472E 00-0.34815919E 00-0.34816343E 00-0.34816676E 00-0.34816837E 00
0001100-0.34816837E 00-0.34816635E 00-0.34816384E 00-0.34815878E 00-0.34815240E 00
0001200-0.34814525E 00-0.34813720E 00-0.34812772E 00-0.34811819E 00-0.34810895E 00
0001300-0.34809959E 00-0.34809214E 00-0.34808528E 00-0.34808105E 00-0.34807968E 00
0001400-0.34807938E 00-0.34808266E 00-0.34808886E 00-0.34809792E 00-0.34810895E 00
0001500-0.34812254E 00-0.34813833E 00-0.34815514E 00-0.34817255E 00-0.34819061E 00
0001600-0.34820777E 00-0.34822440E 00-0.34823895E 00-0.34824985E 00-0.34825855E 00
0001700-0.34826338E 00-0.34826344E 00-0.34825814E 00-0.34824872E 00-0.34823281E 00
0001800-0.34821153E 00-0.34818268E 00-0.34814644E 00-0.34810090E 00-0.34804529E 00
0001900-0.34797645E 00-0.34789050E 00-0.34778368E 00-0.34764940E 00-0.34748036E 00
0002000-0.34726745E 00-0.34699661E 00-0.34665662E 00-0.34622896E 00-0.34569466E 00
0002100-0.34503084E 00-0.34421390E 00-0.34321409E 00-0.34200209E 00-0.34054393E 00
0002200-0.33880419E 00-0.33674645E 00-0.33433187E 00-0.33152121E 00-0.32827592E 00
0002300-0.32455772E 00-0.32032937E 00-0.31555676E 00-0.31020826E 00-0.30425614E 00
0002400-0.29767740E 00-0.29045504E 00-0.28258377E 00-0.27403349E 00-0.26676852E 00
0002500-0.26180476E 00-0.26117957E 00-0.26180476E 00-0.26676852E 00-0.27403349E 00
EOF
```

```
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.19625247E-01 0.19629404E-01 0.19632783E-01 0.19634709E-01 0.19634679E-01
0000200 0.19632507E-01 0.19628525E-01 0.19623309E-01 0.19617721E-01 0.19612759E-01
0000300 0.19609347E-01 0.19608021E-01 0.19609150E-01 0.19612748E-01 0.19618344E-01
0000400 0.19625094E-01 0.19631863E-01 0.19637380E-01 0.19640461E-01 0.19640319E-01
0000500 0.19636650E-01 0.19629724E-01 0.19620445E-01 0.19610185E-01 0.19600771E-01
0000600 0.19593973E-01 0.19591264E-01 0.19593686E-01 0.19601263E-01 0.19613232E-01
0000700 0.19627906E-01 0.19642796E-01 0.19655105E-01 0.19662157E-01 0.19661829E-01
0000800 0.19653130E-01 0.19636597E-01 0.19614346E-01 0.19590016E-01 0.19568361E-01
0000900 0.19554395E-01 0.19552547E-01 0.19565422E-01 0.19592706E-01 0.19630089E-01
0001000 0.19668728E-01 0.19694980E-01 0.19690942E-01 0.19635648E-01 0.19506920E-01
0001100 0.19283954E-01 0.18950250E-01 0.18496674E-01 0.17924245E-01 0.17246176E-01
0001200 0.16488735E-01 0.15690926E-01 0.14902838E-01 0.14183071E-01 0.13596315E-01
0001300 0.13209470E-01 0.13077375E-01 0.13209470E-01 0.13596315E-01 0.14183071E-01
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.34810770E 00-0.34811682E 00-0.34812474E 00-0.34813273E 00-0.34814191E 00
0000200-0.34812564E 00-0.34811872E 00-0.34810537E 00-0.34810477E 00-0.34809887E 00
0000300-0.34814394E 00-0.34815216E 00-0.34814358E 00-0.34814078E 00-0.34812146E 00
0000400-0.34811270E 00-0.34810299E 00-0.34809381E 00-0.34808952E 00-0.34808338E 00
0000500-0.34808904E 00-0.34810001E 00-0.34811330E 00-0.34812611E 00-0.34813738E 00
0000600-0.34814066E 00-0.34813702E 00-0.34812355E 00-0.34810340E 00-0.34807807E 00
0000700-0.34805197E 00-0.34803104E 00-0.34802014E 00-0.34802222E 00-0.34804046E 00
0000800-0.34807277E 00-0.34811765E 00-0.34816843E 00-0.34821945E 00-0.34826189E 00
0000900-0.34828925E 00-0.34829402E 00-0.34827173E 00-0.34821838E 00-0.34812748E 00
0001000-0.34798712E 00-0.34777188E 00-0.34743583E 00-0.34689897E 00-0.34603989E 00
0001100-0.34468532E 00-0.34260154E 00-0.33949673E 00-0.33502609E 00-0.32880378E 00
0001200-0.32042778E 00-0.30950761E 00-0.29569691E 00-0.27873141E 00-0.25894082E 00
0001300-0.24048108E 00-0.23810244E 00-0.24048108E 00-0.25894082E 00-0.27873141E 00
EOF
q
```

ZN NL a=10 DENS.

VEFF

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
```

ZN NL a=1.5 DENS.

```
        TOP RECORD
0000100 0.19616932E-01 0.19614454E-01 0.19613069E-01 0.19613080E-01 0.19614577E-01
0000200 0.19617368E-01 0.19621026E-01 0.19624952E-01 0.19628529E-01 0.19631106E-01
0000300 0.19632157E-01 0.19631427E-01 0.19628979E-01 0.19625206E-01 0.19620642E-01
0000400 0.19616093E-01 0.19612405E-01 0.19610278E-01 0.19610163E-01 0.19612215E-01
0000500 0.19616228E-01 0.19621596E-01 0.19627448E-01 0.19632738E-01 0.19636519E-01
0000600 0.19637931E-01 0.19636560E-01 0.19632474E-01 0.19626170E-01 0.19618593E-01
0000700 0.19611057E-01 0.19604888E-01 0.19601334E-01 0.19601192E-01 0.19604750E-01
0000800 0.19611694E-01 0.19621033E-01 0.19631289E-01 0.19640587E-01 0.19647148E-01
0000900 0.19649528E-01 0.19646872E-01 0.19639168E-01 0.19627344E-01 0.19613151E-01
0001000 0.19598994E-01 0.19587465E-01 0.19581068E-01 0.19581553E-01 0.19589674E-01
0001100 0.19604843E-01 0.19625057E-01 0.19647095E-01 0.19667078E-01 0.19680869E-01
0001200 0.19685011E-01 0.19677322E-01 0.19657683E-01 0.19628257E-01 0.19593555E-01
0001300 0.19559972E-01 0.19534823E-01 0.19525100E-01 0.19535784E-01 0.19568253E-01
0001400 0.19618716E-01 0.19677013E-01 0.19726340E-01 0.19743428E-01 0.19700188E-01
0001500 0.19566014E-01 0.19311287E-01 0.18911380E-01 0.18351041E-01 0.17628174E-01
0001600 0.16756620E-01 0.15767254E-01 0.14706865E-01 0.13635226E-01 0.12620654E-01
0001700 0.11735521E-01 0.11051118E-01 0.10621045E-01 0.10476407E-01 0.10621045E-01
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812659E 00-0.34812689E 00-0.34813768E 00-0.34813166E 00-0.34813094E 00
0000200-0.34812903E 00-0.34812224E 00-0.34810442E 00-0.34809816E 00-0.34810323E 00
0000300-0.34809744E 00-0.34809834E 00-0.34809915E 00-0.34811217E 00-0.34812623E 00
0000400-0.34812444E 00-0.34813517E 00-0.34814101E 00-0.34813792E 00-0.34813106E 00
0000500-0.34811884E 00-0.34810257E 00-0.34809285E 00-0.34807861E 00-0.34807503E 00
0000600-0.34806830E 00-0.34807175E 00-0.34808075E 00-0.34809119E 00-0.34810245E 00
0000700-0.34811342E 00-0.34812015E 00-0.34813368E 00-0.34812367E 00-0.34811831E 00
0000800-0.34809661E 00-0.34807986E 00-0.34806246E 00-0.34804958E 00-0.34804034E 00
0000900-0.34803331E 00-0.34804034E 00-0.34805769E 00-0.34808183E 00-0.34810817E 00
0001000-0.34813398E 00-0.34815162E 00-0.34815937E 00-0.34815294E 00-0.34813446E 00
0001100-0.34810477E 00-0.34806955E 00-0.34803581E 00-0.34801114E 00-0.34800124E 00
0001200-0.34801090E 00-0.34804136E 00-0.34809124E 00-0.34815425E 00-0.34822416E 00
0001300-0.34829056E 00-0.34834427E 00-0.34837568E 00-0.34837770E 00-0.34834456E 00
0001400-0.34826869E 00-0.34813792E 00-0.34792405E 00-0.34757495E 00-0.34699547E 00
0001500-0.34603614E 00-0.34448051E 00-0.34203058E 00-0.33830875E 00-0.33286440E 00
0001600-0.32518971E 00-0.31474942E 00-0.30102038E 00-0.28353900E 00-0.26192731E 00
0001700-0.23618901E 00-0.21352011E 00-0.19808227E 00-0.19593847E 00-0.19808227E 00
EOF
q
```

```
redit potel2
LOADING POTE12
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.19617494E-01 0.19625489E-01 0.19633338E-01 0.19639689E-01 0.19643288E-01
0000200 0.19643381E-01 0.19639682E-01 0.19632645E-01 0.19623242E-01 0.19613057E-01
0000300 0.19603882E-01 0.19597407E-01 0.19595023E-01 0.19597508E-01 0.19604728E-01
0000400 0.19615777E-01 0.19628886E-01 0.19641802E-01 0.19652031E-01 0.19657440E-01
0000500 0.19656502E-01 0.19648738E-01 0.19634802E-01 0.19616626E-01 0.19597005E-01
0000600 0.19579381E-01 0.19567169E-01 0.19563161E-01 0.19569010E-01 0.19584656E-01
0000700 0.19608300E-01 0.19636367E-01 0.19664150E-01 0.19686203E-01 0.19697607E-01
0000800 0.19694775E-01 0.19676309E-01 0.19643784E-01 0.19601807E-01 0.19557681E-01
0000900 0.19520435E-01 0.19499339E-01 0.19502006E-01 0.19532163E-01 0.19587692E-01
0001000 0.19659009E-01 0.19728158E-01 0.19768998E-01 0.19748654E-01 0.19630093E-01
0001100 0.19376308E-01 0.18955085E-01 0.18344317E-01 0.17537035E-01 0.16544934E-01
0001200 0.15400007E-01 0.14153268E-01 0.12870707E-01 0.11627372E-01 0.10500614E-01
0001300 0.95637888E-02 0.88701770E-02 0.84462799E-02 0.83049536E-02 0.84462799E-02
EOF
q
redit potel3
LOADING POTE13
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.34812552E 00-0.34811544E 00-0.34809446E 00-0.34809130E 00-0.34808129E 00
0000200-0.34808809E 00-0.34809995E 00-0.34811777E 00-0.34813857E 00-0.34815431E 00
0000300-0.34816813E 00-0.34818351E 00-0.34817624E 00-0.34816808E 00-0.34814411E 00
0000400-0.34811938E 00-0.34809577E 00-0.34806985E 00-0.34805071E 00-0.34803164E 00
0000500-0.34802973E 00-0.34804070E 00-0.34806126E 00-0.34808600E 00-0.34811193E 00
0000600-0.34813017E 00-0.34813660E 00-0.34812599E 00-0.34809953E 00-0.34805828E 00
0000700-0.34800875E 00-0.34795958E 00-0.34792036E 00-0.34790063E 00-0.34790725E 00
0000800-0.34794331E 00-0.34800828E 00-0.34809524E 00-0.34819537E 00-0.34829503E 00
0000900-0.34838039E 00-0.34843713E 00-0.34845501E 00-0.34842420E 00-0.34833711E 00
0001000-0.34818470E 00-0.34794503E 00-0.34757167E 00-0.34697562E 00-0.34600633E 00
0001100-0.34443438E 00-0.34193194E 00-0.33806974E 00-0.33231616E 00-0.32405376E 00
0001200-0.31261158E 00-0.29731202E 00-0.27752811E 00-0.25276875E 00-0.22258997E 00
0001300-0.19393134E 00-0.17432165E 00-0.16128504E 00-0.15930969E 00-0.16128504E 00
EOF
q
```

ZN NL a=2.0 DENS.

VEFF

```
redit pote14
LOADING POTE14
REKEYED
EDIT
p99
```

ZN NL a=2.5 DENS.

```
        TOP RECORD
0000100 0.19621808E-01 0.19616783E-01 0.19611962E-01 0.19608267E-01 0.19606389E-01
0000200 0.19606780E-01 0.19609500E-01 0.19614141E-01 0.19620057E-01 0.19626260E-01
0000300 0.19631710E-01 0.19635309E-01 0.19636400E-01 0.19634616E-01 0.19630127E-01
0000400 0.19623622E-01 0.19616086E-01 0.19608870E-01 0.19603278E-01 0.19600391E-01
0000500 0.19600917E-01 0.19604981E-01 0.19612093E-01 0.19621171E-01 0.19630749E-01
0000600 0.19639183E-01 0.19644871E-01 0.19646693E-01 0.19644119E-01 0.19637231E-01
0000700 0.19627098E-01 0.19615367E-01 0.19604076E-01 0.19595362E-01 0.19591041E-01
0000800 0.19592281E-01 0.19599363E-01 0.19611478E-01 0.19626845E-01 0.19642968E-01
0000900 0.19656911E-01 0.19665956E-01 0.19667923E-01 0.19661833E-01 0.19648012E-01
0001000 0.19628197E-01 0.19605502E-01 0.19583724E-01 0.19567050E-01 0.19559089E-01
0001100 0.19562274E-01 0.19577201E-01 0.19602403E-01 0.19634277E-01 0.19667547E-01
0001200 0.19695967E-01 0.19713469E-01 0.19715190E-01 0.19698739E-01 0.19664884E-01
0001300 0.19618031E-01 0.19565981E-01 0.19518927E-01 0.19487869E-01 0.19482415E-01
0001400 0.19508418E-01 0.19565415E-01 0.19644722E-01 0.19728038E-01 0.19787539E-01
0001500 0.19787069E-01 0.19685108E-01 0.19439075E-01 0.19010961E-01 0.18373344E-01
0001600 0.17515235E-01 0.16446397E-01 0.15199270E-01 0.13827581E-01 0.12401581E-01
0001700 0.11000652E-01 0.97049475E-02 0.85872784E-02 0.76972134E-02 0.70567541E-02
0001800 0.66720583E-02 0.65444261E-02 0.66720583E-02 0.70567541E-02 0.76972134E-02
EOF
q
redit pote15
LOADING POTE15
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812558E 00-0.34813875E 00-0.34814918E 00-0.34816545E 00-0.34816349E 00
0000200-0.34816402E 00-0.34815812E 00-0.34814483E 00-0.34811747E 00-0.34810138E 00
0000300-0.34809989E 00-0.34809059E 00-0.34808505E 00-0.34808415E 00-0.34809893E 00
0000400-0.34811771E 00-0.34812444E 00-0.34814125E 00-0.34815460E 00-0.34816080E 00
0000500-0.34815848E 00-0.34814793E 00-0.34813142E 00-0.34811825E 00-0.34809297E 00
0000600-0.34808403E 00-0.34806854E 00-0.34807408E 00-0.34808975E 00-0.34811068E 00
0000700-0.34813720E 00-0.34816504E 00-0.34818703E 00-0.34821600E 00-0.34822226E 00
0000800-0.34822387E 00-0.34820086E 00-0.34818041E 00-0.34814930E 00-0.34812033E 00
0000900-0.34809673E 00-0.34807366E 00-0.34806979E 00-0.34808230E 00-0.34810895E 00
0001000-0.34814411E 00-0.34818351E 00-0.34821624E 00-0.34823763E 00-0.34823871E 00
0001100-0.34821898E 00-0.34817761E 00-0.34812099E 00-0.34805781E 00-0.34800011E 00
0001200-0.34795916E 00-0.34794456E 00-0.34796321E 00-0.34801602E 00-0.34809881E 00
0001300-0.34820324E 00-0.34831548E 00-0.34842062E 00-0.34850121E 00-0.34854275E 00
0001400-0.34853333E 00-0.34846312E 00-0.34832203E 00-0.34808952E 00-0.34772313E 00
0001500-0.34713435E 00-0.34617192E 00-0.34459460E 00-0.34205484E 00-0.33808911E 00
0001600-0.33211643E 00-0.32345533E 00-0.31135589E 00-0.29505122E 00-0.27381837E 00
0001700-0.24709123E 00-0.21435738E 00-0.18252170E 00-0.15840048E 00-0.14176351E 00
0001800-0.13082600E 00-0.12866610E 00-0.13082600E 00-0.14176351E 00-0.15840048E 00
EOF
q
```

```
redit pote16
LOADING POTE16   ZN NL a=3.0
REKEYED
EDIT             DENS.
p99
        TOP RECORD
0000100 0.19618697E-01 0.19612800E-01 0.19607931E-01 0.19605048E-01 0.19604776E-01
0000200 0.19607361E-01 0.19612480E-01 0.19619416E-01 0.19627128E-01 0.19634329E-01
0000300 0.19639727E-01 0.19642338E-01 0.19641608E-01 0.19637566E-01 0.19630741E-01
0000400 0.19622248E-01 0.19613579E-01 0.19606296E-01 0.19601781E-01 0.19601040E-01
0000500 0.19604474E-01 0.19611709E-01 0.19621752E-01 0.19632924E-01 0.19643363E-01
0000600 0.19651096E-01 0.19654635E-01 0.19653052E-01 0.19646306E-01 0.19635245E-01
0000700 0.19621570E-01 0.19607596E-01 0.19595798E-01 0.19588467E-01 0.19587222E-01
0000800 0.19592728E-01 0.19604489E-01 0.19620746E-01 0.19638821E-01 0.19655410E-01
0000900 0.19667245E-01 0.19671597E-01 0.19666847E-01 0.19652925E-01 0.19631341E-01
0001000 0.19605272E-01 0.19578930E-01 0.19557074E-01 0.19544125E-01 0.19543327E-01
0001100 0.19556075E-01 0.19581385E-01 0.19615833E-01 0.19653883E-01 0.19688636E-01
0001200 0.19713033E-01 0.19721039E-01 0.19709028E-01 0.19676857E-01 0.19628394E-01
0001300 0.19571424E-01 0.19516833E-01 0.19476943E-01 0.19463114E-01 0.19483216E-01
0001400 0.19538667E-01 0.19622125E-01 0.19715872E-01 0.19791439E-01 0.19810796E-01
0001500 0.19729212E-01 0.19499924E-01 0.19080009E-01 0.18437237E-01 0.17556407E-01
0001600 0.16444623E-01 0.15133508E-01 0.13678137E-01 0.12151748E-01 0.10637537E-01
0001700 0.92188567E-02 0.79695173E-02 0.69371350E-02 0.61395653E-02 0.55774041E-02
0001800 0.52442178E-02 0.51343553E-02 0.52442178E-02 0.55774041E-02 0.61395653E-02
EOF
q
redit pote17
LOADING POTE17
REKEYED          VEFF
EDIT
p99
        TOP RECORD
0000100-0.34812516E 00-0.34813696E 00-0.34815609E 00-0.34815681E 00-0.34816295E 00
0000200-0.34816295E 00-0.34816015E 00-0.34813827E 00-0.34812903E 00-0.34812886E 00
0000300-0.34812313E 00-0.34812236E 00-0.34812605E 00-0.34814334E 00-0.34816629E 00
0000400-0.34817684E 00-0.34819889E 00-0.34821510E 00-0.34822357E 00-0.34822273E 00
0000500-0.34821552E 00-0.34819800E 00-0.34818637E 00-0.34816331E 00-0.34814942E 00
0000600-0.34813261E 00-0.34813100E 00-0.34813923E 00-0.34815848E 00-0.34818143E 00
0000700-0.34820658E 00-0.34822863E 00-0.34825248E 00-0.34825397E 00-0.34825128E 00
0000800-0.34822571E 00-0.34819508E 00-0.34816051E 00-0.34812051E 00-0.34808522E 00
0000900-0.34805280E 00-0.34803849E 00-0.34804124E 00-0.34805983E 00-0.34808886E 00
0001000-0.34812415E 00-0.34815401E 00-0.34817290E 00-0.34817195E 00-0.34814858E 00
0001100-0.34810269E 00-0.34803939E 00-0.34796888E 00-0.34790397E 00-0.34785628E 00
0001200-0.34783947E 00-0.34785932E 00-0.34791940E 00-0.34801495E 00-0.34813702E 00
0001300-0.34827012E 00-0.34839827E 00-0.34850150E 00-0.34856343E 00-0.34857035E 00
0001400-0.34851140E 00-0.34837735E 00-0.34815156E 00-0.34779602E 00-0.34722912E 00
0001500-0.34630311E 00-0.34477919E 00-0.34230357E 00-0.33839583E 00-0.33244264E 00
0001600-0.32371068E 00-0.31137764E 00-0.29458189E 00-0.27249342E 00-0.24441594E 00
0001700-0.20974684E 00-0.17544097E 00-0.14835149E 00-0.12795514E 00-0.11411148E 00
0001800-0.10518706E 00-0.10368896E 00-0.10518706E 00-0.11411148E 00-0.12795514E 00
EOF
q
```

```
redit hote18
LOADING POTE18
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.19632086E-01 0.19625474E-01 0.19618101E-01 0.19611321E-01 0.19606341E-01
0000200 0.19604187E-01 0.19605376E-01 0.19609895E-01 0.19617107E-01 0.19625906E-01
0000300 0.19634847E-01 0.19642364E-01 0.19647047E-01 0.19647952E-01 0.19644760E-01
0000400 0.19637812E-01 0.19628093E-01 0.19617267E-01 0.19607171E-01 0.19599635E-01
0000500 0.19596063E-01 0.19597355E-01 0.19603509E-01 0.19613635E-01 0.19626036E-01
0000600 0.19638598E-01 0.19648977E-01 0.19655067E-01 0.19655470E-01 0.19649591E-01
0000700 0.19638035E-01 0.19622408E-01 0.19605178E-01 0.19589324E-01 0.19577712E-01
0000800 0.19572750E-01 0.19575726E-01 0.19586727E-01 0.19604266E-01 0.19625645E-01
0000900 0.19647170E-01 0.19664973E-01 0.19675415E-01 0.19676059E-01 0.19665927E-01
0001000 0.19645989E-01 0.19619167E-01 0.19589949E-01 0.19563634E-01 0.19545630E-01
0001100 0.19540273E-01 0.19550025E-01 0.19574769E-01 0.19611515E-01 0.19654628E-01
0001200 0.19696612E-01 0.19729245E-01 0.19745037E-01 0.19738868E-01 0.19709229E-01
0001300 0.19659180E-01 0.19596431E-01 0.19532591E-01 0.19481618E-01 0.19457106E-01
0001400 0.19469533E-01 0.19522820E-01 0.19611552E-01 0.19718766E-01 0.19815300E-01
0001500 0.19860655E-01 0.19806042E-01 0.19599255E-01 0.19191325E-01 0.18544190E-01
0001600 0.17638061E-01 0.16477466E-01 0.15094008E-01 0.13545129E-01 0.11908241E-01
0001700 0.10271054E-01 0.87194256E-02 0.73259957E-02 0.61350800E-02 0.51602796E-02
0001800 0.43958798E-02 0.38267553E-02 0.34355880E-02 0.32074044E-02 0.31326201E-02
EOF
q
reditkpote19
LOADING POTE19
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.34812713E 00-0.34813714E 00-0.34814817E 00-0.34816527E 00-0.34816778E 00
0000200-0.34817529E 00-0.34817475E 00-0.34816682E 00-0.34814560E 00-0.34812897E 00
0000300-0.34812003E 00-0.34810692E 00-0.34809834E 00-0.34809768E 00-0.34811395E 00
0000400-0.34813476E 00-0.34814554E 00-0.34816980E 00-0.34818465E 00-0.34819621E 00
0000500-0.34819323E 00-0.34818286E 00-0.34816253E 00-0.34814405E 00-0.34810972E 00
0000600-0.34808439E 00-0.34805316E 00-0.34804070E 00-0.34803939E 00-0.34804863E 00
0000700-0.34806752E 00-0.34809273E 00-0.34811640E 00-0.34814405E 00-0.34815234E 00
0000800-0.34815997E 00-0.34813720E 00-0.34811246E 00-0.34807742E 00-0.34803998E 00
0000900-0.34800494E 00-0.34797466E 00-0.34796590E 00-0.34797859E 00-0.34801251E 00
0001000-0.34806341E 00-0.34812570E 00-0.34818804E 00-0.34824216E 00-0.34827632E 00
0001100-0.34828579E 00-0.34826654E 00-0.34822172E 00-0.34815925E 00-0.34809089E 00
0001200-0.34802973E 00-0.34799021E 00-0.34798193E 00-0.34801096E 00-0.34807676E 00
0001300-0.34817505E 00-0.34829527E 00-0.34842306E 00-0.34854239E 00-0.34863818E 00
0001400-0.34869677E 00-0.34870732E 00-0.34865975E 00-0.34853530E 00-0.34829313E 00
0001500-0.34784395E 00-0.34702921E 00-0.34559160E 00-0.34315252E 00-0.33919781E 00
0001600-0.33307612E 00-0.32401168E 00-0.31113648E 00-0.29354620E 00-0.27033460E 00
0001700-0.24114513E 00-0.20565856E 00-0.16981953E 00-0.13962847E 00-0.11488867E 00
0001800-0.95554233E-01-0.81225812E-01-0.71649969E-01-0.65622151E-01-0.64562201E-01
EOF
q
```

ZN NL a=4.0
DENS.

VEFF

```
redit pote20
LOADING POTE20
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.19615527E-01 0.19607466E-01 0.19601159E-01 0.19597877E-01 0.19598462E-01
0000200 0.19603036E-01 0.19611128E-01 0.19621581E-01 0.19632809E-01 0.19642901E-01
0000300 0.19650128E-01 0.19653201E-01 0.19651454E-01 0.19645024E-01 0.19634873E-01
0000400 0.19622721E-01 0.19610636E-01 0.19600827E-01 0.19595187E-01 0.19594945E-01
0000500 0.19600444E-01 0.19611053E-01 0.19625098E-01 0.19640278E-01 0.19653868E-01
0000600 0.19663360E-01 0.19666728E-01 0.19663002E-01 0.19652270E-01 0.19636095E-01
0000700 0.19616958E-01 0.19598126E-01 0.19582916E-01 0.19574326E-01 0.19574251E-01
0000800 0.19583270E-01 0.19600283E-01 0.19622639E-01 0.19646432E-01 0.19667268E-01
0000900 0.19680914E-01 0.19684028E-01 0.19674994E-01 0.19654226E-01 0.19624338E-01
0001000 0.19589953E-01 0.19556850E-01 0.19531209E-01 0.19518450E-01 0.19522097E-01
0001100 0.19543070E-01 0.19579105E-01 0.19624840E-01 0.19672520E-01 0.19713189E-01
0001200 0.19738097E-01 0.19740589E-01 0.19717593E-01 0.19670777E-01 0.19606903E-01
0001300 0.19537367E-01 0.19476630E-01 0.19439749E-01 0.19439202E-01 0.19481450E-01
0001400 0.19563671E-01 0.19671265E-01 0.19776646E-01 0.19839931E-01 0.19811422E-01
0001500 0.19636571E-01 0.19262590E-01 0.18646378E-01 0.17762512E-01 0.16609985E-01
0001600 0.15216094E-01 0.13635892E-01 0.11946939E-01 0.10239583E-01 0.86047500E-02
0001700 0.71211159E-02 0.58366582E-02 0.47650263E-02 0.38982595E-02 0.32172520E-02
0001800 0.26991412E-02 0.23217581E-02 0.20663075E-02 0.19187452E-02 0.18705663E-02
EOF
q
redit pote21
LOADING POTE21
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.34812182E 00-0.34815288E 00-0.34816438E 00-0.34817785E 00-0.34818059E 00
0000200-0.34818196E 00-0.34816283E 00-0.34815133E 00-0.34815258E 00-0.34814072E 00
0000300-0.34813309E 00-0.34813046E 00-0.34814668E 00-0.34816438E 00-0.34817576E 00
0000400-0.34820229E 00-0.34822232E 00-0.34823757E 00-0.34824169E 00-0.34823740E 00
0000500-0.34821683E 00-0.34819877E 00-0.34816390E 00-0.34814042E 00-0.34810632E 00
0000600-0.34809428E 00-0.34809130E 00-0.34810239E 00-0.34812278E 00-0.34814739E 00
0000700-0.34817779E 00-0.34821397E 00-0.34822708E 00-0.34823525E 00-0.34821188E 00
0000800-0.34818065E 00-0.34813422E 00-0.34808338E 00-0.34803218E 00-0.34797722E 00
0000900-0.34794289E 00-0.34793061E 00-0.34793967E 00-0.34796870E 00-0.34801275E 00
0001000-0.34805965E 00-0.34810144E 00-0.34812480E 00-0.34812331E 00-0.34809160E 00
0001100-0.34803265E 00-0.34795374E 00-0.34786874E 00-0.34779394E 00-0.34774595E 00
0001200-0.34773803E 00-0.34777850E 00-0.34786838E 00-0.34800154E 00-0.34816468E 00
0001300-0.34834021E 00-0.34850478E 00-0.34863555E 00-0.34871083E 00-0.34871280E 00
0001400-0.34862810E 00-0.34844118E 00-0.34812224E 00-0.34760451E 00-0.34675735E 00
0001500-0.34535730E 00-0.34305817E 00-0.33937204E 00-0.33365691E 00-0.32512087E 00
0001600-0.31284606E 00-0.29583454E 00-0.27307475E 00-0.24364555E 00-0.20667130E 00
0001700-0.16884881E 00-0.13683385E 00-0.10992360E 00-0.87721825E-01-0.69819927E-01
0001800-0.56011036E-01-0.45983583E-01-0.39440345E-01-0.35505779E-01-0.34760345E-01
EOF
q
```

ZN NL a=5.0 DENS.

VEFF

```
redit pote22
LOADING POTE22
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.19630365E-01 0.19620314E-01 0.19609492E-01 0.19599877E-01 0.19593295E-01
0000200 0.19591164E-01 0.19594084E-01 0.19601855E-01 0.19613430E-01 0.19626979E-01
0000300 0.19640271E-01 0.19650910E-01 0.19657005E-01 0.19657299E-01 0.19651435E-01
0000400 0.19640192E-01 0.19625306E-01 0.19609280E-01 0.19594900E-01 0.19584760E-01
0000500 0.19580856E-01 0.19584265E-01 0.19594692E-01 0.19610651E-01 0.19629557E-01
0000600 0.19648168E-01 0.19663159E-01 0.19671589E-01 0.19671567E-01 0.19662600E-01
0000700 0.19645784E-01 0.19623686E-01 0.19599952E-01 0.19578781E-01 0.19564189E-01
0000800 0.19559193E-01 0.19565392E-01 0.19582372E-01 0.19607734E-01 0.19637406E-01
0000900 0.19666228E-01 0.19688807E-01 0.19700527E-01 0.19698318E-01 0.19681487E-01
0001000 0.19651901E-01 0.19614033E-01 0.19574214E-01 0.19539729E-01 0.19517519E-01
0001100 0.19512888E-01 0.19528382E-01 0.19562975E-01 0.19611984E-01 0.19667473E-01
0001200 0.19719485E-01 0.19757580E-01 0.19772898E-01 0.19759968E-01 0.19718386E-01
0001300 0.19653413E-01 0.19575939E-01 0.19501064E-01 0.19445665E-01 0.19425120E-01
0001400 0.19449435E-01 0.19519564E-01 0.19624349E-01 0.19738670E-01 0.19823622E-01
0001500 0.19828770E-01 0.19696865E-01 0.19370686E-01 0.18801309E-01 0.17956886E-01
0001600 0.16830288E-01 0.15443835E-01 0.13849713E-01 0.12125030E-01 0.10362230E-01
0001700 0.86560436E-02 0.70896819E-02 0.57151057E-02 0.45487545E-02 0.35839707E-02
0001800 0.28014036E-02 0.21762771E-02 0.16828934E-02 0.12972048E-02 0.99802087E-03
0001900 0.76741702E-03 0.59064967E-03 0.45585330E-03 0.35364018E-03 0.27668802E-03
0002000 0.21936875E-03 0.17742263E-03 0.14769923E-03 0.12794910E-03 0.11667056E-03
0002100 0.11300443E-03 0.11667056E-03 0.12794910E-03 0.14769923E-03 0.17742263E-03
EOF
q
redit pote23
LOADING POTE23
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.34812540E 00-0.34814942E 00-0.34818280E 00-0.34819931E 00-0.34822106E 00
0000200-0.34823191E 00-0.34823328E 00-0.34821171E 00-0.34818888E 00-0.34817284E 00
0000300-0.34814781E 00-0.34812838E 00-0.34811258E 00-0.34812278E 00-0.34814328E 00
0000400-0.34815717E 00-0.34818870E 00-0.34822375E 00-0.34825337E 00-0.34827209E 00
0000500-0.34827298E 00-0.34825778E 00-0.34823877E 00-0.34819621E 00-0.34816468E 00
0000600-0.34811962E 00-0.34809214E 00-0.34808105E 00-0.34808511E 00-0.34810466E 00
0000700-0.34814113E 00-0.34818220E 00-0.34823489E 00-0.34826952E 00-0.34829986E 00
0000800-0.34829473E 00-0.34827858E 00-0.34823954E 00-0.34818685E 00-0.34812754E 00
0000900-0.34806484E 00-0.34802234E 00-0.34800440E 00-0.34801453E 00-0.34805149E 00
0001000-0.34811217E 00-0.34818327E 00-0.34825504E 00-0.34830993E 00-0.34833944E 00
0001100-0.34833241E 00-0.34828740E 00-0.34820962E 00-0.34811229E 00-0.34801209E 00
0001200-0.34792978E 00-0.34788185E 00-0.34788251E 00-0.34793800E 00-0.34804654E 00
0001300-0.34819764E 00-0.34837562E 00-0.34855682E 00-0.34871662E 00-0.34882790E 00
0001400-0.34886718E 00-0.34881514E 00-0.34865415E 00-0.34835559E 00-0.34786010E 00
0001500-0.34704947E 00-0.34571618E 00-0.34353125E 00-0.34002143E 00-0.33455718E 00
0001600-0.32635492E 00-0.31449562E 00-0.29797006E 00-0.27573949E 00-0.24683607E 00
0001700-0.21030873E 00-0.17269069E 00-0.14042979E 00-0.11265033E 00-0.88752687E-01
0001800-0.68152547E-01-0.50349034E-01-0.34914844E-01-0.21498464E-01-0.98065548E-02
0001900 0.40235952E-03 0.93284845E-02 0.17138015E-01 0.23969762E-01 0.29946972E-01
0002000 0.35180595E-01 0.39758921E-01 0.43709923E-01 0.46917994E-01 0.49113516E-01
0002100 0.49871560E-01 0.49113516E-01 0.46917994E-01 0.43709923E-01 0.39758921E-01
EOF
q
```

ZN NL a=10.0 DENS.

VEFF

```
redit pote24
LOADING POTE24
REKEYED
EDIT
p99
```

ZN NL a=15.0 DENS.

```
        TOP RECORD
0000100 0.19631356E-01 0.19620351E-01 0.19608494E-01 0.19597840E-01 0.19590359E-01
0000200 0.19587521E-01 0.19590028E-01 0.19597646E-01 0.19609332E-01 0.19623149E-01
0000300 0.19636720E-01 0.19647621E-01 0.19653834E-01 0.19653991E-01 0.19647781E-01
0000400 0.19635957E-01 0.19620359E-01 0.19603513E-01 0.19588359E-01 0.19577608E-01
0000500 0.19573398E-01 0.19576810E-01 0.19587621E-01 0.19604236E-01 0.19624017E-01
0000600 0.19643605E-01 0.19659579E-01 0.19668799E-01 0.19669339E-01 0.19660648E-01
0000700 0.19643780E-01 0.19621380E-01 0.19597247E-01 0.19575700E-01 0.19560877E-01
0000800 0.19555964E-01 0.19562624E-01 0.19580498E-01 0.19607138E-01 0.19638363E-01
0000900 0.19668858E-01 0.19693065E-01 0.19706141E-01 0.19704886E-01 0.19688468E-01
0001000 0.19658756E-01 0.19620217E-01 0.19579332E-01 0.19543536E-01 0.19520007E-01
0001100 0.19514307E-01 0.19529186E-01 0.19563772E-01 0.19613430E-01 0.19670159E-01
0001200 0.19723866E-01 0.19763842E-01 0.19780956E-01 0.19769404E-01 0.19728504E-01
0001300 0.19663300E-01 0.19584611E-01 0.19507568E-01 0.19449223E-01 0.19425295E-01
0001400 0.19446187E-01 0.19513302E-01 0.19615937E-01 0.19729368E-01 0.19814961E-01
0001500 0.19822419E-01 0.19694451E-01 0.19373573E-01 0.18810365E-01 0.17972425E-01
0001600 0.16851880E-01 0.15470367E-01 0.13879463E-01 0.12156006E-01 0.10392293E-01
0001700 0.86833835E-02 0.71129613E-02 0.57334602E-02 0.45618042E-02 0.35916483E-02
0001800 0.28038893E-02 0.21738957E-02 0.16760514E-02 0.12863218E-02 0.98349364E-03
0001900 0.74957334E-03 0.56972541E-03 0.43196511E-03 0.32675965E-03 0.24661492E-03
0002000 0.18569217E-03 0.13947410E-03 0.10448480E-03 0.78059224E-04 0.58159247E-04
0002100 0.43227716E-04 0.32074546E-04 0.23788845E-04 0.17673156E-04 0.13194478E-04
0002200 0.99488898E-05 0.76348451E-05 0.60326138E-05 0.49878872E-05 0.43992195E-05
0002300 0.42091906E-05 0.43992195E-05 0.49878872E-05 0.60326138E-05 0.76348451E-05
EOF
q
redit pote25
LOADING POTE25
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.34812552E 00-0.34813917E 00-0.34816211E 00-0.34817332E 00-0.34818864E 00
0000200-0.34819525E 00-0.34818858E 00-0.34816056E 00-0.34813958E 00-0.34812260E 00
0000300-0.34809691E 00-0.34807432E 00-0.34805751E 00-0.34805954E 00-0.34807462E 00
0000400-0.34808487E 00-0.34811389E 00-0.34814256E 00-0.34816384E 00-0.34817547E 00
0000500-0.34817785E 00-0.34816384E 00-0.34815019E 00-0.34811276E 00-0.34808058E 00
0000600-0.34804100E 00-0.34802312E 00-0.34801835E 00-0.34802639E 00-0.34805447E 00
0000700-0.34809142E 00-0.34813654E 00-0.34819347E 00-0.34823120E 00-0.34826362E 00
0000800-0.34826404E 00-0.34825289E 00-0.34822172E 00-0.34817410E 00-0.34812194E 00
0000900-0.34806359E 00-0.34802651E 00-0.34801316E 00-0.34802735E 00-0.34806788E 00
0001000-0.34813136E 00-0.34820461E 00-0.34827805E 00-0.34833503E 00-0.34836584E 00
0001100-0.34836030E 00-0.34831733E 00-0.34824234E 00-0.34814793E 00-0.34805125E 00
0001200-0.34797245E 00-0.34792835E 00-0.34793276E 00-0.34799099E 00-0.34810090E 00
0001300-0.34825146E 00-0.34842676E 00-0.34860289E 00-0.34875482E 00-0.34885687E 00
0001400-0.34888458E 00-0.34882015E 00-0.34864479E 00-0.34833223E 00-0.34782404E 00
0001500-0.34700376E 00-0.34566712E 00-0.34348875E 00-0.34000003E 00-0.33457434E 00
0001600-0.32642931E 00-0.31464672E 00-0.29821283E 00-0.27608258E 00-0.24727881E 00
0001700-0.21084195E 00-0.17330968E 00-0.14113885E 00-0.11345017E 00-0.89633763E-01
0001800-0.69097221E-01-0.51329985E-01-0.35896454E-01-0.22432331E-01-0.10629110E-01
0001900-0.22349025E-03 0.90138428E-02 0.17288979E-01 0.24796493E-01 0.31730566E-01
0002000 0.38292702E-01 0.44702407E-01 0.51198009E-01 0.58018185E-01 0.65354943E-01
0002100 0.73272705E-01 0.81604838E-01 0.89906275E-01 0.97551286E-01 0.10398382E 00
0002200 0.10896963E 00 0.11263782E 00 0.11528808E 00 0.11713463E 00 0.11825740E 00
0002300 0.11863720E 00 0.11825740E 00 0.11713463E 00 0.11528808E 00 0.11263782E 00
EOF
q
```

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
```

ZN+ LDA a=0.25 DENS.

```
        TOP RECORD
0000100 0.13365541E-01 0.13365295E-01 0.13365056E-01 0.13364866E-01 0.13364743E-01
0000200 0.13364661E-01 0.13364643E-01 0.13364714E-01 0.13364851E-01 0.13365105E-01
0000300 0.13365421E-01 0.13365820E-01 0.13366304E-01 0.13366874E-01 0.13367474E-01
0000400 0.13368122E-01 0.13368789E-01 0.13369445E-01 0.13370100E-01 0.13370711E-01
0000500 0.13371244E-01 0.13371702E-01 0.13372082E-01 0.13372321E-01 0.13372436E-01
0000600 0.13372410E-01 0.13372280E-01 0.13371997E-01 0.13371561E-01 0.13370998E-01
0000700 0.13370335E-01 0.13369553E-01 0.13368681E-01 0.13367765E-01 0.13366811E-01
0000800 0.13365854E-01 0.13364937E-01 0.13364095E-01 0.13363324E-01 0.13362691E-01
0000900 0.13362166E-01 0.13361830E-01 0.13361707E-01 0.13361763E-01 0.13362046E-01
0001000 0.13362549E-01 0.13363227E-01 0.13364106E-01 0.13365153E-01 0.13366356E-01
0001100 0.13367634E-01 0.13368987E-01 0.13370369E-01 0.13371706E-01 0.13372961E-01
0001200 0.13374098E-01 0.13375048E-01 0.13375763E-01 0.13376214E-01 0.13376370E-01
0001300 0.13376206E-01 0.13375692E-01 0.13374832E-01 0.13373621E-01 0.13372090E-01
0001400 0.13370261E-01 0.13368201E-01 0.13365943E-01 0.13363596E-01 0.13361193E-01
0001500 0.13358839E-01 0.13356630E-01 0.13354670E-01 0.13353039E-01 0.13351832E-01
0001600 0.13351157E-01 0.13351064E-01 0.13351623E-01 0.13352871E-01 0.13354819E-01
0001700 0.13357479E-01 0.13360798E-01 0.13364706E-01 0.13369091E-01 0.13373807E-01
0001800 0.13378683E-01 0.13383523E-01 0.13388030E-01 0.13391931E-01 0.13394907E-01
0001900 0.13396621E-01 0.13396684E-01 0.13394706E-01 0.13390291E-01 0.13383027E-01
0002000 0.13372540E-01 0.13358414E-01 0.13340339E-01 0.13317961E-01 0.13291024E-01
0002100 0.13259333E-01 0.13222743E-01 0.13181206E-01 0.13134748E-01 0.13083518E-01
0002200 0.13027783E-01 0.12967881E-01 0.12904342E-01 0.12837805E-01 0.12768976E-01
0002300 0.12698799E-01 0.12628309E-01 0.12558628E-01 0.12491055E-01 0.12427017E-01
0002400 0.12368042E-01 0.12315735E-01 0.12271848E-01 0.12238197E-01 0.12216613E-01
0002500 0.12209263E-01 0.12216613E-01 0.12238197E-01 0.12271848E-01 0.12315735E-01
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953620E 00-0.26953596E 00-0.26953584E 00-0.26953673E 00-0.26953679E 00
0000200-0.26953882E 00-0.26954871E 00-0.26954949E 00-0.26955086E 00-0.26955158E 00
0000300-0.26955485E 00-0.26955736E 00-0.26955354E 00-0.26956040E 00-0.26956367E 00
0000400-0.26956648E 00-0.26957077E 00-0.26956558E 00-0.26957160E 00-0.26957130E 00
0000500-0.26956934E 00-0.26956987E 00-0.26956850E 00-0.26956743E 00-0.26956612E 00
0000600-0.26956433E 00-0.26956397E 00-0.26956362E 00-0.26956207E 00-0.26955909E 00
0000700-0.26955795E 00-0.26955652E 00-0.26955581E 00-0.26955450E 00-0.26955301E 00
0000800-0.26955169E 00-0.26955062E 00-0.26954919E 00-0.26954770E 00-0.26954544E 00
0000900-0.26954359E 00-0.26954198E 00-0.26953954E 00-0.26953781E 00-0.26953697E 00
0001000-0.26953596E 00-0.26953524E 00-0.26953453E 00-0.26953447E 00-0.26953483E 00
0001100-0.26953548E 00-0.26953566E 00-0.26953620E 00-0.26953757E 00-0.26953918E 00
0001200-0.26954120E 00-0.26954353E 00-0.26954550E 00-0.26954794E 00-0.26955020E 00
0001300-0.26955265E 00-0.26955426E 00-0.26955628E 00-0.26955748E 00-0.26955837E 00
0001400-0.26955837E 00-0.26955831E 00-0.26955682E 00-0.26955462E 00-0.26955235E 00
0001500-0.26954859E 00-0.26954412E 00-0.26953924E 00-0.26953381E 00-0.26952797E 00
0001600-0.26952183E 00-0.26951581E 00-0.26950973E 00-0.26950467E 00-0.26950014E 00
0001700-0.26949692E 00-0.26949489E 00-0.26949459E 00-0.26949531E 00-0.26949811E 00
0001800-0.26950294E 00-0.26950884E 00-0.26951540E 00-0.26952195E 00-0.26952857E 00
0001900-0.26953220E 00-0.26953256E 00-0.26952684E 00-0.26951277E 00-0.26948714E 00
0002000-0.26944602E 00-0.26938546E 00-0.26930070E 00-0.26918638E 00-0.26903635E 00
0002100-0.26884401E 00-0.26860195E 00-0.26830244E 00-0.26793659E 00-0.26749593E 00
0002200-0.26697087E 00-0.26635170E 00-0.26562911E 00-0.26479244E 00-0.26383328E 00
0002300-0.26274198E 00-0.26150984E 00-0.26012951E 00-0.25859451E 00-0.25689930E 00
0002400-0.25504094E 00-0.25301808E 00-0.25083131E 00-0.24861532E 00-0.24564791E 00
0002500-0.24510956E 00-0.24564791E 00-0.24861532E 00-0.25083131E 00-0.25301808E 00
EOF
```

```
redit pote4
LOADING POTE4   ZN+ LDA  a=0.5
REKEYED
EDIT                DENS.
p99
        TOP RECORD
0000100 0.13366435E-01 0.13364721E-01 0.13363350E-01 0.13362508E-01 0.13362356E-01
0000200 0.13362985E-01 0.13364401E-01 0.13366416E-01 0.13368811E-01 0.13371274E-01
0000300 0.13373487E-01 0.13375103E-01 0.13375852E-01 0.13375539E-01 0.13374120E-01
0000400 0.13371680E-01 0.13368495E-01 0.13364870E-01 0.13361342E-01 0.13358362E-01
0000500 0.13356421E-01 0.13355929E-01 0.13357069E-01 0.13359863E-01 0.13364095E-01
0000600 0.13369303E-01 0.13374869E-01 0.13380010E-01 0.13383891E-01 0.13385795E-01
0000700 0.13385128E-01 0.13381656E-01 0.13375476E-01 0.13367102E-01 0.13357453E-01
0000800 0.13347838E-01 0.13339758E-01 0.13334740E-01 0.13334200E-01 0.13339087E-01
0000900 0.13349719E-01 0.13365451E-01 0.13384670E-01 0.13404492E-01 0.13420917E-01
0001000 0.13428859E-01 0.13422456E-01 0.13395458E-01 0.13341699E-01 0.13255790E-01
0001100 0.13133682E-01 0.12973513E-01 0.12776088E-01 0.12545533E-01 0.12289561E-01
0001200 0.12019724E-01 0.11751153E-01 0.11502445E-01 0.11295021E-01 0.11152197E-01
0001300 0.11102211E-01 0.11152197E-01 0.11295021E-01 0.11502445E-01 0.11751153E-01
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT                VEFF
p99
        TOP RECORD
0000100-0.26953423E 00-0.26953000E 00-0.26953083E 00-0.26953202E 00-0.26952720E 00
0000200-0.26953053E 00-0.26953363E 00-0.26953518E 00-0.26953685E 00-0.26954311E 00
0000300-0.26954377E 00-0.26954412E 00-0.26954466E 00-0.26954639E 00-0.26954591E 00
0000400-0.26954520E 00-0.26954430E 00-0.26954192E 00-0.26953804E 00-0.26953220E 00
0000500-0.26952702E 00-0.26952159E 00-0.26951832E 00-0.26951545E 00-0.26951545E 00
0000600-0.26951820E 00-0.26952302E 00-0.26953042E 00-0.26954013E 00-0.26955068E 00
0000700-0.26955998E 00-0.26956743E 00-0.26957119E 00-0.26956892E 00-0.26956052E 00
0000800-0.26954508E 00-0.26952517E 00-0.26950127E 00-0.26947808E 00-0.26945895E 00
0000900-0.26944941E 00-0.26945198E 00-0.26947069E 00-0.26950264E 00-0.26954007E 00
0001000-0.26956832E 00-0.26956040E 00-0.26947480E 00-0.26925719E 00-0.26883072E 00
0001100-0.26810306E 00-0.26695973E 00-0.26527041E 00-0.26289231E 00-0.25967598E 00
0001200-0.25547642E 00-0.25016552E 00-0.24364442E 00-0.23633349E 00-0.22561616E 00
0001300-0.22349507E 00-0.22561616E 00-0.23633349E 00-0.24364442E 00-0.25016552E 00
EOF
q
```

```
redit pote6
LOADING POTE6
REKEYED
EDIT
p99
```

ZN+ LDA a=0.75 DENS.

```
        TOP RECORD
0000100 0.13366722E-01 0.13365429E-01 0.13364166E-01 0.13363015E-01 0.13361994E-01
0000200 0.13361182E-01 0.13360560E-01 0.13360195E-01 0.13360128E-01 0.13360344E-01
0000300 0.13360851E-01 0.13361640E-01 0.13362724E-01 0.13364043E-01 0.13365574E-01
0000400 0.13367273E-01 0.13369098E-01 0.13370987E-01 0.13372861E-01 0.13374660E-01
0000500 0.13376351E-01 0.13377830E-01 0.13379071E-01 0.13380002E-01 0.13380565E-01
0000600 0.13380755E-01 0.13380524E-01 0.13379883E-01 0.13378806E-01 0.13377331E-01
0000700 0.13375476E-01 0.13373300E-01 0.13370849E-01 0.13368189E-01 0.13365436E-01
0000800 0.13362631E-01 0.13359923E-01 0.13357352E-01 0.13355032E-01 0.13353076E-01
0000900 0.13351548E-01 0.13350535E-01 0.13350099E-01 0.13350271E-01 0.13351072E-01
0001000 0.13352543E-01 0.13354618E-01 0.13357282E-01 0.13360478E-01 0.13364106E-01
0001100 0.13368074E-01 0.13372257E-01 0.13376512E-01 0.13380680E-01 0.13384636E-01
0001200 0.13388205E-01 0.13391219E-01 0.13393573E-01 0.13395131E-01 0.13395749E-01
0001300 0.13395362E-01 0.13393909E-01 0.13391379E-01 0.13387807E-01 0.13383206E-01
0001400 0.13377700E-01 0.13371419E-01 0.13364527E-01 0.13357244E-01 0.13349835E-01
0001500 0.13342522E-01 0.13335615E-01 0.13329409E-01 0.13324209E-01 0.13320282E-01
0001600 0.13317924E-01 0.13317343E-01 0.13318744E-01 0.13322249E-01 0.13327923E-01
0001700 0.13335764E-01 0.13345674E-01 0.13357427E-01 0.13370737E-01 0.13385218E-01
0001800 0.13400298E-01 0.13415389E-01 0.13429701E-01 0.13442438E-01 0.13452638E-01
0001900 0.13459276E-01 0.13461296E-01 0.13457537E-01 0.13446841E-01 0.13428066E-01
0002000 0.13400063E-01 0.13361756E-01 0.13312180E-01 0.13250425E-01 0.13175771E-01
0002100 0.13087686E-01 0.12985833E-01 0.12870088E-01 0.12740687E-01 0.12598015E-01
0002200 0.12442868E-01 0.12276344E-01 0.12099840E-01 0.11915099E-01 0.11724155E-01
0002300 0.11529371E-01 0.11333410E-01 0.11139195E-01 0.10949910E-01 0.10768931E-01
0002400 0.10599844E-01 0.10446470E-01 0.10312676E-01 0.10202628E-01 0.10120444E-01
0002500 0.10069691E-01 0.10052614E-01 0.10069691E-01 0.10120444E-01 0.10202628E-01
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953626E 00-0.26953262E 00-0.26953065E 00-0.26952755E 00-0.26952738E 00
0000200-0.26953357E 00-0.26953351E 00-0.26953340E 00-0.26953602E 00-0.26953936E 00
0000300-0.26954341E 00-0.26954091E 00-0.26954681E 00-0.26954550E 00-0.26954556E 00
0000400-0.26955169E 00-0.26955122E 00-0.26955694E 00-0.26955563E 00-0.26955438E 00
0000500-0.26955426E 00-0.26955384E 00-0.26955473E 00-0.26955539E 00-0.26955485E 00
0000600-0.26955521E 00-0.26955700E 00-0.26955700E 00-0.26955575E 00-0.26955634E 00
0000700-0.26955599E 00-0.26955575E 00-0.26955569E 00-0.26955444E 00-0.26955330E 00
0000800-0.26955235E 00-0.26954985E 00-0.26954693E 00-0.26954353E 00-0.26953965E 00
0000900-0.26953626E 00-0.26953185E 00-0.26952821E 00-0.26952475E 00-0.26952255E 00
0001000-0.26951963E 00-0.26951748E 00-0.26951635E 00-0.26951587E 00-0.26951647E 00
0001100-0.26951802E 00-0.26952004E 00-0.26952344E 00-0.26952797E 00-0.26953328E 00
0001200-0.26954025E 00-0.26954693E 00-0.26955462E 00-0.26956201E 00-0.26956987E 00
0001300-0.26957721E 00-0.26958394E 00-0.26959014E 00-0.26959538E 00-0.26959866E 00
0001400-0.26960051E 00-0.26960003E 00-0.26959711E 00-0.26959223E 00-0.26958472E 00
0001500-0.26957506E 00-0.26956290E 00-0.26954877E 00-0.26953292E 00-0.26951593E 00
0001600-0.26949841E 00-0.26948082E 00-0.26946449E 00-0.26944953E 00-0.26943779E 00
0001700-0.26942956E 00-0.26942509E 00-0.26942545E 00-0.26943183E 00-0.26944399E 00
0001800-0.26946157E 00-0.26948351E 00-0.26950961E 00-0.26953751E 00-0.26956457E 00
0001900-0.26958752E 00-0.26960158E 00-0.26960069E 00-0.26957786E 00-0.26952416E 00
0002000-0.26943004E 00-0.26928365E 00-0.26907134E 00-0.26877803E 00-0.26838660E 00
0002100-0.26787829E 00-0.26723206E 00-0.26642525E 00-0.26543385E 00-0.26423293E 00
0002200-0.26279503E 00-0.26109338E 00-0.25910014E 00-0.25678700E 00-0.25412750E 00
0002300-0.25109500E 00-0.24766606E 00-0.24381846E 00-0.23953348E 00-0.23479623E 00
0002400-0.22959709E 00-0.22392982E 00-0.21779567E 00-0.21120107E 00-0.20555174E 00
0002500-0.20175105E 00-0.20121896E 00-0.20175105E 00-0.20555174E 00-0.21120107E 00
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
```

ZN+ LDA a=1.0 DENS.

```
        TOP RECORD
0000100 0.13367061E-01 0.13363246E-01 0.13359800E-01 0.13357207E-01 0.13355926E-01
0000200 0.13356242E-01 0.13358217E-01 0.13361651E-01 0.13366226E-01 0.13371401E-01
0000300 0.13376448E-01 0.13380699E-01 0.13383485E-01 0.13384271E-01 0.13382800E-01
0000400 0.13379078E-01 0.13373423E-01 0.13366487E-01 0.13359066E-01 0.13352238E-01
0000500 0.13346981E-01 0.13344258E-01 0.13344701E-01 0.13348572E-01 0.13355680E-01
0000600 0.13365392E-01 0.13376564E-01 0.13387751E-01 0.13397310E-01 0.13403606E-01
0000700 0.13405260E-01 0.13401404E-01 0.13391811E-01 0.13377111E-01 0.13358727E-01
0000800 0.13338890E-01 0.13320465E-01 0.13306577E-01 0.13300255E-01 0.13303939E-01
0000900 0.13319049E-01 0.13345376E-01 0.13380777E-01 0.13420898E-01 0.13459090E-01
0001000 0.13486482E-01 0.13492461E-01 0.13465330E-01 0.13393175E-01 0.13265051E-01
0001100 0.13072260E-01 0.12809593E-01 0.12476645E-01 0.12078658E-01 0.11627194E-01
0001200 0.11140145E-01 0.10641221E-01 0.10159075E-01 0.97262003E-02 0.93777888E-02
0001300 0.91499574E-02 0.90721548E-02 0.91499574E-02 0.93777888E-02 0.97262003E-02
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953620E 00-0.26952744E 00-0.26952434E 00-0.26952094E 00-0.26951480E 00
0000200-0.26951593E 00-0.26951867E 00-0.26952040E 00-0.26952332E 00-0.26953179E 00
0000300-0.26953608E 00-0.26954019E 00-0.26954579E 00-0.26955193E 00-0.26955450E 00
0000400-0.26955712E 00-0.26955670E 00-0.26955348E 00-0.26954752E 00-0.26953834E 00
0000500-0.26952839E 00-0.26951736E 00-0.26950914E 00-0.26950157E 00-0.26949996E 00
0000600-0.26950210E 00-0.26950926E 00-0.26952159E 00-0.26953882E 00-0.26955885E 00
0000700-0.26957834E 00-0.26959538E 00-0.26960599E 00-0.26960796E 00-0.26959807E 00
0000800-0.26957548E 00-0.26954144E 00-0.26949853E 00-0.26945305E 00-0.26941162E 00
0000900-0.26938432E 00-0.26937783E 00-0.26940089E 00-0.26945317E 00-0.26952827E 00
0001000-0.26960623E 00-0.26965064E 00-0.26959956E 00-0.26936603E 00-0.26882857E 00
0001100-0.26782948E 00-0.26617247E 00-0.26362497E 00-0.25992358E 00-0.25478518E 00
0001200-0.24792278E 00-0.23906791E 00-0.22799617E 00-0.21455485E 00-0.19907498E 00
0001300-0.18487686E 00-0.18279499E 00-0.18487686E 00-0.19907498E 00-0.21455485E 00
EOF
q
```

```
redit potel0
LOADING POTE10
REKEYED
EDIT
p99
```

ZN+ LDA a=2.0 DENS.

```
        TOP RECORD
0000100 0.13373714E-01 0.13366055E-01 0.13358120E-01 0.13351038E-01 0.13345812E-01
0000200 0.13343252E-01 0.13343904E-01 0.13347890E-01 0.13354894E-01 0.13364084E-01
0000300 0.13374392E-01 0.13384450E-01 0.13392821E-01 0.13398208E-01 0.13399612E-01
0000400 0.13396513E-01 0.13388950E-01 0.13377659E-01 0.13363872E-01 0.13349351E-01
0000500 0.13336129E-01 0.13326202E-01 0.13321340E-01 0.13322756E-01 0.13330895E-01
0000600 0.13345279E-01 0.13364524E-01 0.13386354E-01 0.13407856E-01 0.13425849E-01
0000700 0.13437234E-01 0.13439454E-01 0.13430972E-01 0.13411626E-01 0.13382770E-01
0000800 0.13347454E-01 0.13310131E-01 0.13276339E-01 0.13251979E-01 0.13242662E-01
0000900 0.13252720E-01 0.13284236E-01 0.13336286E-01 0.13404187E-01 0.13479184E-01
0001000 0.13548359E-01 0.13595138E-01 0.13600159E-01 0.13542727E-01 0.13402645E-01
0001100 0.13162386E-01 0.12809448E-01 0.12338534E-01 0.11753287E-01 0.11067346E-01
0001200 0.10304265E-01 0.94963089E-02 0.86822100E-02 0.79042204E-02 0.72052404E-02
0001300 0.66259354E-02 0.61968602E-02 0.59343092E-02 0.58465898E-02 0.59343092E-02
EOF
q
redit potel1
LOADING POTE11
REKEYED
EDIT
p99
```

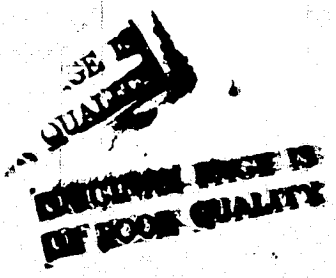
VEFF

```
        TOP RECORD
0000100-0.26953626E 00-0.26951540E 00-0.26950437E 00-0.26949513E 00-0.26948225E 00
0000200-0.26947987E 00-0.26947773E 00-0.26947784E 00-0.26947999E 00-0.26949018E 00
0000300-0.26949453E 00-0.26950461E 00-0.26951659E 00-0.26952982E 00-0.26954001E 00
0000400-0.26954842E 00-0.26955330E 00-0.26955235E 00-0.26954550E 00-0.26953292E 00
0000500-0.26951671E 00-0.26949728E 00-0.26947957E 00-0.26946318E 00-0.26945359E 00
0000600-0.26944989E 00-0.26945484E 00-0.26947045E 00-0.26949489E 00-0.26952618E 00
0000700-0.26956117E 00-0.26959538E 00-0.26962388E 00-0.26964080E 00-0.26964074E 00
0000800-0.26962078E 00-0.26958025E 00-0.26952136E 00-0.26945049E 00-0.26937866E 00
0000900-0.26931965E 00-0.26928854E 00-0.26929992E 00-0.26936269E 00-0.26947707E 00
0001000-0.26962674E 00-0.26977402E 00-0.26984864E 00-0.26974207E 00-0.26929379E 00
0001100-0.26828736E 00-0.26644003E 00-0.26340199E 00-0.25875878E 00-0.25204194E 00
0001200-0.24274856E 00-0.23037291E 00-0.21444374E 00-0.19457060E 00-0.17048848E 00
0001300-0.14730012E 00-0.13110811E 00-0.12036180E 00-0.11846614E 00-0.12036180E 00
EOF
q
```

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.13380539E-01 0.13382759E-01 0.13382833E-01 0.13380654E-01 0.13376422E-01
0000200 0.13370637E-01 0.13364058E-01 0.13357546E-01 0.13352014E-01 0.13348330E-01
0000300 0.13347086E-01 0.13348620E-01 0.13352837E-01 0.13359323E-01 0.13367314E-01
0000400 0.13375800E-01 0.13383623E-01 0.13389651E-01 0.13392981E-01 0.13392951E-01
0000500 0.13389394E-01 0.13382550E-01 0.13373230E-01 0.13362527E-01 0.13351884E-01
0000600 0.13342772E-01 0.13336584E-01 0.13334371E-01 0.13336711E-01 0.13343602E-01
0000700 0.13354409E-01 0.13367847E-01 0.13382256E-01 0.13395663E-01 0.13406076E-01
0000800 0.13411798E-01 0.13411637E-01 0.13405111E-01 0.13392597E-01 0.13375394E-01
0000900 0.13355490E-01 0.13335522E-01 0.13318285E-01 0.13306532E-01 0.13302490E-01
0001000 0.13307463E-01 0.13321664E-01 0.13343967E-01 0.13372056E-01 0.13402481E-01
0001100 0.13431080E-01 0.13453510E-01 0.13465736E-01 0.13464775E-01 0.13449132E-01
0001200 0.13419300E-01 0.13377883E-01 0.13329647E-01 0.13281088E-01 0.13239756E-01
0001300 0.13213404E-01 0.13208847E-01 0.13230719E-01 0.13280306E-01 0.13354555E-01
0001400 0.13445340E-01 0.13539162E-01 0.13617456E-01 0.13657492E-01 0.13633739E-01
0001500 0.13520155E-01 0.13292741E-01 0.12932483E-01 0.12428302E-01 0.11779651E-01
0001600 0.10998085E-01 0.10107782E-01 0.91442093E-02 0.81511587E-02 0.71766600E-02
0001700 0.62682182E-02 0.54679364E-02 0.48038289E-02 0.42878240E-02 0.39220676E-02
0001800 0.37043442E-02 0.36323301E-02 0.37043442E-02 0.39220676E-02 0.42878240E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26953411E 00-0.26954114E 00-0.26955009E 00-0.26955134E 00-0.26955587E 00
0000200-0.26955378E 00-0.26955670E 00-0.26954854E 00-0.26954359E 00-0.26954210E 00
0000300-0.26953733E 00-0.26953495E 00-0.26953381E 00-0.26952970E 00-0.26953328E 00
0000400-0.26953512E 00-0.26953924E 00-0.26954198E 00-0.26954859E 00-0.26955175E 00
0000500-0.26955515E 00-0.26955503E 00-0.26955193E 00-0.26954794E 00-0.26954460E 00
0000600-0.26953703E 00-0.26953661E 00-0.26953262E 00-0.26952726E 00-0.26952428E 00
0000700-0.26952803E 00-0.26952916E 00-0.26953363E 00-0.26954037E 00-0.26954889E 00
0000800-0.26955318E 00-0.26955825E 00-0.26956123E 00-0.26956010E 00-0.26955569E 00
0000900-0.26954526E 00-0.26953328E 00-0.26951832E 00-0.26950622E 00-0.26949233E 00
0001000-0.26948339E 00-0.26947618E 00-0.26947421E 00-0.26947880E 00-0.26949084E 00
0001100-0.26951015E 00-0.26953614E 00-0.26956761E 00-0.26960254E 00-0.26963687E 00
0001200-0.26966578E 00-0.26968336E 00-0.26968539E 00-0.26966757E 00-0.26962906E 00
0001300-0.26957124E 00-0.26950151E 00-0.26943058E 00-0.26937377E 00-0.26934582E 00
0001400-0.26935846E 00-0.26941389E 00-0.26949477E 00-0.26955366E 00-0.26950145E 00
0001500-0.26919192E 00-0.26840955E 00-0.26685190E 00-0.26412106E 00-0.25971723E 00
0001600-0.25304210E 00-0.24342066E 00-0.23013175E 00-0.21245611E 00-0.18973577E 00
0001700-0.16155314E 00-0.13337690E 00-0.11053497E 00-0.92852592E-01-0.80389261E-01
0001800-0.72268784E-01-0.70612133E-01-0.72268784E-01-0.80389261E-01-0.92852592E-01
EOF
q
```

ZN+ LDA a=3.0 DENS.

VEFF




```
redit pote14
LOADING POTE14   ZN+ LDA a=5.0
REKEYED          DENS.
EDIT
p99
        TOP RECORD
0000100 0.13389897E-01 0.13392050E-01 0.13391048E-01 0.13386868E-01 0.13379939E-01
0000200 0.13371054E-01 0.13361279E-01 0.13351940E-01 0.13344370E-01 0.13339639E-01
0000300 0.13338570E-01 0.13341453E-01 0.13348136E-01 0.13357870E-01 0.13369501E-01
0000400 0.13381492E-01 0.13392244E-01 0.13400178E-01 0.13404086E-01 0.13403140E-01
0000500 0.13397235E-01 0.13386898E-01 0.13373308E-01 0.13358150E-01 0.13343494E-01
0000600 0.13331357E-01 0.13323650E-01 0.13321664E-01 0.13326086E-01 0.13336718E-01
0000700 0.13352491E-01 0.13371501E-01 0.13391320E-01 0.13409190E-01 0.13422444E-01
0000800 0.13428863E-01 0.13426963E-01 0.13416398E-01 0.13397969E-01 0.13373613E-01
0000900 0.13346326E-01 0.13319775E-01 0.13297770E-01 0.13283875E-01 0.13280839E-01
0001000 0.13290036E-01 0.13311308E-01 0.13342720E-01 0.13380703E-01 0.13420351E-01
0001100 0.13456039E-01 0.13482057E-01 0.13493463E-01 0.13486929E-01 0.13461255E-01
0001200 0.13418071E-01 0.13361767E-01 0.13299368E-01 0.13239868E-01 0.13193257E-01
0001300 0.13169155E-01 0.13175294E-01 0.13216015E-01 0.13290748E-01 0.13393063E-01
0001400 0.13509870E-01 0.13621595E-01 0.13702881E-01 0.13724234E-01 0.13654333E-01
0001500 0.13463166E-01 0.13125494E-01 0.12624525E-01 0.11955131E-01 0.11126190E-01
0001600 0.10161255E-01 0.90974122E-02 0.79818480E-02 0.68668835E-02 0.58038794E-02
0001700 0.48370175E-02 0.39938726E-02 0.32833719E-02 0.27021605E-02 0.22402275E-02
0001800 0.18849808E-02 0.16237812E-02 0.14456338E-02 0.13421862E-02 0.13083101E-02
EOF
q
redit pote15
LOADING POTE15   VEFF
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26952553E 00-0.26952362E 00-0.26952142E 00-0.26952529E 00-0.26952070E 00
0000200-0.26952583E 00-0.26952052E 00-0.26951545E 00-0.26951420E 00-0.26951128E 00
0000300-0.26950973E 00-0.26951170E 00-0.26950485E 00-0.26950943E 00-0.26950961E 00
0000400-0.26951575E 00-0.26952374E 00-0.26953071E 00-0.26954013E 00-0.26954526E 00
0000500-0.26954865E 00-0.26954871E 00-0.26954871E 00-0.26954442E 00-0.26953417E 00
0000600-0.26952696E 00-0.26951945E 00-0.26950943E 00-0.26950079E 00-0.26949906E 00
0000700-0.26949853E 00-0.26950318E 00-0.26951259E 00-0.26952684E 00-0.26954156E 00
0000800-0.26955557E 00-0.26956838E 00-0.26957500E 00-0.26957601E 00-0.26956576E 00
0000900-0.26954991E 00-0.26952821E 00-0.26950163E 00-0.26947463E 00-0.26945180E 00
0001000-0.26943469E 00-0.26942724E 00-0.26943082E 00-0.26944786E 00-0.26947695E 00
0001100-0.26951557E 00-0.26956129E 00-0.26960933E 00-0.26965332E 00-0.26968729E 00
0001200-0.26970416E 00-0.26969904E 00-0.26966906E 00-0.26961619E 00-0.26954603E 00
0001300-0.26947081E 00-0.26940459E 00-0.26936668E 00-0.26937389E 00-0.26943916E 00
0001400-0.26956421E 00-0.26973087E 00-0.26989180E 00-0.26995778E 00-0.26978248E 00
0001500-0.26914960E 00-0.26775461E 00-0.26519340E 00-0.26095432E 00-0.25441730E 00
0001600-0.24486911E 00-0.23152602E 00-0.21358085E 00-0.19025105E 00-0.16083723E 00
0001700-0.13040465E 00-0.10413253E 00-0.81582844E-01-0.62395237E-01-0.46110131E-01
0001800-0.32847974E-01-0.22505261E-01-0.15075821E-01-0.10362759E-01-0.91489553E-02
EOF
q
```

```
redit potel6
LOADING POTE16
REKEYED
EDIT
p99
```

ZN+ LDA a=10.0 DENS.

```
        TOP RECORD
0000100 0.13384115E-01 0.13392244E-01 0.13397265E-01 0.13398368E-01 0.13395291E-01
0000200 0.13388272E-01 0.13378158E-01 0.13366215E-01 0.13353992E-01 0.13343249E-01
0000300 0.13335492E-01 0.13331939E-01 0.13333313E-01 0.13339579E-01 0.13350192E-01
0000400 0.13363831E-01 0.13378803E-01 0.13393071E-01 0.13404623E-01 0.13411701E-01
0000500 0.13413064E-01 0.13408236E-01 0.13397496E-01 0.13382062E-01 0.13363764E-01
0000600 0.13344988E-01 0.13328351E-01 0.13316255E-01 0.13310663E-01 0.13312757E-01
0000700 0.13322733E-01 0.13339691E-01 0.13361726E-01 0.13386101E-01 0.13409533E-01
0000800 0.13428707E-01 0.13440613E-01 0.13443049E-01 0.13434999E-01 0.13416827E-01
0000900 0.13390310E-01 0.13358600E-01 0.13325769E-01 0.13296414E-01 0.13275001E-01
0001000 0.13265267E-01 0.13269618E-01 0.13288666E-01 0.13320941E-01 0.13363000E-01
0001100 0.13409615E-01 0.13454400E-01 0.13490558E-01 0.13511743E-01 0.13513181E-01
0001200 0.13492379E-01 0.13449844E-01 0.13389394E-01 0.13318099E-01 0.13245568E-01
0001300 0.13183098E-01 0.13142142E-01 0.13132643E-01 0.13161264E-01 0.13229631E-01
0001400 0.13333045E-01 0.13459563E-01 0.13589833E-01 0.13697736E-01 0.13752092E-01
0001500 0.13718918E-01 0.13564929E-01 0.13261300E-01 0.12787670E-01 0.12135882E-01
0001600 0.11312570E-01 0.10340180E-01 0.92557594E-02 0.81075579E-02 0.69496557E-02
0001700 0.58355145E-02 0.48113093E-02 0.39063543E-02 0.31309482E-02 0.24823574E-02
0001800 0.19502214E-02 0.15204542E-02 0.11778632E-02 0.90774382E-03 0.69675455E-03
0001900 0.53329905E-03 0.40760660E-03 0.31164009E-03 0.23891368E-03 0.18428385E-03
0002000 0.14373740E-03 0.11419941E-03 0.93369847E-04 0.79591904E-04 0.71751580E-04
0002100 0.69207948E-04 0.71751580E-04 0.79591904E-04 0.93369847E-04 0.11419941E-03
EOF
q
redit potel7
LOADING POTE17
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953560E 00-0.26955378E 00-0.26957148E 00-0.26958334E 00-0.26959550E 00
0000200-0.26959324E 00-0.26959997E 00-0.26959240E 00-0.26958013E 00-0.26957065E 00
0000300-0.26955873E 00-0.26955003E 00-0.26954269E 00-0.26952726E 00-0.26952797E 00
0000400-0.26952296E 00-0.26952839E 00-0.26953530E 00-0.26954603E 00-0.26955670E 00
0000500-0.26956689E 00-0.26957053E 00-0.26956993E 00-0.26956952E 00-0.26955956E 00
0000600-0.26954472E 00-0.26953536E 00-0.26952124E 00-0.26950568E 00-0.26949161E 00
0000700-0.26948506E 00-0.26948076E 00-0.26948422E 00-0.26949471E 00-0.26951295E 00
0000800-0.26953489E 00-0.26955956E 00-0.26958269E 00-0.26960039E 00-0.26960862E 00
0000900-0.26960492E 00-0.26958883E 00-0.26955968E 00-0.26952153E 00-0.26947755E 00
0001000-0.26943415E 00-0.26939714E 00-0.26937240E 00-0.26936561E 00-0.26937997E 00
0001100-0.26941538E 00-0.26946956E 00-0.26953691E 00-0.26960939E 00-0.26967478E 00
0001200-0.26972163E 00-0.26973653E 00-0.26971120E 00-0.26964092E 00-0.26952887E 00
0001300-0.26938725E 00-0.26923788E 00-0.26910841E 00-0.26903117E 00-0.26903486E 00
0001400-0.26914012E 00-0.26934981E 00-0.26964444E 00-0.26996672E 00-0.27021807E 00
0001500-0.27023900E 00-0.26980054E 00-0.26858920E 00-0.26619554E 00-0.26211119E 00
0001600-0.25573283E 00-0.24637729E 00-0.23330629E 00-0.21576327E 00-0.19301564E 00
0001700-0.16439807E 00-0.13462204E 00-0.10846359E 00-0.85451007E-01-0.65150082E-01
0001800-0.47176819E-01-0.31193919E-01-0.16920190E-01-0.41195154E-02 0.74020140E-02
0001900 0.17801665E-01 0.27202878E-01 0.35698626E-01 0.43351851E-01 0.50195470E-01
0002000 0.56224748E-01 0.61400361E-01 0.65636396E-01 0.68812430E-01 0.70807099E-01
0002100 0.71466029E-01 0.70807099E-01 0.68812430E-01 0.65636396E-01 0.61400361E-01
EOF
q
```

```
redit potel8
LOADING POTE18
REKEYED
EDIT
p99
```

ZN+ LDA a=150 DENS.

```
        TOP RECORD
0000100 0.13386820E-01 0.13394982E-01 0.13399936E-01 0.13400912E-01 0.13397582E-01
0000200 0.13390243E-01 0.13379734E-01 0.13367355E-01 0.13354737E-01 0.13343576E-01
0000300 0.13335500E-01 0.13331734E-01 0.13332956E-01 0.13339244E-01 0.13349935E-01
0000400 0.13363745E-01 0.13378911E-01 0.13393380E-01 0.13405096E-01 0.13412308E-01
0000500 0.13413712E-01 0.13408821E-01 0.13397947E-01 0.13382263E-01 0.13363674E-01
0000600 0.13344590E-01 0.13327617E-01 0.13315257E-01 0.13309497E-01 0.13311565E-01
0000700 0.13321616E-01 0.13338801E-01 0.13361156E-01 0.13385911E-01 0.13409767E-01
0000800 0.13429306E-01 0.13441466E-01 0.13444055E-01 0.13435937E-01 0.13417531E-01
0000900 0.13390616E-01 0.13358358E-01 0.13324916E-01 0.13294946E-01 0.13272997E-01
0001000 0.13262883E-01 0.13267059E-01 0.13286188E-01 0.13318826E-01 0.13361506E-01
0001100 0.13408951E-01 0.13454683E-01 0.13491768E-01 0.13513811E-01 0.13515875E-01
0001200 0.13495386E-01 0.13452820E-01 0.13391957E-01 0.13319883E-01 0.13246320E-01
0001300 0.13182640E-01 0.13140459E-01 0.13129871E-01 0.13157662E-01 0.13225608E-01
0001400 0.13329081E-01 0.13456199E-01 0.13587583E-01 0.13697125E-01 0.13753414E-01
0001500 0.13722420E-01 0.13570651E-01 0.13269134E-01 0.12797385E-01 0.12147095E-01
0001600 0.11324879E-01 0.10353118E-01 0.92688724E-02 0.81203990E-02 0.69617443E-02
0001700 0.58463924E-02 0.48205070E-02 0.39134957E-02 0.31357887E-02 0.24848229E-02
0001800 0.19503641E-02 0.15184190E-02 0.11738401E-02 0.90193748E-03 0.68934937E-03
0001900 0.52443612E-03 0.39736507E-03 0.30002138E-03 0.22582646E-03 0.16952414E-03
0002000 0.12696489E-03 0.94903618E-04 0.70823764E-04 0.52787494E-04 0.39311650E-04
0002100 0.29267045E-04 0.21798187E-04 0.16259975E-04 0.12168086E-04 0.91608272E-05
0002200 0.69699236E-05 0.53983440E-05 0.43037735E-05 0.35865069E-05 0.31809077E-05
0002300 0.30497304E-05 0.31809077E-05 0.35865069E-05 0.43037735E-05 0.53983440E-05
EOF
q
redit potel9
LOADING POTE19
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953620E 00-0.26955515E 00-0.26956958E 00-0.26957881E 00-0.26958817E 00
0000200-0.26958066E 00-0.26958561E 00-0.26957279E 00-0.26955432E 00-0.26953971E 00
0000300-0.26952320E 00-0.26951253E 00-0.26950383E 00-0.26948750E 00-0.26949018E 00
0000400-0.26948684E 00-0.26949358E 00-0.26949960E 00-0.26950651E 00-0.26952291E 00
0000500-0.26953590E 00-0.26954174E 00-0.26954061E 00-0.26954198E 00-0.26953334E 00
0000600-0.26951939E 00-0.26950717E 00-0.26949275E 00-0.26947725E 00-0.26946187E 00
0000700-0.26945829E 00-0.26945478E 00-0.26946074E 00-0.26947522E 00-0.26949781E 00
0000800-0.26952475E 00-0.26955378E 00-0.26958090E 00-0.26960069E 00-0.26961094E 00
0000900-0.26960772E 00-0.26959097E 00-0.26955986E 00-0.26951951E 00-0.26947290E 00
0001000-0.26942784E 00-0.26939154E 00-0.26936877E 00-0.26936579E 00-0.26938683E 00
0001100-0.26942933E 00-0.26949179E 00-0.26956761E 00-0.26964623E 00-0.26971668E 00
0001200-0.26976401E 00-0.26977575E 00-0.26974338E 00-0.26966238E 00-0.26953673E 00
0001300-0.26938117E 00-0.26921892E 00-0.26907969E 00-0.26899743E 00-0.26900232E 00
0001400-0.26911432E 00-0.26933628E 00-0.26964647E 00-0.26998603E 00-0.27025449E 00
0001500-0.27028966E 00-0.26986068E 00-0.26865220E 00-0.26625448E 00-0.26216167E 00
0001600-0.25577343E 00-0.24641371E 00-0.23335427E 00-0.21585119E 00-0.19318479E 00
0001700-0.16470361E 00-0.13506931E 00-0.10900527E 00-0.86047173E-01-0.65764904E-01
0001800-0.47779795E-01-0.31754881E-01-0.17409496E-01-0.45054406E-02 0.71560554E-02
0001900 0.17741021E-01 0.27386054E-01 0.36204677E-01 0.44290867E-01 0.51723160E-01
0002000 0.58506745E-01 0.64874291E-01 0.70696473E-01 0.76070726E-01 0.81029058E-01
0002100 0.85600019E-01 0.89806199E-01 0.93664467E-01 0.97184539E-01 0.10036719E 00
0002200 0.10320216E 00 0.10566121E 00 0.10769814E 00 0.10924143E 00 0.11021340E 00
0002300 0.11054569E 00 0.11021340E 00 0.10924143E 00 0.10769814E 00 0.10566121E 00
EOF
q
```

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
```

ZN+ NL a=0.25 DENS.

```
        TOP RECORD
0000100 0.13364919E-01 0.13364341E-01 0.13363767E-01 0.13363224E-01 0.13362736E-01
0000200 0.13362307E-01 0.13361972E-01 0.13361733E-01 0.13361610E-01 0.13361618E-01
0000300 0.13361726E-01 0.13361972E-01 0.13362344E-01 0.13362814E-01 0.13363373E-01
0000400 0.13364028E-01 0.13364717E-01 0.13365462E-01 0.13366219E-01 0.13366982E-01
0000500 0.13367716E-01 0.13368387E-01 0.13369028E-01 0.13369538E-01 0.13369977E-01
0000600 0.13370290E-01 0.13370492E-01 0.13370547E-01 0.13370510E-01 0.13370335E-01
0000700 0.13370041E-01 0.13369642E-01 0.13369173E-01 0.13368629E-01 0.13368044E-01
0000800 0.13367452E-01 0.13366845E-01 0.13366278E-01 0.13365783E-01 0.13365362E-01
0000900 0.13365060E-01 0.13364870E-01 0.13364863E-01 0.13364989E-01 0.13365280E-01
0001000 0.13365749E-01 0.13366368E-01 0.13367157E-01 0.13368051E-01 0.13369098E-01
0001100 0.13370197E-01 0.13371345E-01 0.13372488E-01 0.13373625E-01 0.13374679E-01
0001200 0.13375603E-01 0.13376404E-01 0.13376977E-01 0.13377316E-01 0.13377406E-01
0001300 0.13377227E-01 0.13376743E-01 0.13375964E-01 0.13374891E-01 0.13373557E-01
0001400 0.13371971E-01 0.13370190E-01 0.13368271E-01 0.13366252E-01 0.13364211E-01
0001500 0.13362236E-01 0.13360385E-01 0.13358783E-01 0.13357442E-01 0.13356507E-01
0001600 0.13356034E-01 0.13356026E-01 0.13356615E-01 0.13357770E-01 0.13359502E-01
0001700 0.13361823E-01 0.13364676E-01 0.13367970E-01 0.13371613E-01 0.13375439E-01
0001800 0.13379313E-01 0.13383001E-01 0.13386261E-01 0.13388842E-01 0.13390448E-01
0001900 0.13390698E-01 0.13389308E-01 0.13385873E-01 0.13380073E-01 0.13371520E-01
0002000 0.13359807E-01 0.13344668E-01 0.13325728E-01 0.13302740E-01 0.13275448E-01
0002100 0.13243683E-01 0.13207369E-01 0.13166413E-01 0.13120908E-01 0.13070978E-01
0002200 0.13016917E-01 0.12959033E-01 0.12897860E-01 0.12833953E-01 0.12768071E-01
0002300 0.12701053E-01 0.12633845E-01 0.12567542E-01 0.12503389E-01 0.12442656E-01
0002400 0.12386788E-01 0.12337301E-01 0.12295816E-01 0.12264043E-01 0.12243666E-01
0002500 0.12236711E-01 0.12243666E-01 0.12264043E-01 0.12295816E-01 0.12337301E-01
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953518E 00-0.26951760E 00-0.26950526E 00-0.26949644E 00-0.26948649E 00
0000200-0.26947945E 00-0.26947629E 00-0.26947182E 00-0.26946920E 00-0.26946801E 00
0000300-0.26946861E 00-0.26947135E 00-0.26947165E 00-0.26947612E 00-0.26947987E 00
0000400-0.26948434E 00-0.26949060E 00-0.26949310E 00-0.26949418E 00-0.26950032E 00
0000500-0.26950657E 00-0.26951385E 00-0.26951557E 00-0.26951814E 00-0.26952052E 00
0000600-0.26952308E 00-0.26952666E 00-0.26953030E 00-0.26953310E 00-0.26953578E 00
0000700-0.26953936E 00-0.26954240E 00-0.26954669E 00-0.26954955E 00-0.26955229E 00
0000800-0.26955515E 00-0.26955819E 00-0.26956010E 00-0.26956183E 00-0.26956290E 00
0000900-0.26956397E 00-0.26956493E 00-0.26956457E 00-0.26956433E 00-0.26956397E 00
0001000-0.26956326E 00-0.26956284E 00-0.26956147E 00-0.26956016E 00-0.26955920E 00
0001100-0.26955777E 00-0.26955646E 00-0.26955491E 00-0.26955372E 00-0.26955289E 00
0001200-0.26955265E 00-0.26955253E 00-0.26955223E 00-0.26955336E 00-0.26955402E 00
0001300-0.26955521E 00-0.26955670E 00-0.26955855E 00-0.26956052E 00-0.26956230E 00
0001400-0.26956463E 00-0.26956671E 00-0.26956803E 00-0.26956964E 00-0.26957107E 00
0001500-0.26957154E 00-0.26957113E 00-0.26957071E 00-0.26957005E 00-0.26956880E 00
0001600-0.26956666E 00-0.26956445E 00-0.26956165E 00-0.26955789E 00-0.26955497E 00
0001700-0.26955092E 00-0.26954705E 00-0.26954377E 00-0.26954043E 00-0.26953709E 00
0001800-0.26953346E 00-0.26952922E 00-0.26952410E 00-0.26951718E 00-0.26950753E 00
0001900-0.26949376E 00-0.26947457E 00-0.26944828E 00-0.26941204E 00-0.26936287E 00
0002000-0.26929760E 00-0.26921302E 00-0.26910377E 00-0.26896554E 00-0.26879293E 00
0002100-0.26857990E 00-0.26831955E 00-0.26800549E 00-0.26762933E 00-0.26718336E 00
0002200-0.26665974E 00-0.26604980E 00-0.26534462E 00-0.26453543E 00-0.26361443E 00
0002300-0.26257312E 00-0.26140487E 00-0.26010138E 00-0.25865704E 00-0.25706744E 00
0002400-0.25532895E 00-0.25344068E 00-0.25139844E 00-0.24934679E 00-0.24655432E 00
0002500-0.24607551E 00-0.24655432E 00-0.24934679E 00-0.25139844E 00-0.25344065E 00
```

```
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.13366405E-01 0.13365142E-01 0.13364159E-01 0.13363674E-01 0.13363805E-01
0000200 0.13364606E-01 0.13366047E-01 0.13367996E-01 0.13370272E-01 0.13372567E-01
0000300 0.13374649E-01 0.13376232E-01 0.13377082E-01 0.13377037E-01 0.13376087E-01
0000400 0.13374273E-01 0.13371795E-01 0.13368949E-01 0.13366114E-01 0.13363700E-01
0000500 0.13362072E-01 0.13361551E-01 0.13362337E-01 0.13364397E-01 0.13367597E-01
0000600 0.13371583E-01 0.13375800E-01 0.13379689E-01 0.13382569E-01 0.13383906E-01
0000700 0.13383247E-01 0.13380434E-01 0.13375565E-01 0.13369132E-01 0.13361908E-01
0000800 0.13354924E-01 0.13349406E-01 0.13346560E-01 0.13347395E-01 0.13352580E-01
0000900 0.13362087E-01 0.13375115E-01 0.13389964E-01 0.13403900E-01 0.13413131E-01
0001000 0.13413049E-01 0.13398439E-01 0.13363708E-01 0.13303537E-01 0.13213351E-01
0001100 0.13089888E-01 0.12931816E-01 0.12740370E-01 0.12519646E-01 0.12277007E-01
0001200 0.12023155E-01 0.11771977E-01 0.11540424E-01 0.11347972E-01 0.11215612E-01
0001300 0.11169437E-01 0.11215612E-01 0.11347972E-01 0.11540424E-01 0.11771977E-01
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26953578E 00-0.26953751E 00-0.26954269E 00-0.26954842E 00-0.26955479E 00
0000200-0.26955920E 00-0.26956433E 00-0.26957077E 00-0.26957393E 00-0.26956850E 00
0000300-0.26957434E 00-0.26957035E 00-0.26957065E 00-0.26957375E 00-0.26957703E 00
0000400-0.26958209E 00-0.26958835E 00-0.26959407E 00-0.26959860E 00-0.26960069E 00
0000500-0.26960105E 00-0.26959723E 00-0.26959151E 00-0.26958269E 00-0.26957178E 00
0000600-0.26956099E 00-0.26955014E 00-0.26954097E 00-0.26953578E 00-0.26953477E 00
0000700-0.26953816E 00-0.26954603E 00-0.26955831E 00-0.26957262E 00-0.26958847E 00
0000800-0.26960266E 00-0.26961607E 00-0.26962650E 00-0.26963371E 00-0.26963645E 00
0000900-0.26963598E 00-0.26963258E 00-0.26962459E 00-0.26960766E 00-0.26957339E 00
0001000-0.26950639E 00-0.26938283E 00-0.26916516E 00-0.26880425E 00-0.26823467E 00
0001100-0.26737529E 00-0.26612997E 00-0.26438886E 00-0.26203412E 00-0.25894284E 00
0001200-0.25499612E 00-0.25008947E 00-0.24411744E 00-0.23756284E 00-0.22770965E 00
0001300-0.22593158E 00-0.22770965E 00-0.23756284E 00-0.24411744E 00-0.25008947E 00
EOF
q
```

ZN+ NL a=0.5 DENS.

VEFF

```
redit pote6
LOADING POTE6
REKEYED
EDIT
p99
```

ZN+ NL a=0.75 DENS.

```
        TOP RECORD
0000100 0.13367295E-01 0.13366167E-01 0.13365034E-01 0.13364010E-01 0.13363115E-01
0000200 0.13362367E-01 0.13361804E-01 0.13361461E-01 0.13361342E-01 0.13361473E-01
0000300 0.13361875E-01 0.13362486E-01 0.13363380E-01 0.13364475E-01 0.13365753E-01
0000400 0.13367195E-01 0.13368722E-01 0.13370331E-01 0.13371907E-01 0.13373472E-01
0000500 0.13374913E-01 0.13376176E-01 0.13377249E-01 0.13378039E-01 0.13378546E-01
0000600 0.13378736E-01 0.13378590E-01 0.13378054E-01 0.13377175E-01 0.13375964E-01
0000700 0.13374437E-01 0.13372626E-01 0.13370588E-01 0.13368394E-01 0.13366081E-01
0000800 0.13363767E-01 0.13361476E-01 0.13359349E-01 0.13357416E-01 0.13355792E-01
0000900 0.13354510E-01 0.13353679E-01 0.13353311E-01 0.13353452E-01 0.13354138E-01
0001000 0.13355363E-01 0.13357118E-01 0.13359364E-01 0.13362061E-01 0.13365109E-01
0001100 0.13368446E-01 0.13371963E-01 0.13375528E-01 0.13379071E-01 0.13382420E-01
0001200 0.13385449E-01 0.13388034E-01 0.13390064E-01 0.13391424E-01 0.13392024E-01
0001300 0.13391823E-01 0.13390739E-01 0.13388775E-01 0.13385955E-01 0.13382323E-01
0001400 0.13377957E-01 0.13372984E-01 0.13367560E-01 0.13361849E-01 0.13356071E-01
0001500 0.13350438E-01 0.13345186E-01 0.13340574E-01 0.13336819E-01 0.13334185E-01
0001600 0.13332874E-01 0.13333056E-01 0.13334874E-01 0.13338406E-01 0.13343673E-01
0001700 0.13350658E-01 0.13359200E-01 0.13369087E-01 0.13380043E-01 0.13391610E-01
0001800 0.13403330E-01 0.13414588E-01 0.13424698E-01 0.13432857E-01 0.13438214E-01
0001900 0.13439823E-01 0.13436731E-01 0.13427861E-01 0.13412256E-01 0.13388805E-01
0002000 0.13356514E-01 0.13314463E-01 0.13261743E-01 0.13197672E-01 0.13121553E-01
0002100 0.13033003E-01 0.12931738E-01 0.12817737E-01 0.12691241E-01 0.12552723E-01
0002200 0.12402933E-01 0.12242906E-01 0.12074020E-01 0.11897873E-01 0.11716399E-01
0002300 0.11531789E-01 0.11346508E-01 0.11163250E-01 0.10984972E-01 0.10814760E-01
0002400 0.10655962E-01 0.10512054E-01 0.10386650E-01 0.10283548E-01 0.10206629E-01
0002500 0.10159124E-01 0.10143165E-01 0.10159124E-01 0.10206629E-01 0.10283548E-01
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953554E 00-0.26952821E 00-0.26953083E 00-0.26953393E 00-0.26953620E 00
0000200-0.26954114E 00-0.26954430E 00-0.26954758E 00-0.26954681E 00-0.26954561E 00
0000300-0.26954633E 00-0.26954526E 00-0.26954633E 00-0.26954663E 00-0.26954722E 00
0000400-0.26954770E 00-0.26954865E 00-0.26954281E 00-0.26954275E 00-0.26954323E 00
0000500-0.26954377E 00-0.26953793E 00-0.26953489E 00-0.26953214E 00-0.26953077E 00
0000600-0.26953030E 00-0.26953077E 00-0.26953161E 00-0.26953292E 00-0.26953506E 00
0000700-0.26953822E 00-0.26954222E 00-0.26954603E 00-0.26954859E 00-0.26955295E 00
0000800-0.26955730E 00-0.26955944E 00-0.26956248E 00-0.26956528E 00-0.26956558E 00
0000900-0.26956648E 00-0.26956606E 00-0.26956499E 00-0.26956332E 00-0.26956034E 00
0001000-0.26955634E 00-0.26955235E 00-0.26954865E 00-0.26954347E 00-0.26953757E 00
0001100-0.26953346E 00-0.26952922E 00-0.26952499E 00-0.26952213E 00-0.26951933E 00
0001200-0.26951832E 00-0.26951939E 00-0.26952124E 00-0.26952428E 00-0.26952940E 00
0001300-0.26953548E 00-0.26954383E 00-0.26955259E 00-0.26956254E 00-0.26957339E 00
0001400-0.26958454E 00-0.26959598E 00-0.26960760E 00-0.26961821E 00-0.26962775E 00
0001500-0.26963675E 00-0.26964450E 00-0.26965058E 00-0.26965541E 00-0.26965797E 00
0001600-0.26965904E 00-0.26965779E 00-0.26965564E 00-0.26965177E 00-0.26964670E 00
0001700-0.26964104E 00-0.26963419E 00-0.26962739E 00-0.26962036E 00-0.26961190E 00
0001800-0.26960391E 00-0.26959383E 00-0.26958036E 00-0.26956183E 00-0.26953578E 00
0001900-0.26949978E 00-0.26944935E 00-0.26937842E 00-0.26928037E 00-0.26914805E 00
0002000-0.26897180E 00-0.26874179E 00-0.26844543E 00-0.26806879E 00-0.26759613E 00
0002100-0.26701152E 00-0.26629722E 00-0.26543123E 00-0.26439351E 00-0.26316327E 00
0002200-0.26171607E 00-0.26002938E 00-0.25807983E 00-0.25584316E 00-0.25329792E 00
0002300-0.25042111E 00-0.24719238E 00-0.24359417E 00-0.23961008E 00-0.23522562E 00
0002400-0.23043138E 00-0.22522020E 00-0.21959341E 00-0.21353662E 00-0.20840955E 00
0002500-0.20490766E 00-0.20446002E 00-0.20490766E 00-0.20840955E 00-0.21353662E 00
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.13366994E-01 0.13364006E-01 0.13361320E-01 0.13359331E-01 0.13358388E-01
0000200 0.13358705E-01 0.13360322E-01 0.13363145E-01 0.13366856E-01 0.13370998E-01
0000300 0.13375081E-01 0.13378493E-01 0.13380721E-01 0.13381328E-01 0.13380110E-01
0000400 0.13377093E-01 0.13372492E-01 0.13366830E-01 0.13360810E-01 0.13355214E-01
0000500 0.13350893E-01 0.13348568E-01 0.13348762E-01 0.13351709E-01 0.13357256E-01
0000600 0.13364863E-01 0.13373636E-01 0.13382442E-01 0.13389971E-01 0.13394952E-01
0000700 0.13396345E-01 0.13393462E-01 0.13386250E-01 0.13375245E-01 0.13361707E-01
0000800 0.13347499E-01 0.13334893E-01 0.13326403E-01 0.13324324E-01 0.13330456E-01
0000900 0.13345461E-01 0.13368707E-01 0.13397839E-01 0.13428468E-01 0.13454277E-01
0001000 0.13467118E-01 0.13457403E-01 0.13414662E-01 0.13328560E-01 0.13189696E-01
0001100 0.12990914E-01 0.12728367E-01 0.12402516E-01 0.12018967E-01 0.11588894E-01
0001200 0.11129014E-01 0.10661077E-01 0.10211185E-01 0.98087043E-02 0.94855092E-02
0001300 0.92743821E-02 0.92024244E-02 0.92743821E-02 0.94855092E-02 0.98087043E-02
EOF
q
reditkpote9
LOADING POTE9
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26953614E 00-0.26954222E 00-0.26955110E 00-0.26955712E 00-0.26956218E 00
0000200-0.26956123E 00-0.26956308E 00-0.26955801E 00-0.26955479E 00-0.26954132E 00
0000300-0.26953769E 00-0.26952958E 00-0.26952404E 00-0.26952291E 00-0.26952535E 00
0000400-0.26953238E 00-0.26954180E 00-0.26955211E 00-0.26956230E 00-0.26956981E 00
0000500-0.26957345E 00-0.26957130E 00-0.26956421E 00-0.26955074E 00-0.26953340E 00
0000600-0.26951474E 00-0.26949519E 00-0.26947862E 00-0.26946872E 00-0.26946646E 00
0000700-0.26947433E 00-0.26949102E 00-0.26951748E 00-0.26955050E 00-0.26958823E 00
0000800-0.26962572E 00-0.26966190E 00-0.26969284E 00-0.26971734E 00-0.26973355E 00
0000900-0.26974303E 00-0.26974660E 00-0.26974380E 00-0.26973194E 00-0.26970077E 00
0001000-0.26963031E 00-0.26948524E 00-0.26920807E 00-0.26871938E 00-0.26790828E 00
0001100-0.26663482E 00-0.26472920E 00-0.26199281E 00-0.25820798E 00-0.25314814E 00
0001200-0.24658722E 00-0.23831826E 00-0.22816747E 00-0.21601045E 00-0.20212895E 00
0001300-0.18927366E 00-0.18763685E 00-0.18927366E 00-0.20212895E 00-0.21601045E 00
EOF
q
```

ZN+ NL a=1.0 DENS.

VEFF

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
```

ZN+ NL a=20
DENS.

```
        TOP RECORD
0000100 0.13372555E-01 0.13366833E-01 0.13360873E-01 0.13355523E-01 0.13351582E-01
0000200 0.13349745E-01 0.13350405E-01 0.13353679E-01 0.13359282E-01 0.13366636E-01
0000300 0.13374839E-01 0.13382807E-01 0.13389405E-01 0.13393618E-01 0.13394624E-01
0000400 0.13392005E-01 0.13385814E-01 0.13376616E-01 0.13365399E-01 0.13353590E-01
0000500 0.13342790E-01 0.13334613E-01 0.13330448E-01 0.13331316E-01 0.13337515E-01
0000600 0.13348706E-01 0.13363771E-01 0.13380870E-01 0.13397746E-01 0.13411842E-01
0000700 0.13420749E-01 0.13422534E-01 0.13416052E-01 0.13401300E-01 0.13379604E-01
0000800 0.13353504E-01 0.13326734E-01 0.13303757E-01 0.13289303E-01 0.13287604E-01
0000900 0.13301712E-01 0.13332590E-01 0.13378460E-01 0.13434280E-01 0.13491385E-01
0001000 0.13537634E-01 0.13557699E-01 0.13534147E-01 0.13448600E-01 0.13283536E-01
0001100 0.13024259E-01 0.12660820E-01 0.12190085E-01 0.11617023E-01 0.10955472E-01
0001200 0.10227878E-01 0.94641708E-02 0.86996034E-02 0.79722367E-02 0.73205642E-02
0001300 0.67812912E-02 0.63819699E-02 0.61375424E-02 0.60559139E-02 0.61375424E-02
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953602E 00-0.26954961E 00-0.26956272E 00-0.26957440E 00-0.26958334E 00
0000200-0.26958883E 00-0.26958692E 00-0.26958144E 00-0.26957196E 00-0.26954788E 00
0000300-0.26953548E 00-0.26951081E 00-0.26949459E 00-0.26948547E 00-0.26948333E 00
0000400-0.26949030E 00-0.26950455E 00-0.26952398E 00-0.26954514E 00-0.26956487E 00
0000500-0.26958042E 00-0.26958662E 00-0.26958364E 00-0.26956856E 00-0.26954317E 00
0000600-0.26950991E 00-0.26947111E 00-0.26943314E 00-0.26940185E 00-0.26938289E 00
0000700-0.26937926E 00-0.26939410E 00-0.26942819E 00-0.26947856E 00-0.26954335E 00
0000800-0.26961493E 00-0.26968956E 00-0.26976001E 00-0.26982230E 00-0.26987100E 00
0000900-0.26990592E 00-0.26992828E 00-0.26994091E 00-0.26994443E 00-0.26993406E 00
0001000-0.26989293E 00-0.26978391E 00-0.26953936E 00-0.26905406E 00-0.26817495E 00
0001100-0.26669693E 00-0.26435900E 00-0.26084691E 00-0.25580275E 00-0.24883932E 00
0001200-0.23956084E 00-0.22759235E 00-0.21260756E 00-0.19437134E 00-0.17264932E 00
0001300-0.15222347E 00-0.13815331E 00-0.12874687E 00-0.12733430E 00-0.12874687E 00
EOF
q
```

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p99
```

ZN+ NL a=3.0 DENS.

```
        TOP RECORD
0000100 0.13378926E-01 0.13381027E-01 0.13381340E-01 0.13379741E-01 0.13376456E-01
0000200 0.13371825E-01 0.13366479E-01 0.13361130E-01 0.13356525E-01 0.13353381E-01
0000300 0.13352156E-01 0.13353165E-01 0.13356395E-01 0.13361514E-01 0.13367906E-01
0000400 0.13374783E-01 0.13381209E-01 0.13386283E-01 0.13389248E-01 0.13389513E-01
0000500 0.13386957E-01 0.13381761E-01 0.13374500E-01 0.13366111E-01 0.13357673E-01
0000600 0.13350386E-01 0.13345331E-01 0.13343435E-01 0.13345137E-01 0.13350427E-01
0000700 0.13358835E-01 0.13369400E-01 0.13380781E-01 0.13391372E-01 0.13399635E-01
0000800 0.13404168E-01 0.13404008E-01 0.13398733E-01 0.13388649E-01 0.13374761E-01
0000900 0.13358660E-01 0.13342448E-01 0.13328373E-01 0.13318628E-01 0.13315015E-01
0001000 0.13318595E-01 0.13329506E-01 0.13346896E-01 0.13368834E-01 0.13392575E-01
0001100 0.13414804E-01 0.13432007E-01 0.13441090E-01 0.13439782E-01 0.13427094E-01
0001200 0.13403699E-01 0.13372019E-01 0.13336230E-01 0.13301805E-01 0.13275005E-01
0001300 0.13262033E-01 0.13267964E-01 0.13295822E-01 0.13345435E-01 0.13412643E-01
0001400 0.13488661E-01 0.13560060E-01 0.13608992E-01 0.13614230E-01 0.13552528E-01
0001500 0.13400894E-01 0.13138849E-01 0.12751237E-01 0.12230780E-01 0.11580009E-01
0001600 0.10812439E-01 0.99524297E-02 0.90336241E-02 0.80960691E-02 0.71824752E-02
0001700 0.63343309E-02 0.55883303E-02 0.49691163E-02 0.44874251E-02 0.41454919E-02
0001800 0.39416924E-02 0.38742700E-02 0.39416924E-02 0.41454919E-02 0.44874251E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953614E 00-0.26953244E 00-0.26953340E 00-0.26953930E 00-0.26954955E 00
0000200-0.26955998E 00-0.26956993E 00-0.26957989E 00-0.26958990E 00-0.26959628E 00
0000300-0.26959789E 00-0.26958418E 00-0.26957655E 00-0.26956815E 00-0.26954597E 00
0000400-0.26953483E 00-0.26951939E 00-0.26950955E 00-0.26951694E 00-0.26951689E 00
0000500-0.26952440E 00-0.26954156E 00-0.26955909E 00-0.26958203E 00-0.26960558E 00
0000600-0.26962340E 00-0.26963258E 00-0.26963609E 00-0.26963145E 00-0.26961589E 00
0000700-0.26958662E 00-0.26956224E 00-0.26952994E 00-0.26950395E 00-0.26948559E 00
0000800-0.26947606E 00-0.26947844E 00-0.26949239E 00-0.26951492E 00-0.26954365E 00
0000900-0.26957446E 00-0.26960230E 00-0.26962125E 00-0.26962817E 00-0.26961929E 00
0001000-0.26959425E 00-0.26955438E 00-0.26950330E 00-0.26944762E 00-0.26939535E 00
0001100-0.26935351E 00-0.26932901E 00-0.26932824E 00-0.26935399E 00-0.26940501E 00
0001200-0.26948053E 00-0.26957303E 00-0.26967704E 00-0.26978290E 00-0.26988328E 00
0001300-0.26996911E 00-0.27003670E 00-0.27008498E 00-0.27011544E 00-0.27013087E 00
0001400-0.27013206E 00-0.27010918E 00-0.27003360E 00-0.26984280E 00-0.26943350E 00
0001500-0.26864475E 00-0.26725090E 00-0.26495481E 00-0.26138699E 00-0.25611228E 00
0001600-0.24864376E 00-0.23846787E 00-0.22507721E 00-0.20800960E 00-0.18690735E 00
0001700-0.16145241E 00-0.13642961E 00-0.11655122E 00-0.10149401E 00-0.91212511E-01
0001800-0.84532499E-01-0.83414495E-01-0.84532499E-01-0.91212511E-01-0.10149401E 00
EOF
q
```

```
redit pote14
LOADING POTE14
REKEYED
EDIT
p99
```

ZN^{+} NL a=5.0 DENS.

```
        TOP RECORD
0000100 0.13387125E-01 0.13389595E-01 0.13389386E-01 0.13386466E-01 0.13381127E-01
0000200 0.13373997E-01 0.13366010E-01 0.13358198E-01 0.13351612E-01 0.13347268E-01
0000300 0.13345808E-01 0.13347603E-01 0.13352577E-01 0.13360158E-01 0.13369441E-01
0000400 0.13379246E-01 0.13388209E-01 0.13395112E-01 0.13398807E-01 0.13398688E-01
0000500 0.13394520E-01 0.13386723E-01 0.13376147E-01 0.13364162E-01 0.13352346E-01
0000600 0.13342381E-01 0.13335809E-01 0.13333753E-01 0.13336785E-01 0.13344847E-01
0000700 0.13357092E-01 0.13372045E-01 0.13387825E-01 0.13402168E-01 0.13412938E-01
0000800 0.13418287E-01 0.13417013E-01 0.13408732E-01 0.13394024E-01 0.13374429E-01
0000900 0.13352316E-01 0.13330568E-01 0.13312347E-01 0.13300482E-01 0.13297230E-01
0001000 0.13303772E-01 0.13319999E-01 0.13344422E-01 0.13374172E-01 0.13405353E-01
0001100 0.13433419E-01 0.13453875E-01 0.13462823E-01 0.13457689E-01 0.13437755E-01
0001200 0.13404571E-01 0.13361998E-01 0.13315972E-01 0.13274040E-01 0.13244338E-01
0001300 0.13234485E-01 0.13250224E-01 0.13294078E-01 0.13364118E-01 0.13453044E-01
0001400 0.13547663E-01 0.13629079E-01 0.13673432E-01 0.13653487E-01 0.13540946E-01
0001500 0.13309341E-01 0.12937296E-01 0.12411781E-01 0.11730947E-01 0.10905791E-01
0001600 0.99605620E-02 0.89310296E-02 0.78613013E-02 0.67989901E-02 0.57899468E-02
0001700 0.48731752E-02 0.40728711E-02 0.33967798E-02 0.28418503E-02 0.23991240E-02
0001800 0.20572578E-02 0.18049113E-02 0.16322238E-02 0.15316957E-02 0.14987395E-02
EOF
q
redit pote15
LOADING POTE15
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953495E 00-0.26952213E 00-0.26951951E 00-0.26952207E 00-0.26952946E 00
0000200-0.26954240E 00-0.26955962E 00-0.26957786E 00-0.26959121E 00-0.26960057E 00
0000300-0.26958984E 00-0.26958758E 00-0.26958096E 00-0.26955432E 00-0.26953989E 00
0000400-0.26951647E 00-0.26949430E 00-0.26949310E 00-0.26948726E 00-0.26949269E 00
0000500-0.26950634E 00-0.26953191E 00-0.26956320E 00-0.26959348E 00-0.26962548E 00
0000600-0.26964575E 00-0.26965845E 00-0.26966023E 00-0.26965350E 00-0.26962215E 00
0000700-0.26959342E 00-0.26955116E 00-0.26951110E 00-0.26947773E 00-0.26945424E 00
0000800-0.26944494E 00-0.26945114E 00-0.26947224E 00-0.26950532E 00-0.26954538E 00
0000900-0.26958781E 00-0.26962423E 00-0.26964873E 00-0.26965576E 00-0.26964188E 00
0001000-0.26960701E 00-0.26955181E 00-0.26948357E 00-0.26941186E 00-0.26934505E 00
0001100-0.26929462E 00-0.26926893E 00-0.26927435E 00-0.26931262E 00-0.26938564E 00
0001200-0.26948655E 00-0.26960957E 00-0.26974469E 00-0.26988208E 00-0.27000993E 00
0001300-0.27012002E 00-0.27020735E 00-0.27027053E 00-0.27031273E 00-0.27033740E 00
0001400-0.27034235E 00-0.27031106E 00-0.27019316E 00-0.26989764E 00-0.26927119E 00
0001500-0.26808840E 00-0.26604170E 00-0.26273555E 00-0.25768936E 00-0.25034964E 00
0001600-0.24011075E 00-0.22634727E 00-0.20845479E 00-0.18591028E 00-0.15821904E 00
0001700-0.12999779E 00-0.10582542E 00-0.85305452E-01-0.68240345E-01-0.54420736E-01
0001800-0.43689977E-01-0.35840202E-01-0.30668877E-01-0.27513415E-01-0.26909012E-01
EOF
q
```

```
redit pote16
LOADING POTE16   ZN+ NL  a=10.0
REKEYED          DENS.
EDIT
p99
        TOP RECORD
0000100 0.13382163E-01 0.13389461E-01 0.13394173E-01 0.13395648E-01 0.13393492E-01
0000200 0.13387885E-01 0.13379466E-01 0.13369240E-01 0.13358515E-01 0.13348717E-01
0000300 0.13341229E-01 0.13337161E-01 0.13337228E-01 0.13341583E-01 0.13349824E-01
0000400 0.13360970E-01 0.13373658E-01 0.13386171E-01 0.13396814E-01 0.13403982E-01
0000500 0.13406519E-01 0.13403833E-01 0.13396084E-01 0.13384040E-01 0.13369221E-01
0000600 0.13353497E-01 0.13339076E-01 0.13328020E-01 0.13322081E-01 0.13322424E-01
0000700 0.13329327E-01 0.13342291E-01 0.13359834E-01 0.13379794E-01 0.13399504E-01
0000800 0.13416182E-01 0.13427231E-01 0.13430715E-01 0.13425533E-01 0.13411812E-01
0000900 0.13390873E-01 0.13365105E-01 0.13337817E-01 0.13312772E-01 0.13293728E-01
0001000 0.13283886E-01 0.13285428E-01 0.13299048E-01 0.13323810E-01 0.13357054E-01
0001100 0.13394672E-01 0.13431530E-01 0.13462067E-01 0.13481196E-01 0.13484910E-01
0001200 0.13471194E-01 0.13440479E-01 0.13395894E-01 0.13343275E-01 0.13290517E-01
0001300 0.13246827E-01 0.13221454E-01 0.13222165E-01 0.13253745E-01 0.13316505E-01
0001400 0.13405103E-01 0.13507761E-01 0.13606165E-01 0.13676137E-01 0.13689116E-01
0001500 0.13614435E-01 0.13422351E-01 0.13087600E-01 0.12593016E-01 0.11932712E-01
0001600 0.11114515E-01 0.10160532E-01 0.91059580E-02 0.79958066E-02 0.68799928E-02
0001700 0.58075190E-02 0.48206039E-02 0.39460547E-02 0.31932755E-02 0.25598481E-02
0001800 0.20363533E-02 0.16099305E-02 0.12666502E-02 0.99297240E-03 0.77655772E-03
0001900 0.60661975E-03 0.47401967E-03 0.37119025E-03 0.29198360E-03 0.23148602E-03
0002000 0.18583429E-03 0.15204697E-03 0.12787824E-03 0.11170120E-03 0.10241690E-03
0002100 0.99391356E-04 0.10241690E-03 0.11170120E-03 0.12787824E-03 0.15204697E-03
EOF
q
redit pote17
LOADING POTE17
REKEYED          VEFF
EDIT
p99
        TOP RECORD
0000100-0.26953602E 00-0.26951641E 00-0.26950210E 00-0.26949650E 00-0.26949912E 00
0000200-0.26951134E 00-0.26952857E 00-0.26955050E 00-0.26957327E 00-0.26959193E 00
0000300-0.26960641E 00-0.26960242E 00-0.26959872E 00-0.26958704E 00-0.26956004E 00
0000400-0.26953411E 00-0.26950008E 00-0.26947027E 00-0.26945657E 00-0.26944280E 00
0000500-0.26943952E 00-0.26944989E 00-0.26947045E 00-0.26950067E 00-0.26953596E 00
0000600-0.26957142E 00-0.26960218E 00-0.26962876E 00-0.26963913E 00-0.26963735E 00
0000700-0.26961005E 00-0.26957786E 00-0.26952845E 00-0.26947874E 00-0.26943368E 00
0000800-0.26939791E 00-0.26937908E 00-0.26937896E 00-0.26939785E 00-0.26943451E 00
0000900-0.26948392E 00-0.26954025E 00-0.26959419E 00-0.26963854E 00-0.26966429E 00
0001000-0.26966643E 00-0.26964217E 00-0.26959157E 00-0.26952016E 00-0.26943803E 00
0001100-0.26935554E 00-0.26928556E 00-0.26923937E 00-0.26922721E 00-0.26925248E 00
0001200-0.26931816E 00-0.26941937E 00-0.26955074E 00-0.26970148E 00-0.26986045E 00
0001300-0.27001309E 00-0.27014923E 00-0.27025986E 00-0.27034056E 00-0.27039200E 00
0001400-0.27041894E 00-0.27042294E 00-0.27039456E 00-0.27029598E 00-0.27005041E 00
0001500-0.26951861E 00-0.26849097E 00-0.26667202E 00-0.26367319E 00-0.25901568E 00
0001600-0.25213796E 00-0.24241638E 00-0.22919261E 00-0.21181440E 00-0.18969446E 00
0001700-0.16225517E 00-0.13399297E 00-0.10934311E 00-0.87763429E-01-0.68892121E-01
0001800-0.52364789E-01-0.37860695E-01-0.25107499E-01-0.13870984E-01-0.39528944E-02
0001900 0.48157610E-02 0.12579907E-01 0.19466925E-01 0.25590993E-01 0.31060945E-01
0002000 0.35975561E-01 0.40405814E-01 0.44339404E-01 0.47598112E-01 0.49845960E-01
0002100 0.50629880E-01 0.49845960E-01 0.47598112E-01 0.44339404E-01 0.40405814E-01
EOF
q
-
```

```
reqit pote18
LOADING POTE18
REKEYED
EDIT
p99
```

ZN+ NL a=15.0 DENS.

```
        TOP RECORD
0000100 0.13383869E-01 0.13391186E-01 0.13395797E-01 0.13397049E-01 0.13394549E-01
0000200 0.13388492E-01 0.13379559E-01 0.13368785E-01 0.13357490E-01 0.13347194E-01
0000300 0.13339270E-01 0.13334908E-01 0.13334829E-01 0.13339221E-01 0.13347641E-01
0000400 0.13359129E-01 0.13372228E-01 0.13385218E-01 0.13396293E-01 0.13403844E-01
0000500 0.13406649E-01 0.13404112E-01 0.13396338E-01 0.13384122E-01 0.13369013E-01
0000600 0.13352919E-01 0.13338100E-01 0.13326690E-01 0.13320524E-01 0.13320759E-01
0000700 0.13327803E-01 0.13341062E-01 0.13359107E-01 0.13379693E-01 0.13400119E-01
0000800 0.13417505E-01 0.13429157E-01 0.13433076E-01 0.13428118E-01 0.13414353E-01
0000900 0.13393100E-01 0.13366781E-01 0.13338756E-01 0.13312917E-01 0.13293065E-01
0001000 0.13282560E-01 0.13283622E-01 0.13297059E-01 0.13321985E-01 0.13355732E-01
0001100 0.13394140E-01 0.13432041E-01 0.13463736E-01 0.13483983E-01 0.13488669E-01
0001200 0.13475604E-01 0.13445131E-01 0.13400324E-01 0.13346955E-01 0.13293009E-01
0001300 0.13247762E-01 0.13220601E-01 0.13219506E-01 0.13249461E-01 0.13310991E-01
0001400 0.13398968E-01 0.13501741E-01 0.13601139E-01 0.13673007E-01 0.13688754E-01
0001500 0.13617579E-01 0.13429541E-01 0.13099097E-01 0.12608692E-01 0.11952210E-01
0001600 0.11137065E-01 0.10185111E-01 0.91313459E-02 0.80207437E-02 0.69032684E-02
0001700 0.58281049E-02 0.48377551E-02 0.39592907E-02 0.32023755E-02 0.25647797E-02
0001800 0.20372418E-02 0.16069973E-02 0.12601658E-02 0.98322262E-03 0.76380558E-03
0001900 0.59108250E-03 0.45584212E-03 0.35042455E-03 0.26856759E-03 0.20521722E-03
0002000 0.15633751E-03 0.11873341E-03 0.89890716E-04 0.67840840E-04 0.51047609E-04
0002100 0.38314232E-04 0.28708848E-04 0.21505868E-04 0.16140941E-04 0.12177396E-04
0002200 0.92807986E-05 0.71994164E-05 0.57483994E-05 0.47970461E-05 0.42589136E-05
0002300 0.40848490E-05 0.42589136E-05 0.47970461E-05 0.57483994E-05 0.71994164E-05
EOF
q
```

```
redit pote19
LOADING POTE19
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26953602E 00-0.26950717E 00-0.26949179E 00-0.26948059E 00-0.26947826E 00
0000200-0.26948434E 00-0.26950353E 00-0.26952589E 00-0.26955068E 00-0.26956886E 00
0000300-0.26958328E 00-0.26957929E 00-0.26957631E 00-0.26956499E 00-0.26953942E 00
0000400-0.26951450E 00-0.26948160E 00-0.26945317E 00-0.26944065E 00-0.26942688E 00
0000500-0.26942718E 00-0.26943815E 00-0.26946324E 00-0.26949918E 00-0.26953924E 00
0000600-0.26957965E 00-0.26961529E 00-0.26964146E 00-0.26965868E 00-0.26965576E 00
0000700-0.26962811E 00-0.26960051E 00-0.26955217E 00-0.26950365E 00-0.26946002E 00
0000800-0.26942611E 00-0.26940882E 00-0.26941079E 00-0.26943254E 00-0.26947182E 00
0000900-0.26952463E 00-0.26958436E 00-0.26964170E 00-0.26968938E 00-0.26971787E 00
0001000-0.26972181E 00-0.26969886E 00-0.26964808E 00-0.26957566E 00-0.26949155E 00
0001100-0.26940632E 00-0.26933253E 00-0.26928288E 00-0.26926696E 00-0.26928854E 00
0001200-0.26935107E 00-0.26944935E 00-0.26957828E 00-0.26972735E 00-0.26988477E 00
0001300-0.27003682E 00-0.27017188E 00-0.27028155E 00-0.27036017E 00-0.27040911E 00
0001400-0.27043247E 00-0.27043205E 00-0.27039903E 00-0.27029669E 00-0.27004927E 00
0001500-0.26951915E 00-0.26849884E 00-0.26669335E 00-0.26371711E 00-0.25909263E 00
0001600-0.25225979E 00-0.24259573E 00-0.22944218E 00-0.21214622E 00-0.19011956E 00
0001700-0.16278231E 00-0.13462406E 00-0.11007231E 00-0.88582337E-01-0.69786727E-01
0001800-0.53315666E-01-0.38842097E-01-0.26085127E-01-0.14800400E-01-0.47752000E-02
0001900 0.41779503E-02 0.12230098E-01 0.19542828E-01 0.26276026E-01 0.32596603E-01
0002000 0.38685352E-01 0.44739779E-01 0.50968308E-01 0.57562236E-01 0.64643621E-01
0002100 0.72187841E-01 0.79952240E-01 0.87483108E-01 0.94245374E-01 0.99844098E-01
0002200 0.10418087E 00 0.10742295E 00 0.10981655E 00 0.11151797E 00 0.11256123E 00
0002300 0.11291438E 00 0.11256123E 00 0.11151797E 00 0.10981655E 00 0.10742295E 00
EOF
q
```

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
```

MG LDA a=0.25 DENS.

```
        TOP RECORD
0000100 0.12826622E-01 0.12826402E-01 0.12826260E-01 0.12826171E-01 0.12826134E-01
0000200 0.12826167E-01 0.12826297E-01 0.12826510E-01 0.12826789E-01 0.12827154E-01
0000300 0.12827598E-01 0.12828123E-01 0.12828685E-01 0.12829300E-01 0.12829974E-01
0000400 0.12830637E-01 0.12831286E-01 0.12831915E-01 0.12832493E-01 0.12833018E-01
0000500 0.12833443E-01 0.12833782E-01 0.12834001E-01 0.12834098E-01 0.12834057E-01
0000600 0.12833882E-01 0.12833580E-01 0.12833137E-01 0.12832589E-01 0.12831915E-01
0000700 0.12831148E-01 0.12830321E-01 0.12829423E-01 0.12828521E-01 0.12827624E-01
0000800 0.12826741E-01 0.12825921E-01 0.12825213E-01 0.12824584E-01 0.12824111E-01
0000900 0.12823801E-01 0.12823675E-01 0.12823727E-01 0.12823977E-01 0.12824431E-01
0001000 0.12825057E-01 0.12825888E-01 0.12826845E-01 0.12827951E-01 0.12829162E-01
0001100 0.12830433E-01 0.12831707E-01 0.12832973E-01 0.12834139E-01 0.12835227E-01
0001200 0.12836162E-01 0.12836851E-01 0.12837324E-01 0.12837507E-01 0.12837391E-01
0001300 0.12836959E-01 0.12836214E-01 0.12835141E-01 0.12833763E-01 0.12832079E-01
0001400 0.12830157E-01 0.12828063E-01 0.12825847E-01 0.12823548E-01 0.12821283E-01
0001500 0.12819104E-01 0.12817141E-01 0.12815457E-01 0.12814123E-01 0.12813263E-01
0001600 0.12812920E-01 0.12813170E-01 0.12814056E-01 0.12815595E-01 0.12817804E-01
0001700 0.12820650E-01 0.12824092E-01 0.12828056E-01 0.12832411E-01 0.12837037E-01
0001800 0.12841728E-01 0.12846284E-01 0.12850445E-01 0.12853965E-01 0.12856476E-01
0001900 0.12857717E-01 0.12857292E-01 0.12854867E-01 0.12850031E-01 0.12842443E-01
0002000 0.12831736E-01 0.12817565E-01 0.12799598E-01 0.12777589E-01 0.12751229E-01
0002100 0.12720402E-01 0.12684990E-01 0.12644935E-01 0.12600295E-01 0.12551248E-01
0002200 0.12498010E-01 0.12440931E-01 0.12380537E-01 0.12317345E-01 0.12252174E-01
0002300 0.12185793E-01 0.12119193E-01 0.12053430E-01 0.11989757E-01 0.11929452E-01
0002400 0.11873949E-01 0.11824779E-01 0.11783537E-01 0.11751924E-01 0.11731680E-01
0002500 0.11724766E-01 0.11731680E-01 0.11751924E-01 0.11783537E-01 0.11824779E-01
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26224053E 00-0.26223946E 00-0.26223952E 00-0.26224035E 00-0.26224124E 00
0000200-0.26224399E 00-0.26225418E 00-0.26225406E 00-0.26225436E 00-0.26225567E 00
0000300-0.26225919E 00-0.26226258E 00-0.26225799E 00-0.26226610E 00-0.26226825E 00
0000400-0.26227146E 00-0.26227605E 00-0.26227015E 00-0.26227814E 00-0.26227874E 00
0000500-0.26227510E 00-0.26227367E 00-0.26227248E 00-0.26227129E 00-0.26227027E 00
0000600-0.26226807E 00-0.26226783E 00-0.26226735E 00-0.26226568E 00-0.26226300E 00
0000700-0.26226205E 00-0.26226026E 00-0.26225913E 00-0.26225799E 00-0.26225644E 00
0000800-0.26225507E 00-0.26225418E 00-0.26225269E 00-0.26225102E 00-0.26224869E 00
0000900-0.26224697E 00-0.26224530E 00-0.26224267E 00-0.26224124E 00-0.26224017E 00
0001000-0.26223946E 00-0.26223850E 00-0.26223791E 00-0.26223791E 00-0.26223832E 00
0001100-0.26223880E 00-0.26223922E 00-0.26223958E 00-0.26224113E 00-0.26224267E 00
0001200-0.26224440E 00-0.26224685E 00-0.26224875E 00-0.26225138E 00-0.26225322E 00
0001300-0.26225579E 00-0.26225704E 00-0.26225895E 00-0.26226008E 00-0.26226050E 00
0001400-0.26226044E 00-0.26226032E 00-0.26225883E 00-0.26225656E 00-0.26225424E 00
0001500-0.26225013E 00-0.26224613E 00-0.26224130E 00-0.26223600E 00-0.26223016E 00
0001600-0.26222420E 00-0.26221818E 00-0.26221240E 00-0.26220775E 00-0.26220357E 00
0001700-0.26220071E 00-0.26219898E 00-0.26219893E 00-0.26219976E 00-0.26220280E 00
0001800-0.26220787E 00-0.26221353E 00-0.26222026E 00-0.26222706E 00-0.26223344E 00
0001900-0.26223701E 00-0.26223731E 00-0.26223183E 00-0.26221794E 00-0.26219279E 00
0002000-0.26215219E 00-0.26209271E 00-0.26200980E 00-0.26189768E 00-0.26175070E 00
0002100-0.26156276E 00-0.26132637E 00-0.26103401E 00-0.26067674E 00-0.26024723E 00
0002200-0.25973517E 00-0.25913215E 00-0.25842839E 00-0.25761372E 00-0.25668043E 00
0002300-0.25561875E 00-0.25442040E 00-0.25307828E 00-0.25158608E 00-0.24993867E 00
0002400-0.24813318E 00-0.24616849E 00-0.24404448E 00-0.24189264E 00-0.23901159E 00
0002500-0.23848885E 00-0.23901159E 00-0.24189264E 00-0.24404448E 00-0.24616849E 00
EOF
```


```
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12826283E-01 0.12824900E-01 0.12823950E-01 0.12823656E-01 0.12824073E-01
0000200 0.12825184E-01 0.12826942E-01 0.12829117E-01 0.12831457E-01 0.12833681E-01
0000300 0.12835439E-01 0.12836453E-01 0.12836520E-01 0.12835581E-01 0.12833625E-01
0000400 0.12830824E-01 0.12827527E-01 0.12824077E-01 0.12820933E-01 0.12818601E-01
0000500 0.12817435E-01 0.12817737E-01 0.12819588E-01 0.12822945E-01 0.12827463E-01
0000600 0.12832657E-01 0.12837850E-01 0.12842324E-01 0.12845319E-01 0.12846254E-01
0000700 0.12844644E-01 0.12840401E-01 0.12833774E-01 0.12825347E-01 0.12816105E-01
0000800 0.12807317E-01 0.12800381E-01 0.12796722E-01 0.12797516E-01 0.12803532E-01
0000900 0.12814853E-01 0.12830749E-01 0.12849443E-01 0.12868088E-01 0.12882814E-01
0001000 0.12888812E-01 0.12880586E-01 0.12852389E-01 0.12798537E-01 0.12714136E-01
0001100 0.12595665E-01 0.12441482E-01 0.12252551E-01 0.12032863E-01 0.11789732E-01
0001200 0.11534002E-01 0.11279929E-01 0.11044923E-01 0.10849040E-01 0.10714240E-01
0001300 0.10667056E-01 0.10714240E-01 0.10849040E-01 0.11044923E-01 0.11279929E-01
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26223838E 00-0.26223481E 00-0.26223624E 00-0.26223713E 00-0.26223236E 00
0000200-0.26223701E 00-0.26223963E 00-0.26223928E 00-0.26223874E 00-0.26224780E 00
0000300-0.26224512E 00-0.26224583E 00-0.26224619E 00-0.26224774E 00-0.26224667E 00
0000400-0.26224571E 00-0.26224464E 00-0.26224285E 00-0.26223928E 00-0.26223379E 00
0000500-0.26222920E 00-0.26222444E 00-0.26222229E 00-0.26221991E 00-0.26222038E 00
0000600-0.26222306E 00-0.26222771E 00-0.26223469E 00-0.26224375E 00-0.26225358E 00
0000700-0.26226240E 00-0.26226968E 00-0.26227355E 00-0.26227260E 00-0.26226604E 00
0000800-0.26225322E 00-0.26223576E 00-0.26221466E 00-0.26219326E 00-0.26217538E 00
0000900-0.26216567E 00-0.26216614E 00-0.26218122E 00-0.26220727E 00-0.26223838E 00
0001000-0.26226038E 00-0.26224798E 00-0.26216221E 00-0.26195049E 00-0.26153970E 00
0001100-0.26083934E 00-0.25973839E 00-0.25810814E 00-0.25580770E 00-0.25268823E 00
0001200-0.24860519E 00-0.24342924E 00-0.23706073E 00-0.22990841E 00-0.21940786E 00
0001300-0.21732706E 00-0.21940786E 00-0.22990841E 00-0.23706073E 00-0.24342924E 00
EOF
q
-
```

MG LDA a=0.5 DENS.

VEFF

```
redit pote6
LOADING POTE6
REKEYED
EDIT
p 99
```

MG LDA a=0.75 DENS.

```
        TOP RECORD
0000100 0.12825694E-01 0.12824558E-01 0.12823526E-01 0.12822665E-01 0.12822006E-01
0000200 0.12821548E-01 0.12821358E-01 0.12821432E-01 0.12821775E-01 0.12822405E-01
0000300 0.12823313E-01 0.12824442E-01 0.12825802E-01 0.12827344E-01 0.12829032E-01
0000400 0.12830805E-01 0.12832601E-01 0.12834389E-01 0.12836080E-01 0.12837630E-01
0000500 0.12838975E-01 0.12840066E-01 0.12840852E-01 0.12841288E-01 0.12841370E-01
0000600 0.12841038E-01 0.12840327E-01 0.12839232E-01 0.12837749E-01 0.12835927E-01
0000700 0.12833808E-01 0.12831446E-01 0.12828927E-01 0.12826294E-01 0.12823638E-01
0000800 0.12821067E-01 0.12818668E-01 0.12816519E-01 0.12814689E-01 0.12813274E-01
0000900 0.12812328E-01 0.12811929E-01 0.12812104E-01 0.12812883E-01 0.12814246E-01
0001000 0.12816217E-01 0.12818720E-01 0.12821734E-01 0.12825139E-01 0.12828879E-01
0001100 0.12832835E-01 0.12836862E-01 0.12840860E-01 0.12844630E-01 0.12848094E-01
0001200 0.12851056E-01 0.12853410E-01 0.12855038E-01 0.12855813E-01 0.12855686E-01
0001300 0.12854565E-01 0.12852438E-01 0.12849323E-01 0.12845226E-01 0.12840282E-01
0001400 0.12834545E-01 0.12828194E-01 0.12821414E-01 0.12814417E-01 0.12807436E-01
0001500 0.12800731E-01 0.12794569E-01 0.12789246E-01 0.12784988E-01 0.12782097E-01
0001600 0.12780782E-01 0.12781236E-01 0.12783624E-01 0.12788009E-01 0.12794461E-01
0001700 0.12802888E-01 0.12813188E-01 0.12825117E-01 0.12838360E-01 0.12852497E-01
0001800 0.12867033E-01 0.12881272E-01 0.12894567E-01 0.12906086E-01 0.12914911E-01
0001900 0.12920123E-01 0.12920681E-01 0.12915533E-01 0.12903601E-01 0.12883853E-01
0002000 0.12855213E-01 0.12816709E-01 0.12767468E-01 0.12706667E-01 0.12633685E-01
0002100 0.12548074E-01 0.12449510E-01 0.12337975E-01 0.12213670E-01 0.12077041E-01
0002200 0.11928819E-01 0.11770081E-01 0.11602137E-01 0.11426631E-01 0.11245519E-01
0002300 0.11060994E-01 0.10875531E-01 0.10691885E-01 0.10513034E-01 0.10342140E-01
0002400 0.10182582E-01 0.10037888E-01 0.99117272E-02 0.98079555E-02 0.97305030E-02
0002500 0.96826628E-02 0.96665882E-02 0.96826628E-02 0.97305030E-02 0.98079555E-02
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p 99
```

VEFF

```
        TOP RECORD
0000100-0.26224059E 00-0.26223665E 00-0.26223475E 00-0.26223177E 00-0.26223075E 00
0000200-0.26223832E 00-0.26223743E 00-0.26223725E 00-0.26223940E 00-0.26224345E 00
0000300-0.26224822E 00-0.26224482E 00-0.26225156E 00-0.26224995E 00-0.26224929E 00
0000400-0.26225543E 00-0.26225364E 00-0.26226121E 00-0.26225895E 00-0.26225644E 00
0000500-0.26205531E 00-0.26225495E 00-0.26225603E 00-0.26225650E 00-0.26225567E 00
0000600-0.26225561E 00-0.26225746E 00-0.26225728E 00-0.26225585E 00-0.26225626E 00
0000700-0.26225573E 00-0.26225519E 00-0.26225531E 00-0.26225364E 00-0.26225281E 00
0000800-0.26225179E 00-0.26224971E 00-0.26224715E 00-0.26224369E 00-0.26224005E 00
0000900-0.26223683E 00-0.26223290E 00-0.26222968E 00-0.26222652E 00-0.26222461E 00
0001000-0.26222181E 00-0.26221997E 00-0.26221919E 00-0.26221877E 00-0.26221961E 00
0001100-0.26222098E 00-0.26222295E 00-0.26222628E 00-0.26223063E 00-0.26223552E 00
0001200-0.26224220E 00-0.26224869E 00-0.26225597E 00-0.26226324E 00-0.26227093E 00
0001300-0.26227790E 00-0.26228476E 00-0.26229089E 00-0.26229572E 00-0.26229924E 00
0001400-0.26230145E 00-0.26230127E 00-0.26229888E 00-0.26229483E 00-0.26228791E 00
0001500-0.26227897E 00-0.26226807E 00-0.26225537E 00-0.26224041E 00-0.26222438E 00
0001600-0.26220781E 00-0.26219153E 00-0.26217616E 00-0.26216161E 00-0.26215023E 00
0001700-0.26214206E 00-0.26213741E 00-0.26213706E 00-0.26214224E 00-0.26215309E 00
0001800-0.26216888E 00-0.26218861E 00-0.26221228E 00-0.26223814E 00-0.26226217E 00
0001900-0.26228279E 00-0.26229483E 00-0.26229239E 00-0.26226854E 00-0.26221532E 00
0002000-0.26212305E 00-0.26198030E 00-0.26177382E 00-0.26148927E 00-0.26110959E 00
0002100-0.26061678E 00-0.25999045E 00-0.25920826E 00-0.25824708E 00-0.25708199E 00
0002200-0.25568688E 00-0.25403482E 00-0.25209886E 00-0.24985147E 00-0.24726611E 00
0002300-0.24431676E 00-0.24098033E 00-0.23723495E 00-0.23306215E 00-0.22844714E 00
0002400-0.22338015E 00-0.21785539E 00-0.21187335E 00-0.20544094E 00-0.19992149E 00
0002500-0.19621396E 00-0.19569445E 00-0.19621396E 00-0.19992149E 00-0.20544094E 00
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12825228E-01 0.12821775E-01 0.12819011E-01 0.12817394E-01 0.12817174E-01
0000200 0.12818534E-01 0.12821361E-01 0.12825362E-01 0.12830105E-01 0.12834989E-01
0000300 0.12839321E-01 0.12842506E-01 0.12843996E-01 0.12843467E-01 0.12840793E-01
0000400 0.12836162E-01 0.12830041E-01 0.12823150E-01 0.12816358E-01 0.12810662E-01
0000500 0.12806911E-01 0.12805872E-01 0.12807984E-01 0.12813263E-01 0.12821361E-01
0000600 0.12831438E-01 0.12842294E-01 0.12852494E-01 0.12860548E-01 0.12864958E-01
0000700 0.12864687E-01 0.12859076E-01 0.12848236E-01 0.12833003E-01 0.12814939E-01
0000800 0.12796331E-01 0.12779910E-01 0.12768544E-01 0.12764961E-01 0.12771193E-01
0000900 0.12788184E-01 0.12815394E-01 0.12850452E-01 0.12888886E-01 0.12924179E-01
0001000 0.12947898E-01 0.12950040E-01 0.12919739E-01 0.12846064E-01 0.12719035E-01
0001100 0.12530882E-01 0.12277067E-01 0.11957549E-01 0.11577487E-01 0.11147879E-01
0001200 0.10685556E-01 0.10212768E-01 0.97564049E-02 0.93469508E-02 0.90174936E-02
0001300 0.88020787E-02 0.87285303E-02 0.88020787E-02 0.90174936E-02 0.93469508E-02
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26224053E 00-0.26223069E 00-0.26222730E 00-0.26222253E 00-0.26221448E 00
0000200-0.26221579E 00-0.26221770E 00-0.26221955E 00-0.26222074E 00-0.26223153E 00
0000300-0.26223266E 00-0.26223791E 00-0.26224363E 00-0.26225001E 00-0.26225245E 00
0000400-0.26225531E 00-0.26225543E 00-0.26225299E 00-0.26224858E 00-0.26224089E 00
0000500-0.26223308E 00-0.26222420E 00-0.26221836E 00-0.26221317E 00-0.26221365E 00
0000600-0.26221669E 00-0.26222444E 00-0.26223677E 00-0.26225299E 00-0.26227152E 00
0000700-0.26229012E 00-0.26230633E 00-0.26231718E 00-0.26232046E 00-0.26231337E 00
0000800-0.26229495E 00-0.26226628E 00-0.26222903E 00-0.26218808E 00-0.26215070E 00
0000900-0.26212442E 00-0.26211524E 00-0.26213199E 00-0.26217413E 00-0.26223612E 00
0001000-0.26229984E 00-0.26233172E 00-0.26227361E 00-0.26204276E 00-0.26152319E 00
0001100-0.26056260E 00-0.25897020E 00-0.25651795E 00-0.25294638E 00-0.24797410E 00
0001200-0.24131429E 00-0.23269719E 00-0.22189492E 00-0.20875138E 00-0.19358540E 00
0001300-0.17966580E 00-0.17762214E 00-0.17966580E 00-0.19358540E 00-0.20875138E 00
EOF
q
```

MG LDA a=1.0
DENS.

VEFF

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12837525E-01 0.12836032E-01 0.12833603E-01 0.12830529E-01 0.12827173E-01
0000200 0.12823954E-01 0.12821328E-01 0.12819637E-01 0.12819171E-01 0.12820091E-01
0000300 0.12822311E-01 0.12825631E-01 0.12829646E-01 0.12833796E-01 0.12837626E-01
0000400 0.12840550E-01 0.12842145E-01 0.12842096E-01 0.12840323E-01 0.12836952E-01
0000500 0.12832381E-01 0.12827069E-01 0.12821764E-01 0.12817156E-01 0.12813929E-01
0000600 0.12812611E-01 0.12813531E-01 0.12816697E-01 0.12821816E-01 0.12828365E-01
0000700 0.12835518E-01 0.12842346E-01 0.12847867E-01 0.12851212E-01 0.12851737E-01
0000800 0.12849066E-01 0.12843296E-01 0.12834948E-01 0.12824882E-01 0.12814377E-01
0000900 0.12804840E-01 0.12797642E-01 0.12794051E-01 0.12794971E-01 0.12800686E-01
0001000 0.12810994E-01 0.12824859E-01 0.12840800E-01 0.12856748E-01 0.12870438E-01
0001100 0.12879595E-01 0.12882307E-01 0.12877356E-01 0.12864303E-01 0.12843959E-01
0001200 0.12818243E-01 0.12790147E-01 0.12763560E-01 0.12742829E-01 0.12732171E-01
0001300 0.12735177E-01 0.12754072E-01 0.12789015E-01 0.12837648E-01 0.12894694E-01
0001400 0.12951784E-01 0.12997653E-01 0.13018612E-01 0.12999382E-01 0.12924340E-01
0001500 0.12778897E-01 0.12551270E-01 0.12234055E-01 0.11825852E-01 0.11332359E-01
0001600 0.10766990E-01 0.10150585E-01 0.95105954E-02 0.88794492E-02 0.82926676E-02
0001700 0.77871121E-02 0.73988475E-02 0.71555153E-02 0.70735365E-02 0.71555153E-02
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26224053E 00-0.26223969E 00-0.26223528E 00-0.26223278E 00-0.26223439E 00
0000200-0.26222473E 00-0.26223022E 00-0.26222199E 00-0.26221114E 00-0.26220816E 00
0000300-0.26220363E 00-0.26221353E 00-0.26221919E 00-0.26221019E 00-0.26222134E 00
0000400-0.26221877E 00-0.26222694E 00-0.26223201E 00-0.26222956E 00-0.26223773E 00
0000500-0.26224005E 00-0.26223511E 00-0.26222509E 00-0.26222306E 00-0.26221955E 00
0000600-0.26220822E 00-0.26220977E 00-0.26220745E 00-0.26220369E 00-0.26219988E 00
0000700-0.26220793E 00-0.26220685E 00-0.26221335E 00-0.26222104E 00-0.26222938E 00
0000800-0.26223660E 00-0.26224041E 00-0.26224065E 00-0.26223594E 00-0.26222640E 00
0000900-0.26221269E 00-0.26219648E 00-0.26217902E 00-0.26216406E 00-0.26215309E 00
0001000-0.26214933E 00-0.26215482E 00-0.26216924E 00-0.26219332E 00-0.26222545E 00
0001100-0.26226145E 00-0.26229692E 00-0.26232648E 00-0.26234382E 00-0.26234460E 00
0001200-0.26232368E 00-0.26228046E 00-0.26221710E 00-0.26213980E 00-0.26205891E 00
0001300-0.26198930E 00-0.26194632E 00-0.26194441E 00-0.26199740E 00-0.26210767E 00
0001400-0.26226920E 00-0.26245606E 00-0.26262110E 00-0.26268589E 00-0.26253831E 00
0001500-0.26202285E 00-0.26093876E 00-0.25903910E 00-0.25603050E 00-0.25158286E 00
0001600-0.24534094E 00-0.23694575E 00-0.22605604E 00-0.21238005E 00-0.19570446E 00
0001700-0.17621338E 00-0.15902650E 00-0.14729583E 00-0.14541936E 00-0.14729583E 00
EOF
q
```

MG LDA a=1.5 DENS.

VEFF

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p99
```

MG LDA a=2.0 DENS.

```
        TOP RECORD
0000100 0.12828801E-01 0.12821160E-01 0.12814041E-01 0.12808438E-01 0.12805186E-01
0000200 0.12804858E-01 0.12807664E-01 0.12813427E-01 0.12821544E-01 0.12831103E-01
0000300 0.12840841E-01 0.12849480E-01 0.12855727E-01 0.12858581E-01 0.12857348E-01
0000400 0.12851872E-01 0.12842562E-01 0.12830395E-01 0.12816798E-01 0.12803566E-01
0000500 0.12792572E-01 0.12785599E-01 0.12784023E-01 0.12788609E-01 0.12799382E-01
0000600 0.12815479E-01 0.12835234E-01 0.12856212E-01 0.12875631E-01 0.12890495E-01
0000700 0.12898132E-01 0.12896504E-01 0.12884628E-01 0.12862857E-01 0.12833040E-01
0000800 0.12798399E-01 0.12763426E-01 0.12733411E-01 0.12713857E-01 0.12709629E-01
0000900 0.12724306E-01 0.12759198E-01 0.12812704E-01 0.12879737E-01 0.12951430E-01
0001000 0.13015203E-01 0.13055246E-01 0.13053413E-01 0.12990542E-01 0.12848120E-01
0001100 0.12610357E-01 0.12266189E-01 0.11811361E-01 0.11249851E-01 0.10594834E-01
0001200 0.98686032E-02 0.91014616E-02 0.83296672E-02 0.75927749E-02 0.69309399E-02
0001300 0.63823946E-02 0.59760585E-02 0.57273544E-02 0.56442469E-02 0.57273544E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26224059E 00-0.26221710E 00-0.26220369E 00-0.26219350E 00-0.26217997E 00
0000200-0.26217687E 00-0.26217479E 00-0.26217449E 00-0.26217651E 00-0.26218772E 00
0000300-0.26219136E 00-0.26220173E 00-0.26221412E 00-0.26222771E 00-0.26223761E 00
0000400-0.26224631E 00-0.26225126E 00-0.26225102E 00-0.26224536E 00-0.26223415E 00
0000500-0.26221973E 00-0.26220280E 00-0.26218790E 00-0.26217407E 00-0.26216680E 00
0000600-0.26216495E 00-0.26217091E 00-0.26218659E 00-0.26221025E 00-0.26224023E 00
0000700-0.26227343E 00-0.26230574E 00-0.26233280E 00-0.26234943E 00-0.26235056E 00
0000800-0.26233339E 00-0.26229721E 00-0.26224381E 00-0.26217908E 00-0.26211298E 00
0000900-0.26205790E 00-0.26202786E 00-0.26203626E 00-0.26209158E 00-0.26219404E 00
0001000-0.26232868E 00-0.26245958E 00-0.26252019E 00-0.26240641E 00-0.26196420E 00
0001100-0.26098466E 00-0.25919402E 00-0.25625247E 00-0.25175571E 00-0.24524510E 00
0001200-0.23622692E 00-0.22420251E 00-0.20870590E 00-0.18934870E 00-0.16586673E 00
0001300-0.14321256E 00-0.12741637E 00-0.11693496E 00-0.11508375E 00-0.11693496E 00
EOF
q
```

```
redit pote14
LOADING POTE14
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12840677E-01 0.12841612E-01 0.12840837E-01 0.12838341E-01 0.12834370E-01
0000200 0.12829449E-01 0.12824148E-01 0.12819201E-01 0.12815300E-01 0.12813020E-01
0000300 0.12812808E-01 0.12814794E-01 0.12818817E-01 0.12824513E-01 0.12831155E-01
0000400 0.12837932E-01 0.12843940E-01 0.12848344E-01 0.12850426E-01 0.12849782E-01
0000500 0.12846351E-01 0.12840413E-01 0.12832563E-01 0.12823846E-01 0.12815278E-01
0000600 0.12808092E-01 0.12803331E-01 0.12801830E-01 0.12803964E-01 0.12809735E-01
0000700 0.12818601E-01 0.12829561E-01 0.12841243E-01 0.12852129E-01 0.12860622E-01
0000800 0.12865353E-01 0.12865368E-01 0.12860268E-01 0.12850281E-01 0.12836371E-01
0000900 0.12820095E-01 0.12803521E-01 0.12788925E-01 0.12778498E-01 0.12774125E-01
0001000 0.12777016E-01 0.12787551E-01 0.12804978E-01 0.12827612E-01 0.12852788E-01
0001100 0.12877226E-01 0.12897287E-01 0.12909573E-01 0.12911294E-01 0.12900811E-01
0001200 0.12878042E-01 0.12844574E-01 0.12803901E-01 0.12761049E-01 0.12722209E-01
0001300 0.12694057E-01 0.12682848E-01 0.12693480E-01 0.12728442E-01 0.12786951E-01
0001400 0.12864169E-01 0.12950778E-01 0.13033029E-01 0.13093088E-01 0.13110142E-01
0001500 0.13061859E-01 0.12926336E-01 0.12684554E-01 0.12322724E-01 0.11834756E-01
0001600 0.11224102E-01 0.10504633E-01 0.97005665E-02 0.88448934E-02 0.79767741E-02
0001700 0.71381368E-02 0.63701272E-02 0.57095587E-02 0.51823370E-02 0.48015453E-02
0001800 0.45721009E-02 0.44958591E-02 0.45721009E-02 0.48015453E-02 0.51823370E-02
EOF
q
redit pote15
LOADING POTE15
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26224053E 00-0.26224148E 00-0.26224923E 00-0.26225543E 00-0.26225448E 00
0000200-0.26226121E 00-0.26225299E 00-0.26226050E 00-0.26225471E 00-0.26224679E 00
0000300-0.26224262E 00-0.26223892E 00-0.26224262E 00-0.26224488E 00-0.26223886E 00
0000400-0.26225042E 00-0.26224959E 00-0.26225805E 00-0.26226187E 00-0.26226187E 00
0000500-0.26226908E 00-0.26227367E 00-0.26227164E 00-0.26226556E 00-0.26226085E 00
0000600-0.26225185E 00-0.26223892E 00-0.26223379E 00-0.26222479E 00-0.26221591E 00
0000700-0.26221156E 00-0.26221806E 00-0.26221961E 00-0.26222676E 00-0.26223707E 00
0000800-0.26224965E 00-0.26226175E 00-0.26227051E 00-0.26227540E 00-0.26227331E 00
0000900-0.26226389E 00-0.26224750E 00-0.26222503E 00-0.26219797E 00-0.26217139E 00
0001000-0.26214772E 00-0.26213139E 00-0.26212656E 00-0.26213384E 00-0.26215607E 00
0001100-0.26219153E 00-0.26223713E 00-0.26228774E 00-0.26233691E 00-0.26237577E 00
0001200-0.26239622E 00-0.26239043E 00-0.26235437E 00-0.26228714E 00-0.26219314E 00
0001300-0.26208347E 00-0.26197499E 00-0.26188874E 00-0.26184690E 00-0.26187128E 00
0001400-0.26197463E 00-0.26215959E 00-0.26240891E 00-0.26267952E 00-0.26289141E 00
0001500-0.26292390E 00-0.26259995E 00-0.26168180E 00-0.25986362E 00-0.25677013E 00
0001600-0.25196141E 00-0.24494576E 00-0.23520046E 00-0.22220224E 00-0.20546389E 00
0001700-0.18458247E 00-0.15960097E 00-0.13516647E 00-0.11594987E 00-0.10240483E 00
0001800-0.93485653E-01-0.91802061E-01-0.93485653E-01-0.10240483E 00-0.11594987E 00
EOF
q
```

MG LDA a=2.5 DENS.

VEFF

```
redit pote16
LOADING POTE16
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12843218E-01 0.12843050E-01 0.12840811E-01 0.12836687E-01 0.12831174E-01
0000200 0.12824927E-01 0.12818791E-01 0.12813605E-01 0.12810122E-01 0.12808930E-01
0000300 0.12810331E-01 0.12814272E-01 0.12820330E-01 0.12827836E-01 0.12835909E-01
0000400 0.12843430E-01 0.12849402E-01 0.12852889E-01 0.12853321E-01 0.12850419E-01
0000500 0.12844414E-01 0.12835879E-01 0.12825873E-01 0.12815632E-01 0.12806546E-01
0000600 0.12799934E-01 0.12796845E-01 0.12797948E-01 0.12803353E-01 0.12812637E-01
0000700 0.12824807E-01 0.12838401E-01 0.12851648E-01 0.12862731E-01 0.12869909E-01
0000800 0.12871906E-01 0.12868036E-01 0.12858313E-01 0.12843616E-01 0.12825545E-01
0000900 0.12806308E-01 0.12788475E-01 0.12774661E-01 0.12767162E-01 0.12767635E-01
0001000 0.12776814E-01 0.12794264E-01 0.12818433E-01 0.12846593E-01 0.12875292E-01
0001100 0.12900520E-01 0.12918308E-01 0.12925278E-01 0.12919176E-01 0.12899276E-01
0001200 0.12866706E-01 0.12824610E-01 0.12777939E-01 0.12733068E-01 0.12697104E-01
0001300 0.12677073E-01 0.12678765E-01 0.12705818E-01 0.12758542E-01 0.12833159E-01
0001400 0.12921177E-01 0.13009284E-01 0.13079654E-01 0.13110813E-01 0.13079073E-01
0001500 0.12960508E-01 0.12733266E-01 0.12380302E-01 0.11891991E-01 0.11268444E-01
0001600 0.10520943E-01 0.96723475E-02 0.87559372E-02 0.78127310E-02 0.68876706E-02
0001700 0.60253777E-02 0.52654892E-02 0.46345405E-02 0.41439719E-02 0.37960298E-02
0001800 0.35888117E-02 0.35202529E-02 0.35888117E-02 0.37960298E-02 0.41439719E-02
EOF
q
redit pote17
LOADING POTE17
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26223838E 00-0.26224488E 00-0.26225328E 00-0.26225358E 00-0.26225799E 00
0000200-0.26225579E 00-0.26225972E 00-0.26225078E 00-0.26224488E 00-0.26224309E 00
0000300-0.26223874E 00-0.26223826E 00-0.26223695E 00-0.26223207E 00-0.26223743E 00
0000400-0.26223731E 00-0.26224190E 00-0.26224458E 00-0.26224911E 00-0.26225251E 00
0000500-0.26225609E 00-0.26225513E 00-0.26225251E 00-0.26224881E 00-0.26224601E 00
0000600-0.26223856E 00-0.26224005E 00-0.26223749E 00-0.26223296E 00-0.26223034E 00
0000700-0.26223570E 00-0.26223552E 00-0.26224023E 00-0.26224649E 00-0.26225412E 00
0000800-0.26225656E 00-0.26226032E 00-0.26226217E 00-0.26226068E 00-0.26225656E 00
0000900-0.26224732E 00-0.26223785E 00-0.26222670E 00-0.26221901E 00-0.26220965E 00
0001000-0.26220506E 00-0.26220083E 00-0.26220071E 00-0.26220506E 00-0.26221508E 00
0001100-0.26223058E 00-0.26225191E 00-0.26227820E 00-0.26230896E 00-0.26234096E 00
0001200-0.26237011E 00-0.26239115E 00-0.26239991E 00-0.26239109E 00-0.26236224E 00
0001300-0.26231337E 00-0.26224905E 00-0.26217735E 00-0.26211202E 00-0.26206648E 00
0001400-0.26205337E 00-0.26207668E 00-0.26212311E 00-0.26215023E 00-0.26207668E 00
0001500-0.26176506E 00-0.26100999E 00-0.25952047E 00-0.25690985E 00-0.25268888E 00
0001600-0.24626803E 00-0.23697764E 00-0.22409880E 00-0.20691103E 00-0.18475276E 00
0001700-0.15721452E 00-0.12968969E 00-0.10739601E 00-0.90149522E-01-0.77998817E-01
0001800-0.70084155E-01-0.68469822E-01-0.70084155E-01-0.77998817E-01-0.90149522E-01
EOF
q
```

MG LDA a=3.0 DENS.

VEFF

```
redit pote18
LOADING POTE18
REKEYED
EDIT
p99
```

MG LDA a=4.0 DENS.

```
        TOP RECORD
0000100 0.12843456E-01 0.12847025E-01 0.12848258E-01 0.12846902E-01 0.12843084E-01
0000200 0.12837213E-01 0.12830034E-01 0.12822479E-01 0.12815617E-01 0.12810398E-01
0000300 0.12807697E-01 0.12808058E-01 0.12811571E-01 0.12817971E-01 0.12826562E-01
0000400 0.12836330E-01 0.12846056E-01 0.12854375E-01 0.12860145E-01 0.12862395E-01
0000500 0.12860637E-01 0.12854837E-01 0.12845516E-01 0.12833711E-01 0.12820859E-01
0000600 0.12808587E-01 0.12798563E-01 0.12792300E-01 0.12790829E-01 0.12794629E-01
0000700 0.12803473E-01 0.12816481E-01 0.12832083E-01 0.12848321E-01 0.12862939E-01
0000800 0.12873765E-01 0.12878992E-01 0.12877423E-01 0.12868699E-01 0.12853414E-01
0000900 0.12833100E-01 0.12810189E-01 0.12787603E-01 0.12768537E-01 0.12755979E-01
0001000 0.12752298E-01 0.12758866E-01 0.12775756E-01 0.12801632E-01 0.12833737E-01
0001100 0.12868114E-01 0.12900110E-01 0.12924798E-01 0.12937721E-01 0.12935571E-01
0001200 0.12916774E-01 0.12881901E-01 0.12834027E-01 0.12778498E-01 0.12722708E-01
0001300 0.12675215E-01 0.12644835E-01 0.12639310E-01 0.12664050E-01 0.12720831E-01
0001400 0.12806658E-01 0.12912948E-01 0.13025437E-01 0.13124146E-01 0.13184670E-01
0001500 0.13179619E-01 0.13081033E-01 0.12863319E-01 0.12506295E-01 0.11998408E-01
0001600 0.11339292E-01 0.10541320E-01 0.96296743E-02 0.86406171E-02 0.76181161E-02
0001700 0.66092126E-02 0.56584626E-02 0.48031956E-02 0.40668882E-02 0.34580538E-02
0001800 0.29753346E-02 0.26121596E-02 0.23603404E-02 0.22125279E-02 0.21639012E-02
EOF
q
redit pote19
LOADING POTE19
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26224053E 00-0.26224744E 00-0.26226044E 00-0.26226848E 00-0.26227450E 00
0000200-0.26228684E 00-0.26228178E 00-0.26229084E 00-0.26228482E 00-0.26227421E 00
0000300-0.26227283E 00-0.26227057E 00-0.26227349E 00-0.26227653E 00-0.26226842E 00
0000400-0.26227862E 00-0.26228184E 00-0.26229030E 00-0.26230007E 00-0.26230413E 00
0000500-0.26231539E 00-0.26232129E 00-0.26231986E 00-0.26231074E 00-0.26230359E 00
0000600-0.26228899E 00-0.26226985E 00-0.26225770E 00-0.26224232E 00-0.26222843E 00
0000700-0.26221442E 00-0.26221496E 00-0.26221186E 00-0.26221555E 00-0.26222491E 00
0000800-0.26223838E 00-0.26225328E 00-0.26226670E 00-0.26227647E 00-0.26227897E 00
0000900-0.26227415E 00-0.26225907E 00-0.26223612E 00-0.26220602E 00-0.26217413E 00
0001000-0.26214331E 00-0.26211983E 00-0.26210827E 00-0.26211089E 00-0.26213092E 00
0001100-0.26216787E 00-0.26221865E 00-0.26227736E 00-0.26233691E 00-0.26238769E 00
0001200-0.26241910E 00-0.26242107E 00-0.26238656E 00-0.26231325E 00-0.26220441E 00
0001300-0.26207119E 00-0.26193321E 00-0.26181626E 00-0.26174694E 00-0.26175600E 00
0001400-0.26186383E 00-0.26208061E 00-0.26239610E 00-0.26277333E 00-0.26313627E 00
0001500-0.26336300E 00-0.26327127E 00-0.26260841E 00-0.26104224E 00-0.25815648E 00
0001600-0.25345302E 00-0.24636275E 00-0.23626542E 00-0.22251886E 00-0.20449728E 00
0001700-0.18197244E 00-0.15479499E 00-0.12705654E 00-0.10294473E 00-0.82476377E-01
0001800-0.65768898E-01-0.52745700E-01-0.43484770E-01-0.37519481E-01-0.36152065E-01
EOF
q
```

```
redit pote20
LOADING POTE20
REKEYED
EDIT
p99
```

MG LDA a=5.0 DENS.

```
        TOP RECORD
0000100 0.12852564E-01 0.12851290E-01 0.12847044E-01 0.12840264E-01 0.12831688E-01
0000200 0.12822364E-01 0.12813497E-01 0.12806285E-01 0.12801748E-01 0.12800623E-01
0000300 0.12803260E-01 0.12809459E-01 0.12818530E-01 0.12829483E-01 0.12840904E-01
0000400 0.12851283E-01 0.12859195E-01 0.12863420E-01 0.12863211E-01 0.12858309E-01
0000500 0.12849163E-01 0.12836706E-01 0.12822479E-01 0.12808308E-01 0.12796100E-01
0000600 0.12787633E-01 0.12784310E-01 0.12786906E-01 0.12795437E-01 0.12809154E-01
0000700 0.12826513E-01 0.12845378E-01 0.12863297E-01 0.12877714E-01 0.12886386E-01
0000800 0.12887675E-01 0.12880836E-01 0.12866188E-01 0.12845121E-01 0.12820017E-01
0000900 0.12794003E-01 0.12770679E-01 0.12753461E-01 0.12745306E-01 0.12748193E-01
0001000 0.12762662E-01 0.12787826E-01 0.12821142E-01 0.12858666E-01 0.12895510E-01
0001100 0.12926359E-01 0.12946103E-01 0.12950692E-01 0.12937687E-01 0.12906976E-01
0001200 0.12860905E-01 0.12804478E-01 0.12744851E-01 0.12690786E-01 0.12651578E-01
0001300 0.12635827E-01 0.12650002E-01 0.12697112E-01 0.12775503E-01 0.12877867E-01
0001400 0.12990903E-01 0.13095420E-01 0.13167117E-01 0.13178233E-01 0.13099749E-01
0001500 0.12904186E-01 0.12568846E-01 0.12079064E-01 0.11431091E-01 0.10634113E-01
0001600 0.97108409E-02 0.86963475E-02 0.76348744E-02 0.65752752E-02 0.55654459E-02
0001700 0.46466403E-02 0.38446832E-02 0.31680430E-02 0.26137161E-02 0.21724717E-02
0001800 0.18326242E-02 0.15824053E-02 0.14115542E-02 0.13122628E-02 0.12797338E-02
EOF
q
redit pote21
LOADING POTE21
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26223016E 00-0.26222730E 00-0.26222533E 00-0.26222861E 00-0.26222241E 00
0000200-0.26222944E 00-0.26222360E 00-0.26221752E 00-0.26221585E 00-0.26221234E 00
0000300-0.26221335E 00-0.26221585E 00-0.26220691E 00-0.26221490E 00-0.26221263E 00
0000400-0.26222038E 00-0.26222837E 00-0.26223314E 00-0.26224339E 00-0.26224852E 00
0000500-0.26225185E 00-0.26225048E 00-0.26225042E 00-0.26224619E 00-0.26223576E 00
0000600-0.26222944E 00-0.26222324E 00-0.26221371E 00-0.26220405E 00-0.26220548E 00
0000700-0.26220429E 00-0.26221001E 00-0.26222003E 00-0.26223445E 00-0.26224858E 00
0000800-0.26226223E 00-0.26227397E 00-0.26227975E 00-0.26228017E 00-0.26226944E 00
0000900-0.26225358E 00-0.26223254E 00-0.26220709E 00-0.26218188E 00-0.26216179E 00
0001000-0.26214689E 00-0.26214182E 00-0.26214778E 00-0.26216596E 00-0.26219571E 00
0001100-0.26223397E 00-0.26227874E 00-0.26232493E 00-0.26236695E 00-0.26239896E 00
0001200-0.26241463E 00-0.26240987E 00-0.26238179E 00-0.26233226E 00-0.26226693E 00
0001300-0.26219714E 00-0.26213616E 00-0.26210219E 00-0.26211089E 00-0.26217425E 00
0001400-0.26229364E 00-0.26245099E 00-0.26260066E 00-0.26265609E 00-0.26247591E 00
0001500-0.26184952E 00-0.26048219E 00-0.25798088E 00-0.25384897E 00-0.24748325E 00
0001600-0.23818880E 00-0.22520304E 00-0.20773834E 00-0.18503118E 00-0.15639889E 00
0001700-0.12677622E 00-0.10120797E 00-0.79266071E-01-0.60598012E-01-0.44747900E-01
0001800-0.31844188E-01-0.21783859E-01-0.14557019E-01-0.99732205E-02-0.87928586E-02
EOF
q
```

```
redit pote22
LOADING POTE22
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12808029E-01 0.12807380E-01 0.12809552E-01 0.12814343E-01 0.12821224E-01
0000200 0.12829397E-01 0.12837831E-01 0.12845375E-01 0.12850985E-01 0.12853898E-01
0000300 0.12853552E-01 0.12849823E-01 0.12843139E-01 0.12834217E-01 0.12824163E-01
0000400 0.12814246E-01 0.12805823E-01 0.12800083E-01 0.12797922E-01 0.12799796E-01
0000500 0.12805652E-01 0.12814872E-01 0.12826417E-01 0.12838811E-01 0.12850463E-01
0000600 0.12859736E-01 0.12865238E-01 0.12866057E-01 0.12861751E-01 0.12852658E-01
0000700 0.12839686E-01 0.12824405E-01 0.12808729E-01 0.12794744E-01 0.12784470E-01
0000800 0.12779493E-01 0.12780823E-01 0.12788713E-01 0.12802482E-01 0.12820642E-01
0000900 0.12841020E-01 0.12861006E-01 0.12877848E-01 0.12889035E-01 0.12892663E-01
0001000 0.12887683E-01 0.12874201E-01 0.12853451E-01 0.12827780E-01 0.12800410E-01
0001100 0.12775067E-01 0.12755461E-01 0.12744881E-01 0.12745596E-01 0.12758523E-01
0001200 0.12782920E-01 0.12816358E-01 0.12854896E-01 0.12893438E-01 0.12926333E-01
0001300 0.12948100E-01 0.12954224E-01 0.12941886E-01 0.12910653E-01 0.12862775E-01
0001400 0.12803264E-01 0.12739655E-01 0.12681205E-01 0.12637876E-01 0.12619030E-01
0001500 0.12631927E-01 0.12680210E-01 0.12762602E-01 0.12871839E-01 0.12994260E-01
0001600 0.13109926E-01 0.13193455E-01 0.13215855E-01 0.13146818E-01 0.12957875E-01
0001700 0.12625728E-01 0.12135722E-01 0.11484515E-01 0.10681681E-01 0.97502731E-02
0001800 0.87254606E-02 0.76513141E-02 0.65761060E-02 0.55469945E-02 0.46044029E-02
0001900 0.37741854E-02 0.30657172E-02 0.24768030E-02 0.19982550E-02 0.16175820E-02
0002000 0.13215016E-02 0.10975222E-02 0.93485066E-03 0.82487613E-03 0.76138065E-03
0002100 0.74063917E-03 0.76138065E-03 0.82487613E-03 0.93485066E-03 0.10975222E-02
EOF
q
redit pote23
LOADING POTE23
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26224053E 00-0.26222903E 00-0.26222795E 00-0.26222575E 00-0.26222396E 00
0000200-0.26223087E 00-0.26223838E 00-0.26224262E 00-0.26224530E 00-0.26225543E 00
0000300-0.26226091E 00-0.26225942E 00-0.26226902E 00-0.26225770E 00-0.26226354E 00
0000400-0.26225656E 00-0.26224482E 00-0.26223761E 00-0.26222879E 00-0.26222533E 00
0000500-0.26222056E 00-0.26220864E 00-0.26221567E 00-0.26221317E 00-0.26222038E 00
0000600-0.26222658E 00-0.26223171E 00-0.26224524E 00-0.26225370E 00-0.26225758E 00
0000700-0.26225144E 00-0.26225168E 00-0.26224089E 00-0.26222557E 00-0.26221353E 00
0000800-0.26219773E 00-0.26218224E 00-0.26216894E 00-0.26216847E 00-0.26216495E 00
0000900-0.26217139E 00-0.26218486E 00-0.26220530E 00-0.26222968E 00-0.26225537E 00
0001000-0.26227945E 00-0.26229793E 00-0.26230884E 00-0.26230919E 00-0.26229918E 00
0001100-0.26227832E 00-0.26225120E 00-0.26221985E 00-0.26219004E 00-0.26216710E 00
0001200-0.26215380E 00-0.26215404E 00-0.26216906E 00-0.26219684E 00-0.26223290E 00
0001300-0.26227307E 00-0.26230800E 00-0.26233011E 00-0.26233059E 00-0.26230323E 00
0001400-0.26224583E 00-0.26216131E 00-0.26206034E 00-0.26196021E 00-0.26188517E 00
0001500-0.26186001E 00-0.26191264E 00-0.26205915E 00-0.26230627E 00-0.26263756E 00
0001600-0.26301116E 00-0.26334798E 00-0.26352483E 00-0.26336485E 00-0.26262480E 00
0001700-0.26098990E 00-0.25814271E 00-0.25368172E 00-0.24704677E 00-0.23761123E 00
0001800-0.22470242E 00-0.20763361E 00-0.18573827E 00-0.15840793E 00-0.12978619E 00
0001900-0.10409272E 00-0.81266105E-01-0.61303739E-01-0.43929689E-01-0.28934158E-01
0002000-0.16170546E-01-0.55971295E-02 0.27735673E-02 0.88391602E-02 0.12675527E-01
0002100 0.13741203E-01 0.12675527E-01 0.88391602E-02 0.27735673E-02-0.55971295E-02
EOF
q
```

MG LDA a=6.0 DENS.

VEFF

```
redit pote24
LOADING POTE24
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12852475E-01 0.12857102E-01 0.12858085E-01 0.12855157E-01 0.12848601E-01
0000200 0.12839202E-01 0.12828138E-01 0.12816846E-01 0.12806866E-01 0.12799658E-01
0000300 0.12796346E-01 0.12797549E-01 0.12803338E-01 0.12813162E-01 0.12825888E-01
0000400 0.12839939E-01 0.12853492E-01 0.12864679E-01 0.12871835E-01 0.12873791E-01
0000500 0.12869954E-01 0.12860488E-01 0.12846369E-01 0.12829244E-01 0.12811180E-01
0000600 0.12794606E-01 0.12781814E-01 0.12774732E-01 0.12774680E-01 0.12782045E-01
0000700 0.12796324E-01 0.12815982E-01 0.12838669E-01 0.12861528E-01 0.12881432E-01
0000800 0.12895450E-01 0.12901265E-01 0.12897480E-01 0.12883898E-01 0.12861684E-01
0000900 0.12833212E-01 0.12801938E-01 0.12771986E-01 0.12747582E-01 0.12732584E-01
0001000 0.12729898E-01 0.12740925E-01 0.12765326E-01 0.12800906E-01 0.12843654E-01
0001100 0.12888186E-01 0.12928311E-01 0.12957811E-01 0.12971301E-01 0.12965068E-01
0001200 0.12937773E-01 0.12890961E-01 0.12829222E-01 0.12759969E-01 0.12692720E-01
0001300 0.12638129E-01 0.12606647E-01 0.12606848E-01 0.12643903E-01 0.12718130E-01
0001400 0.12823697E-01 0.12948174E-01 0.13072323E-01 0.13170958E-01 0.13214506E-01
0001500 0.13171319E-01 0.13010766E-01 0.12706731E-01 0.12241296E-01 0.11607982E-01
0001600 0.10814086E-01 0.98814033E-02 0.88451803E-02 0.77507719E-02 0.66487715E-02
0001700 0.55890568E-02 0.46146810E-02 0.37530453E-02 0.30137945E-02 0.23944436E-02
0001800 0.18853468E-02 0.14733388E-02 0.11441803E-02 0.88405004E-03 0.68037631E-03
0001900 0.52219362E-03 0.40026125E-03 0.30692853E-03 0.23602380E-03 0.18263387E-03
0002000 0.14291718E-03 0.11392287E-03 0.93439245E-04 0.79870064E-04 0.72140509E-04
0002100 0.69631453E-04 0.72140509E-04 0.79870064E-04 0.93439245E-04 0.11392287E-03
EOF
q
redit pote25
LOADING POTE25
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26223993E 00-0.26226473E 00-0.26228625E 00-0.26229972E 00-0.26231480E 00
0000200-0.26231086E 00-0.26232046E 00-0.26231110E 00-0.26229602E 00-0.26228631E 00
0000300-0.26227319E 00-0.26226759E 00-0.26225972E 00-0.26223952E 00-0.26224416E 00
0000400-0.26223457E 00-0.26224053E 00-0.26224649E 00-0.26225078E 00-0.26226026E 00
0000500-0.26226783E 00-0.26226723E 00-0.26226228E 00-0.26226050E 00-0.26224762E 00
0000600-0.26222908E 00-0.26221877E 00-0.26220429E 00-0.26218814E 00-0.26217312E 00
0000700-0.26217151E 00-0.26216489E 00-0.26216924E 00-0.26217997E 00-0.26219773E 00
0000800-0.26221865E 00-0.26224178E 00-0.26226270E 00-0.26227820E 00-0.26228505E 00
0000900-0.26228005E 00-0.26226354E 00-0.26223540E 00-0.26219928E 00-0.26215822E 00
0001000-0.26211894E 00-0.26208657E 00-0.26206601E 00-0.26206279E 00-0.26208031E 00
0001100-0.26211751E 00-0.26217216E 00-0.26223940E 00-0.26231015E 00-0.26237476E 00
0001200-0.26242054E 00-0.26243621E 00-0.26241356E 00-0.26234865E 00-0.26224440E 00
0001300-0.26211387E 00-0.26197755E 00-0.26186132E 00-0.26179677E 00-0.26181042E 00
0001400-0.26192170E 00-0.26213294E 00-0.26242387E 00-0.26273924E 00-0.26298159E 00
0001500-0.26299632E 00-0.26256043E 00-0.26136816E 00-0.25902277E 00-0.25502920E 00
0001600-0.24880195E 00-0.23967654E 00-0.22693539E 00-0.20984310E 00-0.18768728E 00
0001700-0.15982091E 00-0.13082737E 00-0.10535568E 00-0.82947433E-01-0.63180029E-01
0001800-0.45678884E-01-0.30117612E-01-0.16221646E-01-0.37610659E-02 0.74531473E-02
0001900 0.17573982E-01 0.26721768E-01 0.34987055E-01 0.42431135E-01 0.49086239E-01
0002000 0.54947179E-01 0.59976492E-01 0.64091563E-01 0.67174733E-01 0.69110513E-01
0002100 0.69749653E-01 0.69110513E-01 0.67174733E-01 0.64091563E-01 0.59976492E-01
EOF
q
```

MG LDA a=10.0 DENS.

VEFF

```
redit pote26
LOADING POTE26
REKEYED
EDIT
p99
```

MG LDA a=15.0 DENS.

```
        TOP RECORD
0000100 0.12853801E-01 0.12858428E-01 0.12859318E-01 0.12856226E-01 0.12849394E-01
0000200 0.12839634E-01 0.12828112E-01 0.12816358E-01 0.12805928E-01 0.12798265E-01
0000300 0.12794564E-01 0.12795515E-01 0.12801133E-01 0.12810882E-01 0.12823634E-01
0000400 0.12837768E-01 0.12851436E-01 0.12862746E-01 0.12870010E-01 0.12872025E-01
0000500 0.12868147E-01 0.12858592E-01 0.12844298E-01 0.12826905E-01 0.12808558E-01
0000600 0.12791639E-01 0.12778603E-01 0.12771331E-01 0.12771167E-01 0.12778562E-01
0000700 0.12792990E-01 0.12812946E-01 0.12836047E-01 0.12859367E-01 0.12879770E-01
0000800 0.12894243E-01 0.12900393E-01 0.12896821E-01 0.12883302E-01 0.12860939E-01
0000900 0.12832168E-01 0.12800477E-01 0.12770042E-01 0.12745176E-01 0.12729786E-01
0001000 0.12726851E-01 0.12737878E-01 0.12762558E-01 0.12798663E-01 0.12842186E-01
0001100 0.12887675E-01 0.12928873E-01 0.12959436E-01 0.12973834E-01 0.12968257E-01
0001200 0.12941260E-01 0.12894370E-01 0.12832113E-01 0.12761939E-01 0.12693476E-01
0001300 0.12637492E-01 0.12604572E-01 0.12603495E-01 0.12639571E-01 0.12713246E-01
0001400 0.12318839E-01 0.12943935E-01 0.13069320E-01 0.13169773E-01 0.13215575E-01
0001500 0.13174932E-01 0.13017036E-01 0.12715578E-01 0.12252461E-01 0.11621077E-01
0001600 0.10828607E-01 0.98968484E-02 0.88609681E-02 0.77663623E-02 0.66635981E-02
0001700 0.56025647E-02 0.46263449E-02 0.37624200E-02 0.30206121E-02 0.23986141E-02
0001800 0.18869289E-02 0.14724936E-02 0.11411223E-02 0.87900832E-03 0.67356043E-03
0001900 0.51377527E-03 0.39033149E-03 0.29551238E-03 0.22304550E-03 0.16790313E-03
0002000 0.12610483E-03 0.94528732E-04 0.70746552E-04 0.52883042E-04 0.39498453E-04
0002100 0.29493749E-04 0.22033710E-04 0.16486752E-04 0.12377286E-04 0.93492336E-05
0002200 0.71377526E-05 0.55478395E-05 0.44383250E-05 0.37101163E-05 0.32978687E-05
0002300 0.31644622E-05 0.32978687E-05 0.37101163E-05 0.44383250E-05 0.55478395E-05
EOF
q
redit pote27
LOADING POTE27
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26224053E 00-0.26226771E 00-0.26228744E 00-0.26229930E 00-0.26231289E 00
0000200-0.26230597E 00-0.26231289E 00-0.26229930E 00-0.26227850E 00-0.26226443E 00
0000300-0.26224548E 00-0.26223677E 00-0.26222676E 00-0.26220590E 00-0.26221025E 00
0000400-0.26220310E 00-0.26220888E 00-0.26221383E 00-0.26221627E 00-0.26223117E 00
0000500-0.26224172E 00-0.26224458E 00-0.26224017E 00-0.26223999E 00-0.26223016E 00
0000600-0.26221335E 00-0.26220071E 00-0.26218575E 00-0.26216900E 00-0.26215261E 00
0000700-0.26215225E 00-0.26214755E 00-0.26215452E 00-0.26216942E 00-0.26219213E 00
0000800-0.26221907E 00-0.26224744E 00-0.26227379E 00-0.26229292E 00-0.26230264E 00
0000900-0.26229936E 00-0.26228315E 00-0.26225317E 00-0.26221490E 00-0.26217139E 00
0001000-0.26213008E 00-0.26209748E 00-0.26207906E 00-0.26208013E 00-0.26210397E 00
0001100-0.26214945E 00-0.26221317E 00-0.26228946E 00-0.26236826E 00-0.26243824E 00
0001200-0.26248509E 00-0.26249731E 00-0.26246625E 00-0.26238835E 00-0.26226741E 00
0001300-0.26211917E 00-0.26196545E 00-0.26183510E 00-0.26176196E 00-0.26177353E 00
0001400-0.26188999E 00-0.26211292E 00-0.26242083E 00-0.26275551E 00-0.26301843E 00
0001500-0.26305157E 00-0.26262951E 00-0.26144522E 00-0.25910026E 00-0.25510180E 00
0001600-0.24886805E 00-0.23974180E 00-0.22701633E 00-0.20996988E 00-0.18790478E 00
0001700-0.16018975E 00-0.13135326E 00-0.10598546E 00-0.83635092E-01-0.63886225E-01
0001800-0.46369568E-01-0.30760851E-01-0.16786277E-01-0.42144507E-02 0.71479715E-02
0001900 0.17462183E-01 0.28611157E-01 0.35455417E-01 0.43336418E-01 0.50580643E-01
0002000 0.57251588E-01 0.63401520E-01 0.69077849E-01 0.74317813E-01 0.79153061E-01
0002100 0.83610952E-01 0.87713540E-01 0.91476977E-01 0.94911158E-01 0.98016381E-01
0002200 0.10078186E 00 0.10318083E 00 0.10516787E 00 0.10667223E 00 0.10761994E 00
0002300 0.10794365E 00 0.10761994E 00 0.10667223E 00 0.10516787E 00 0.10318083E 00
EOF
q
```

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
```

MG NL a=0.25 DENS.

```
        TOP RECORD
0000100 0.12825221E-01 0.12824725E-01 0.12824260E-01 0.12823828E-01 0.12823500E-01
0000200 0.12823217E-01 0.12823034E-01 0.12822963E-01 0.12823001E-01 0.12823135E-01
0000300 0.12823392E-01 0.12823731E-01 0.12824185E-01 0.12824699E-01 0.12825280E-01
0000400 0.12825925E-01 0.12826599E-01 0.12827266E-01 0.12827937E-01 0.12828566E-01
0000500 0.12829144E-01 0.12829661E-01 0.12830086E-01 0.12830421E-01 0.12830671E-01
0000600 0.12830775E-01 0.12830809E-01 0.12830690E-01 0.12830462E-01 0.12830164E-01
0000700 0.12829762E-01 0.12829296E-01 0.12828775E-01 0.12828209E-01 0.12827650E-01
0000800 0.12827091E-01 0.12826558E-01 0.12826126E-01 0.12825746E-01 0.12825482E-01
0000900 0.12825344E-01 0.12825362E-01 0.12825523E-01 0.12825824E-01 0.12826309E-01
0001000 0.12826934E-01 0.12827694E-01 0.12828603E-01 0.12829598E-01 0.12830678E-01
0001100 0.12831803E-01 0.12832951E-01 0.12834057E-01 0.12835097E-01 0.12836047E-01
0001200 0.12836836E-01 0.12837444E-01 0.12837861E-01 0.12838006E-01 0.12837894E-01
0001300 0.12837499E-01 0.12836833E-01 0.12835883E-01 0.12834676E-01 0.12833204E-01
0001400 0.12831554E-01 0.12829736E-01 0.12827836E-01 0.12825869E-01 0.12823936E-01
0001500 0.12822099E-01 0.12820449E-01 0.12819052E-01 0.12817971E-01 0.12817319E-01
0001600 0.12817103E-01 0.12817398E-01 0.12818255E-01 0.12819666E-01 0.12821633E-01
0001700 0.12824133E-01 0.12827128E-01 0.12830485E-01 0.12834139E-01 0.12837943E-01
0001800 0.12841687E-01 0.12845196E-01 0.12848243E-01 0.12850549E-01 0.12851816E-01
0001900 0.12851771E-01 0.12850039E-01 0.12846336E-01 0.12840267E-01 0.12831520E-01
0002000 0.12819793E-01 0.12804709E-01 0.12786027E-01 0.12763485E-01 0.12736849E-01
0002100 0.12706012E-01 0.12670845E-01 0.12631342E-01 0.12587585E-01 0.12539711E-01
0002200 0.12487985E-01 0.12432754E-01 0.12374464E-01 0.12313705E-01 0.12251154E-01
0002300 0.12187593E-01 0.12123968E-01 0.12061276E-01 0.12000643E-01 0.11943340E-01
0002400 0.11890631E-01 0.11844013E-01 0.11804972E-01 0.11775065E-01 0.11755906E-01
0002500 0.11749372E-01 0.11755906E-01 0.11775065E-01 0.11804972E-01 0.11844013E-01
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26223958E 00-0.26222128E 00-0.26220882E 00-0.26219988E 00-0.26219273E 00
0000200-0.26218963E 00-0.26219225E 00-0.26218617E 00-0.26218235E 00-0.26218081E 00
0000300-0.26218271E 00-0.26218581E 00-0.26218182E 00-0.26219118E 00-0.26219404E 00
0000400-0.26219785E 00-0.26220417E 00-0.26220101E 00-0.26221138E 00-0.26221603E 00
0000500-0.26221526E 00-0.26221716E 00-0.26221931E 00-0.26222140E 00-0.26222390E 00
0000600-0.26222634E 00-0.26222986E 00-0.26223302E 00-0.26223594E 00-0.26223850E 00
0000700-0.26224184E 00-0.26224452E 00-0.26224816E 00-0.26225066E 00-0.26225293E 00
0000800-0.26225597E 00-0.26225853E 00-0.26226014E 00-0.26226205E 00-0.26226246E 00
0000900-0.26226348E 00-0.26226389E 00-0.26226324E 00-0.26226318E 00-0.26226276E 00
0001000-0.26226228E 00-0.26226127E 00-0.26226050E 00-0.26225990E 00-0.26225829E 00
0001100-0.26225746E 00-0.26225674E 00-0.26225531E 00-0.26225543E 00-0.26225477E 00
0001200-0.26225477E 00-0.26225615E 00-0.26225615E 00-0.26225764E 00-0.26225907E 00
0001300-0.26226050E 00-0.26226193E 00-0.26226407E 00-0.26226574E 00-0.26226783E 00
0001400-0.26226944E 00-0.26227146E 00-0.26227260E 00-0.26227349E 00-0.26227432E 00
0001500-0.26227349E 00-0.26227313E 00-0.26227212E 00-0.26227057E 00-0.26226830E 00
0001600-0.26226515E 00-0.26226193E 00-0.26225805E 00-0.26225501E 00-0.26225078E 00
0001700-0.26224750E 00-0.26224440E 00-0.26224118E 00-0.26223737E 00-0.26223469E 00
0001800-0.26223248E 00-0.26222914E 00-0.26222497E 00-0.26221925E 00-0.26221138E 00
0001900-0.26219910E 00-0.26218194E 00-0.26215786E 00-0.26212394E 00-0.26207751E 00
0002000-0.26201493E 00-0.26193303E 00-0.26182753E 00-0.26169360E 00-0.26152563E 00
0002100-0.26131791E 00-0.26106429E 00-0.26075757E 00-0.26039010E 00-0.25995469E 00
0002200-0.25944316E 00-0.25884783E 00-0.25815940E 00-0.25736946E 00-0.25647110E 00
0002300-0.25545543E 00-0.25431573E 00-0.25304514E 00-0.25163865E 00-0.25009084E 00
0002400-0.24839866E 00-0.24656177E 00-0.24457645E 00-0.24258149E 00-0.23987156E 00
0002500-0.23940498E 00-0.23987156E 00-0.24258149E 00-0.24457645E 00-0.24656177E 00
EOF
```

```
---
q
redit pote4
LOADING POTE4   MG NL a=0.5
REKEYED
EDIT            DENS.
p99
        TOP RECORD
0000100 0.12826394E-01 0.12825292E-01 0.12824647E-01 0.12824588E-01 0.12825176E-01
0000200 0.12826417E-01 0.12828212E-01 0.12830365E-01 0.12832668E-01 0.12834869E-01
0000300 0.12836654E-01 0.12837786E-01 0.12838122E-01 0.12837555E-01 0.12836114E-01
0000400 0.12833945E-01 0.12831282E-01 0.12828473E-01 0.12825850E-01 0.12823865E-01
0000500 0.12822803E-01 0.12822904E-01 0.12824267E-01 0.12826841E-01 0.12830362E-01
0000600 0.12834407E-01 0.12838461E-01 0.12841951E-01 0.12844235E-01 0.12844890E-01
0000700 0.12843519E-01 0.12840122E-01 0.12834862E-01 0.12828313E-01 0.12821272E-01
0000800 0.12814790E-01 0.12810014E-01 0.12808055E-01 0.12809798E-01 0.12815718E-01
0000900 0.12825675E-01 0.12838766E-01 0.12853228E-01 0.12866259E-01 0.12874305E-01
0001000 0.12872934E-01 0.12857206E-01 0.12821969E-01 0.12762327E-01 0.12674123E-01
0001100 0.12554478E-01 0.12402348E-01 0.12219023E-01 0.12008555E-01 0.11777945E-01
0001200 0.11537317E-01 0.11299737E-01 0.11081092E-01 0.10899600E-01 0.10774963E-01
0001300 0.10731447E-01 0.10774963E-01 0.10899600E-01 0.11081092E-01 0.11299737E-01
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT            VEFF
p99
        TOP RECORD
0000100-0.26223987E 00-0.26223290E 00-0.26224071E 00-0.26224399E 00-0.26224720E 00
0000200-0.26225716E 00-0.26226276E 00-0.26226598E 00-0.26226401E 00-0.26227331E 00
0000300-0.26227319E 00-0.26227403E 00-0.26227593E 00-0.26227993E 00-0.26228440E 00
0000400-0.26228923E 00-0.26229435E 00-0.26229882E 00-0.26230180E 00-0.26230168E 00
0000500-0.26229966E 00-0.26229405E 00-0.26228750E 00-0.26227766E 00-0.26226753E 00
0000600-0.26225793E 00-0.26224911E 00-0.26224399E 00-0.26224256E 00-0.26224560E 00
0000700-0.26225245E 00-0.26226372E 00-0.26227719E 00-0.26229262E 00-0.26230729E 00
0000800-0.26231939E 00-0.26232934E 00-0.26233441E 00-0.26233524E 00-0.26233321E 00
0000900-0.26232857E 00-0.26232022E 00-0.26230979E 00-0.26229137E 00-0.26225829E 00
0001000-0.26219487E 00-0.26207727E 00-0.26186949E 00-0.26152331E 00-0.26097441E 00
0001100-0.26[illegible]304E 00-0.25893539E 00-0.25724393E 00-0.25495243E 00-0.25194150E 00
0001200-0.24[illegible]9617E 00-0.24331313E 00-0.23749441E 00-0.23110306E 00-0.22153002E 00
0001300-0.21978581E 00-0.22153002E 00-0.23110306E 00-0.23749441E 00-0.24331313E 00
EOF
q
```

```
redit pote6
LOADING POTE6
REKEYED
EDIT
p99
```

MG NL a=075 DENS.

```
        TOP RECORD
0000100 0.12825619E-01 0.12824561E-01 0.12823604E-01 0.12822781E-01 0.12822114E-01
0000200 0.12821656E-01 0.12821395E-01 0.12821373E-01 0.12821592E-01 0.12822043E-01
0000300 0.12822721E-01 0.12823615E-01 0.12824707E-01 0.12825944E-01 0.12827314E-01
0000400 0.12828756E-01 0.12830231E-01 0.12831692E-01 0.12833081E-01 0.12834359E-01
0000500 0.12835439E-01 0.12836315E-01 0.12836955E-01 0.12837321E-01 0.12837380E-01
0000600 0.12837112E-01 0.12836535E-01 0.12835618E-01 0.12834381E-01 0.12832895E-01
0000700 0.12831129E-01 0.12829218E-01 0.12827113E-01 0.12824975E-01 0.12822807E-01
0000800 0.12820691E-01 0.12818731E-01 0.12816984E-01 0.12815494E-01 0.12814358E-01
0000900 0.12813620E-01 0.12813322E-01 0.12813494E-01 0.12814172E-01 0.12815338E-01
0001000 0.12816988E-01 0.12819089E-01 0.12821592E-01 0.12824442E-01 0.12827571E-01
0001100 0.12830861E-01 0.12834210E-01 0.12837537E-01 0.12840692E-01 0.12843598E-01
0001200 0.12846094E-01 0.12848098E-01 0.12849536E-01 0.12850292E-01 0.12850299E-01
0001300 0.12849558E-01 0.12847986E-01 0.12845665E-01 0.12842592E-01 0.12838848E-01
0001400 0.12834515E-01 0.12829751E-01 0.12824710E-01 0.12819543E-01 0.12814470E-01
0001500 0.12809701E-01 0.12805451E-01 0.12801949E-01 0.12799393E-01 0.12797982E-01
0001600 0.12797896E-01 0.12799278E-01 0.12802225E-01 0.12806762E-01 0.12812875E-01
0001700 0.12820497E-01 0.12829427E-01 0.12839455E-01 0.12850258E-01 0.12861397E-01
0001800 0.12872372E-01 0.12882601E-01 0.12891404E-01 0.12898058E-01 0.12901708E-01
0001900 0.12901496E-01 0.12896512E-01 0.12885790E-01 0.12868445E-01 0.12843437E-01
0002000 0.12809966E-01 0.12767136E-01 0.12714222E-01 0.12650535E-01 0.12575593E-01
0002100 0.12489021E-01 0.12390658E-01 0.12280546E-01 0.12158930E-01 0.12026317E-01
0002200 0.11883445E-01 0.11731356E-01 0.11571307E-01 0.11404835E-01 0.11233736E-01
0002300 0.11060070E-01 0.10886122E-01 0.10714352E-01 0.10547534E-01 0.10388464E-01
0002400 0.10240261E-01 0.10106076E-01 0.99892765E-02 0.98933317E-02 0.98217800E-02
0002500 0.97776130E-02 0.97627826E-02 0.97776130E-02 0.98217800E-02 0.98933317E-02
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26223987E 00-0.26223248E 00-0.26223189E 00-0.26223207E 00-0.26223236E 00
0000200-0.26223582E 00-0.26223397E 00-0.26223290E 00-0.26223540E 00-0.26223814E 00
0000300-0.26224262E 00-0.26223779E 00-0.26224321E 00-0.26223850E 00-0.26223594E 00
0000400-0.26223868E 00-0.26223266E 00-0.26223999E 00-0.26223469E 00-0.26222914E 00
0000500-0.26222551E 00-0.26222163E 00-0.26221907E 00-0.26221734E 00-0.26221573E 00
0000600-0.26221544E 00-0.26221657E 00-0.26221716E 00-0.26221919E 00-0.26222295E 00
0000700-0.26222473E 00-0.26222873E 00-0.26223290E 00-0.26223636E 00-0.26224035E 00
0000800-0.26224375E 00-0.26224679E 00-0.26224989E 00-0.26225030E 00-0.26225138E 00
0000900-0.26225197E 00-0.26225060E 00-0.26224875E 00-0.26224583E 00-0.26224273E 00
0001000-0.26223856E 00-0.26223445E 00-0.26222986E 00-0.26222408E 00-0.26221901E 00
0001100-0.26221430E 00-0.26220977E 00-0.26220709E 00-0.26220417E 00-0.26220280E 00
0001200-0.26220393E 00-0.26220471E 00-0.26220787E 00-0.26221347E 00-0.26222014E 00
0001300-0.26222724E 00-0.26223809E 00-0.26224911E 00-0.26226044E 00-0.26227421E 00
0001400-0.26228946E 00-0.26230252E 00-0.26231647E 00-0.26233149E 00-0.26234412E 00
0001500-0.26235682E 00-0.26236826E 00-0.26237845E 00-0.26238602E 00-0.26239341E 00
0001600-0.26239818E 00-0.26240057E 00-0.26240349E 00-0.26240307E 00-0.26240301E 00
0001700-0.26240063E 00-0.26239771E 00-0.26239395E 00-0.26238906E 00-0.26238424E 00
0001800-0.26237673E 00-0.26236629E 00-0.26235205E 00-0.26233250E 00-0.26230377E 00
0001900-0.26226360E 00-0.26220685E 00-0.26212865E 00-0.26202297E 00-0.26188111E 00
0002000-0.26169437E 00-0.26145315E 00-0.26114601E 00-0.26075900E 00-0.26027769E 00
0002100-0.25968647E 00-0.25896692E 00-0.25810176E 00-0.25707132E 00-0.25585347E 00
0002200-0.25442827E 00-0.25277543E 00-0.25087047E 00-0.24869162E 00-0.24622166E 00
0002300-0.24343836E 00-0.24032122E 00-0.23685622E 00-0.23302841E 00-0.22882313E 00
0002400-0.22423142E 00-0.21924859E 00-0.21387637E 00-0.20809615E 00-0.20321208E 00
0002500-0.19986981E 00-0.19944793E 00-0.19986981E 00-0.20321208E 00-0.20809615E 00
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
```

MG NL a=1.0 DENS.

```
        TOP RECORD
0000100 0.12825370E-01 0.12822498E-01 0.12820259E-01 0.12818962E-01 0.12818817E-01
0000200 0.12819964E-01 0.12822323E-01 0.12825646E-01 0.12829561E-01 0.12833588E-01
0000300 0.12837168E-01 0.12839802E-01 0.12841031E-01 0.12840621E-01 0.12838427E-01
0000400 0.12834657E-01 0.12829673E-01 0.12824085E-01 0.12818594E-01 0.12814023E-01
0000500 0.12811065E-01 0.12810361E-01 0.12812253E-01 0.12816790E-01 0.12823645E-01
0000600 0.12832128E-01 0.12841284E-01 0.12849923E-01 0.12856789E-01 0.12860741E-01
0000700 0.12860890E-01 0.12856785E-01 0.12848552E-01 0.12836892E-01 0.12823220E-01
0000800 0.12809388E-01 0.12797683E-01 0.12790427E-01 0.12789730E-01 0.12797043E-01
0000900 0.12812812E-01 0.12836158E-01 0.12864485E-01 0.12893476E-01 0.12916915E-01
0001000 0.12926962E-01 0.12914561E-01 0.12869988E-01 0.12783580E-01 0.12646809E-01
0001100 0.12453198E-01 0.12199473E-01 0.11886336E-01 0.11519376E-01 0.11109214E-01
0001200 0.10671709E-01 0.10227412E-01 0.98008178E-02 0.94196051E-02 0.91137104E-02
0001300 0.89140013E-02 0.88459179E-02 0.89140013E-02 0.91137104E-02 0.94196051E-02
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26224035E 00-0.26223874E 00-0.26224732E 00-0.26224941E 00-0.26224482E 00
0000200-0.26224625E 00-0.26224339E 00-0.26223981E 00-0.26222819E 00-0.26222688E 00
0000300-0.26221853E 00-0.26221418E 00-0.26221335E 00-0.26221687E 00-0.26222312E 00
0000400-0.26223290E 00-0.26224458E 00-0.26225621E 00-0.26226699E 00-0.26227415E 00
0000500-0.26227836E 00-0.26227677E 00-0.26227200E 00-0.26226223E 00-0.26225114E 00
0000600-0.26223981E 00-0.26223004E 00-0.26222503E 00-0.26222748E 00-0.26223719E 00
0000700-0.26225525E 00-0.26226142E 00-0.26231343E 00-0.26234913E 00-0.26238477E 00
0000800-0.26241696E 00-0.26244289E 00-0.26246029E 00-0.26246750E 00-0.26246625E 00
0000900-0.26245803E 00-0.26244318E 00-0.26242584E 00-0.26240158E 00-0.26236296E 00
0001000-0.26229940E 00-0.26214826E 00-0.26188350E 00-0.26141661E 00-0.26063991E 00
0001100-0.25941676E 00-0.25757873E 00-0.25493121E 00-0.25125879E 00-0.24633658E 00
0001200-0.23993999E 00-0.23186433E 00-0.22193903E 00-0.21004355E 00-0.19645798E 00
0001300-0.18390107E 00-0.18226755E 00-0.18390107E 00-0.19645798E 00-0.21004355E 00
EOF
```

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
```

MG NL a=1.5 DENS.

```
        TOP RECORD
0000100 0.12836862E-01 0.12835786E-01 0.12833908E-01 0.12831453E-01 0.12828715E-01
0000200 0.12826037E-01 0.12823831E-01 0.12822349E-01 0.12821831E-01 0.12822412E-01
0000300 0.12824059E-01 0.12826588E-01 0.12829714E-01 0.12832988E-01 0.12836017E-01
0000400 0.12838326E-01 0.12839571E-01 0.12839481E-01 0.12838036E-01 0.12835283E-01
0000500 0.12831565E-01 0.12827296E-01 0.12822982E-01 0.12819253E-01 0.12816641E-01
0000600 0.12815550E-01 0.12816228E-01 0.12818716E-01 0.12822773E-01 0.12827955E-01
0000700 0.12833655E-01 0.12839094E-01 0.12843508E-01 0.12846198E-01 0.12846656E-01
0000800 0.12844581E-01 0.12840088E-01 0.12833547E-01 0.12825683E-01 0.12817468E-01
0000900 0.12810025E-01 0.12804441E-01 0.12801707E-01 0.12802500E-01 0.12807064E-01
0001000 0.12815177E-01 0.12826085E-01 0.12838531E-01 0.12850937E-01 0.12861524E-01
0001100 0.12868591E-01 0.12870666E-01 0.12866896E-01 0.12857087E-01 0.12842037E-01
0001200 0.12823384E-01 0.12803618E-01 0.12785830E-01 0.12773432E-01 0.12769647E-01
0001300 0.12776952E-01 0.12796585E-01 0.12828015E-01 0.12868419E-01 0.12912519E-01
0001400 0.12952354E-01 0.12977593E-01 0.12975905E-01 0.12933828E-01 0.12837794E-01
0001500 0.12675442E-01 0.12437075E-01 0.12117106E-01 0.11715349E-01 0.11237949E-01
0001600 0.10697763E-01 0.10114193E-01 0.95122643E-02 0.89213215E-02 0.83734691E-02
0001700 0.79020970E-02 0.75403042E-02 0.73135570E-02 0.72372593E-02 0.73135570E-02
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26224029E 00-0.26224267E 00-0.26224351E 00-0.26224238E 00-0.26225114E 00
0000200-0.26224464E 00-0.26225656E 00-0.26225412E 00-0.26224536E 00-0.26224077E 00
0000300-0.26223058E 00-0.26222873E 00-0.26222235E 00-0.26220548E 00-0.26220852E 00
0000400-0.26220012E 00-0.26220053E 00-0.26219982E 00-0.26219761E 00-0.26220673E 00
0000500-0.26221442E 00-0.26222032E 00-0.26222795E 00-0.26223892E 00-0.26224416E 00
0000600-0.26224160E 00-0.26224375E 00-0.26223832E 00-0.26222605E 00-0.26220804E 00
0000700-0.26219767E 00-0.26218039E 00-0.26216888E 00-0.26216257E 00-0.26216316E 00
0000800-0.26217002E 00-0.26218283E 00-0.26220042E 00-0.26222003E 00-0.26223952E 00
0000900-0.26225573E 00-0.26226616E 00-0.26226884E 00-0.26226389E 00-0.26224977E 00
0001000-0.26222950E 00-0.26220566E 00-0.26217997E 00-0.26215875E 00-0.26214445E 00
0001100-0.26214027E 00-0.26214808E 00-0.26216918E 00-0.26220262E 00-0.26224625E 00
0001200-0.26229638E 00-0.26234961E 00-0.26240128E 00-0.26244855E 00-0.26248944E 00
0001300-0.26252264E 00-0.26255023E 00-0.26257271E 00-0.26259315E 00-0.26260799E 00
0001400-0.26260823E 00-0.26257044E 00-0.26245278E 00-0.26218581E 00-0.26166940E 00
0001500-0.26076591E 00-0.25929767E 00-0.25704771E 00-0.25376457E 00-0.24916929E 00
0001600-0.24297071E 00-0.23487961E 00-0.22463048E 00-0.21200061E 00-0.19681501E 00
0001700-0.17915154E 00-0.16372526E 00-0.15316224E 00-0.15170753E 00-0.15316224E 00
EOF
q
```

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12828421E-01 0.12822859E-01 0.12817740E-01 0.12813836E-01 0.12811780E-01
0000200 0.12812011E-01 0.12814693E-01 0.12819640E-01 0.12826454E-01 0.12834314E-01
0000300 0.12842286E-01 0.12849331E-01 0.12854453E-01 0.12856867E-01 0.12856014E-01
0000400 0.12851793E-01 0.12844533E-01 0.12835037E-01 0.12824427E-01 0.12814093E-01
0000500 0.12805562E-01 0.12800224E-01 0.12799159E-01 0.12802962E-01 0.12811612E-01
0000600 0.12824390E-01 0.12839966E-01 0.12856402E-01 0.12871429E-01 0.12882791E-01
0000700 0.12888357E-01 0.12886673E-01 0.12877099E-01 0.12860123E-01 0.12837417E-01
0000800 0.12811765E-01 0.12786910E-01 0.12767155E-01 0.12756784E-01 0.12759432E-01
0000900 0.12777437E-01 0.12811057E-01 0.12857884E-01 0.12912456E-01 0.12965962E-01
0001000 0.13006486E-01 0.13019420E-01 0.12988355E-01 0.12896389E-01 0.12727659E-01
0001100 0.12469135E-01 0.12112502E-01 0.11655726E-01 0.11104383E-01 0.10472093E-01
0001200 0.97803250E-02 0.90571269E-02 0.83353110E-02 0.76501295E-02 0.70371255E-02
0001300 0.65301768E-02 0.61548688E-02 0.59251301E-02 0.58484003E-02 0.59251301E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26224023E 00-0.26225436E 00-0.26227266E 00-0.26228422E 00-0.26228976E 00
0000200-0.26229841E 00-0.26229644E 00-0.26228690E 00-0.26227057E 00-0.26226008E 00
0000300-0.26223713E 00-0.26222372E 00-0.26221627E 00-0.26221704E 00-0.26222616E 00
0000400-0.26224285E 00-0.26226598E 00-0.26229334E 00-0.26232141E 00-0.26234585E 00
0000500-0.26236421E 00-0.26237196E 00-0.26236969E 00-0.26235473E 00-0.26232982E 00
0000600-0.26229823E 00-0.26226234E 00-0.26222914E 00-0.26220334E 00-0.26218921E 00
0000700-0.26218992E 00-0.26220840E 00-0.26224345E 00-0.26229346E 00-0.26235467E 00
0000800-0.26242113E 00-0.26248866E 00-0.26255113E 00-0.26260382E 00-0.26264590E 00
0000900-0.26267606E 00-0.26269537E 00-0.26270902E 00-0.26271462E 00-0.26270771E 00
0001000-0.26266843E 00-0.26255786E 00-0.26230484E 00-0.26180387E 00-0.26090336E 00
0001100-0.25940186E 00-0.25704712E 00-0.25353837E 00-0.24853677E 00-0.24167806E 00
0001200-0.23259419E 00-0.22093874E 00-0.20641214E 00-0.18880159E 00-0.16788715E 00
0001300-0.14824939E 00-0.13472098E 00-0.12566626E 00-0.12431830E 00-0.12566626E 00
EOF
q
```

MG NL a=2.0 DENS.

VEFF

```
redit pote14
LOADING POTE14
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12839492E-01 0.12840416E-01 0.12839831E-01 0.12837816E-01 0.12834575E-01
0000200 0.12830470E-01 0.12826029E-01 0.12821849E-01 0.12818452E-01 0.12816373E-01
0000300 0.12815937E-01 0.12817297E-01 0.12820352E-01 0.12824774E-01 0.12829993E-01
0000400 0.12835387E-01 0.12840200E-01 0.12843754E-01 0.12845505E-01 0.12845088E-01
0000500 0.12842432E-01 0.12837753E-01 0.12831565E-01 0.12824606E-01 0.12817774E-01
0000600 0.12812033E-01 0.12808207E-01 0.12806922E-01 0.12808569E-01 0.12813061E-01
0000700 0.12820035E-01 0.12828682E-01 0.12837950E-01 0.12846559E-01 0.12853306E-01
0000800 0.12857109E-01 0.12857169E-01 0.12853198E-01 0.12845404E-01 0.12834534E-01
0000900 0.12821797E-01 0.12808871E-01 0.12797486E-01 0.12789425E-01 0.12786128E-01
0001000 0.12788545E-01 0.12796912E-01 0.12810644E-01 0.12828354E-01 0.12847982E-01
0001100 0.12866892E-01 0.12882318E-01 0.12891635E-01 0.12892786E-01 0.12884717E-01
0001200 0.12867488E-01 0.12842689E-01 0.12813278E-01 0.12783412E-01 0.12758035E-01
0001300 0.12742341E-01 0.12741044E-01 0.12757435E-01 0.12792654E-01 0.12844831E-01
0001400 0.12908656E-01 0.12974866E-01 0.13030488E-01 0.13059199E-01 0.13042312E-01
0001500 0.12960210E-01 0.12794074E-01 0.12528062E-01 0.12151390E-01 0.11660386E-01
0001600 0.11059873E-01 0.10363951E-01 0.95955543E-02 0.87850504E-02 0.79678968E-02
0001700 0.71816221E-02 0.64630806E-02 0.58455318E-02 0.53525977E-02 0.49963854E-02
0001800 0.47816224E-02 0.47102608E-02 0.47816224E-02 0.49963854E-02 0.53525977E-02
EOF
q
redit pote15
LOADING POTE15
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26224041E 00-0.26223212E 00-0.26223451E 00-0.26224053E 00-0.26224554E 00
0000200-0.26225990E 00-0.26226199E 00-0.26227975E 00-0.26228452E 00-0.26227880E 00
0000300-0.26227802E 00-0.26227134E 00-0.26226938E 00-0.26226139E 00-0.26223654E 00
0000400-0.26223266E 00-0.26221621E 00-0.26221007E 00-0.26220870E 00-0.26220506E 00
0000500-0.26221502E 00-0.26223028E 00-0.26224345E 00-0.26225454E 00-0.26227444E 00
0000600-0.26228803E 00-0.26229000E 00-0.26229489E 00-0.26228750E 00-0.26227361E 00
0000700-0.26224738E 00-0.26222974E 00-0.26220411E 00-0.26218015E 00-0.26216298E 00
0000800-0.26215482E 00-0.26215684E 00-0.26216930E 00-0.26219040E 00-0.26221788E 00
0000900-0.26224869E 00-0.26227725E 00-0.26230043E 00-0.26231331E 00-0.26231462E 00
0001000-0.26230103E 00-0.26227552E 00-0.26224035E 00-0.26219791E 00-0.26215661E 00
0001100-0.26212204E 00-0.26209915E 00-0.26209289E 00-0.26210696E 00-0.26214129E 00
0001200-0.26219457E 00-0.26226306E 00-0.26234180E 00-0.26242501E 00-0.26250660E 00
0001300-0.26258111E 00-0.26264638E 00-0.26270139E 00-0.26274705E 00-0.26278841E 00
0001400-0.26282614E 00-0.26285756E 00-0.26286507E 00-0.26280969E 00-0.26261872E 00
0001500-0.26218021E 00-0.26133049E 00-0.25984907E 00-0.25745767E 00-0.25382137E 00
0001600-0.24855828E 00-0.24125624E 00-0.23149353E 00-0.21886814E 00-0.20303416E 00
0001700-0.18371350E 00-0.16093308E 00-0.13901478E 00-0.12218553E 00-0.11061412E 00
0001800-0.10297006E 00-0.10177785E 00-0.10297006E 00-0.11061412E 00-0.12218553E 00
EOF
q
```

MG NL a=2.5 DENS.

VEFF

```
redit pote16
LOADING POTE16
REKEYED
EDIT
p99
```

MG NL a=3.0 DENS.

```
        TOP RECORD
0000100 0.12841653E-01 0.12841474E-01 0.12839492E-01 0.12835883E-01 0.12831032E-01
0000200 0.12825530E-01 0.12820054E-01 0.12815289E-01 0.12811895E-01 0.12810316E-01
0000300 0.12810856E-01 0.12813494E-01 0.12817893E-01 0.12823552E-01 0.12829717E-01
0000400 0.12835532E-01 0.12840226E-01 0.12843013E-01 0.12843430E-01 0.12841269E-01
0000500 0.12836646E-01 0.12830090E-01 0.12822356E-01 0.12814440E-01 0.12807481E-01
0000600 0.12802452E-01 0.12800246E-01 0.12801386E-01 0.12805995E-01 0.12813728E-01
0000700 0.12823790E-01 0.12835033E-01 0.12846079E-01 0.12855425E-01 0.12861751E-01
0000800 0.12863986E-01 0.12861557E-01 0.12854524E-01 0.12843490E-01 0.12829751E-01
0000900 0.12815069E-01 0.12801468E-01 0.12791030E-01 0.12785587E-01 0.12786422E-01
0001000 0.12794092E-01 0.12808260E-01 0.12827575E-01 0.12849879E-01 0.12872368E-01
0001100 0.12891792E-01 0.12905091E-01 0.12909666E-01 0.12903851E-01 0.12887377E-01
0001200 0.12861501E-01 0.12829114E-01 0.12794577E-01 0.12763325E-01 0.12741257E-01
0001300 0.12733892E-01 0.12745500E-01 0.12778137E-01 0.12830716E-01 0.12898326E-01
0001400 0.12971815E-01 0.13037745E-01 0.13078827E-01 0.13074908E-01 0.13004344E-01
0001500 0.12846041E-01 0.12581728E-01 0.12198266E-01 0.11690058E-01 0.11060640E-01
0001600 0.10323741E-01 0.95027909E-02 0.86295567E-02 0.77413954E-02 0.68778731E-02
0001700 0.60772710E-02 0.53733811E-02 0.47890022E-02 0.43341629E-02 0.40111132E-02
0001800 0.38184703E-02 0.37547175E-02 0.38184703E-02 0.40111132E-02 0.43341629E-02
EOF
q
redit pote17
LOADING POTE17
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26224041E 00-0.26223552E 00-0.26223654E 00-0.26223350E 00-0.26224482E 00
0000200-0.26224291E 00-0.26225632E 00-0.26225537E 00-0.26224679E 00-0.26224321E 00
0000300-0.26223350E 00-0.26222181E 00-0.26221013E 00-0.26217806E 00-0.26216835E 00
0000400-0.26214510E 00-0.26213479E 00-0.26212919E 00-0.26212668E 00-0.26213837E 00
0000500-0.26215196E 00-0.26217085E 00-0.26219249E 00-0.26221704E 00-0.26224041E 00
0000600-0.26225412E 00-0.26226759E 00-0.26226777E 00-0.26226056E 00-0.26224238E 00
0000700-0.26222682E 00-0.26220173E 00-0.26218259E 00-0.26217067E 00-0.26216835E 00
0000800-0.26217669E 00-0.26219684E 00-0.26222771E 00-0.26226586E 00-0.26230896E 00
0000900-0.26235056E 00-0.26238638E 00-0.26241088E 00-0.26242197E 00-0.26241571E 00
0001000-0.26239330E 00-0.26235747E 00-0.26231104E 00-0.26226240E 00-0.26221836E 00
0001100-0.26218581E 00-0.26217073E 00-0.26217818E 00-0.26220971E 00-0.26226431E 00
0001200-0.26233840E 00-0.26242656E 00-0.26252252E 00-0.26261783E 00-0.26270491E 00
0001300-0.26277947E 00-0.26283830E 00-0.26287961E 00-0.26290900E 00-0.26292795E 00
0001400-0.26293677E 00-0.26292276E 00-0.26285470E 00-0.26266575E 00-0.26224929E 00
0001500-0.26144272E 00-0.26002324E 00-0.25770003E 00-0.25411695E 00-0.24885851E 00
0001600-0.24146503E 00-0.23145652E 00-0.21836305E 00-0.20176059E 00-0.18132609E 00
0001700-0.15676516E 00-0.13265312E 00-0.11349577E 00-0.98980963E-01-0.89068890E-01
0001800-0.82618713E-01-0.81550360E-01-0.82618713E-01-0.89068890E-01-0.98980963E-01
EOF
q
```

```
redit pote18
LOADING POTE18
REKEYED
EDIT
p99
```

MG NL a=4.0 DENS.

```
        TOP RECORD
0000100 0.12841970E-01 0.12845132E-01 0.12846366E-01 0.12845449E-01 0.12842439E-01
0000200 0.12837715E-01 0.12831844E-01 0.12825571E-01 0.12819745E-01 0.12815177E-01
0000300 0.12812581E-01 0.12812421E-01 0.12814801E-01 0.12819551E-01 0.12826145E-01
0000400 0.12833778E-01 0.12841452E-01 0.12848128E-01 0.12852844E-01 0.12854792E-01
0000500 0.12853548E-01 0.12849066E-01 0.12841754E-01 0.12832381E-01 0.12822092E-01
0000600 0.12812205E-01 0.12804043E-01 0.12798823E-01 0.12797322E-01 0.12800027E-01
0000700 0.12806769E-01 0.12816854E-01 0.12829114E-01 0.12841962E-01 0.12853641E-01
0000800 0.12862429E-01 0.12866866E-01 0.12865946E-01 0.12859393E-01 0.12847677E-01
0000900 0.12831956E-01 0.12814131E-01 0.12796547E-01 0.12781706E-01 0.12771938E-01
0001000 0.12769159E-01 0.12774423E-01 0.12787789E-01 0.12808159E-01 0.12833353E-01
0001100 0.12860276E-01 0.12885217E-01 0.12904432E-01 0.12914471E-01 0.12912907E-01
0001200 0.12898725E-01 0.12872703E-01 0.12837537E-01 0.12797747E-01 0.12759376E-01
0001300 0.12729313E-01 0.12714352E-01 0.12720224E-01 0.12750398E-01 0.12805071E-01
0001400 0.12880143E-01 0.12966737E-01 0.13050873E-01 0.13113964E-01 0.13133653E-01
0001500 0.13085473E-01 0.12944952E-01 0.12690265E-01 0.12305040E-01 0.11781015E-01
0001600 0.11120215E-01 0.10336019E-01 0.94529800E-02 0.85050762E-02 0.75324588E-02
0001700 0.65775029E-02 0.56800805E-02 0.48735738E-02 0.41790232E-02 0.36039576E-02
0001800 0.31471222E-02 0.28026679E-02 0.25633418E-02 0.24226306E-02 0.23763126E-02
EOF
q
redit pote19
LOADING POTE19
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.26224029E 00-0.26222843E 00-0.26223201E 00-0.26223588E 00-0.26224583E 00
0000200-0.26226801E 00-0.26227719E 00-0.26230466E 00-0.26231492E 00-0.26232094E 00
0000300-0.26232833E 00-0.26232421E 00-0.26232201E 00-0.26231056E 00-0.26228446E 00
0000400-0.26227164E 00-0.26224774E 00-0.26223224E 00-0.26222318E 00-0.26221508E 00
0000500-0.26222467E 00-0.26223457E 00-0.26224959E 00-0.26226556E 00-0.26228690E 00
0000600-0.26230502E 00-0.26231766E 00-0.26232839E 00-0.26232338E 00-0.26230699E 00
0000700-0.26227671E 00-0.26224649E 00-0.26220477E 00-0.26216799E 00-0.26213670E 00
0000800-0.26211667E 00-0.26210910E 00-0.26211637E 00-0.26213813E 00-0.26217180E 00
0000900-0.26221329E 00-0.26225764E 00-0.26229990E 00-0.26233190E 00-0.26235062E 00
0001000-0.26235163E 00-0.26233482E 00-0.26230115E 00-0.26225394E 00-0.26220030E 00
0001100-0.26214838E 00-0.26210511E 00-0.26207846E 00-0.26207411E 00-0.26209480E 00
0001200-0.26214105E 00-0.26221043E 00-0.26229763E 00-0.26239765E 00-0.26250273E 00
0001300-0.26260638E 00-0.26270396E 00-0.26279318E 00-0.26287329E 00-0.26295137E 00
0001400-0.26303071E 00-0.26311463E 00-0.26319289E 00-0.26323378E 00-0.26317030E 00
0001500-0.26288992E 00-0.26221919E 00-0.26091814E 00-0.25867438E 00-0.25510138E 00
0001600-0.24974895E 00-0.24211675E 00-0.23167902E 00-0.21791857E 00-0.20034033E 00
0001700-0.17881644E 00-0.15323734E 00-0.12756616E 00-0.10578787E 00-0.87831438E-01
0001800-0.73704481E-01-0.63159704E-01-0.56055587E-01-0.51536500E-01-0.50738353E-01
EOF
q
```

```
redit pote20
LOADING POTE20
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12850251E-01 0.12849282E-01 0.12845688E-01 0.12839757E-01 0.12832142E-01
0000200 0.12823708E-01 0.12815461E-01 0.12808427E-01 0.12803517E-01 0.12801372E-01
0000300 0.12802303E-01 0.12806278E-01 0.12812760E-01 0.12821004E-01 0.12829840E-01
0000400 0.12838110E-01 0.12844570E-01 0.12848262E-01 0.12848493E-01 0.12845024E-01
0000500 0.12838092E-01 0.12828503E-01 0.12817409E-01 0.12806278E-01 0.12796648E-01
0000600 0.12790013E-01 0.12787472E-01 0.12789693E-01 0.12796782E-01 0.12808152E-01
0000700 0.12822576E-01 0.12838416E-01 0.12853649E-01 0.12866259E-01 0.12874372E-01
0000800 0.12876656E-01 0.12872461E-01 0.12861982E-01 0.12846265E-01 0.12827244E-01
0000900 0.12807384E-01 0.12789484E-01 0.12776412E-01 0.12770474E-01 0.12773264E-01
0001000 0.12785252E-01 0.12805700E-01 0.12832530E-01 0.12862612E-01 0.12891967E-01
0001100 0.12916315E-01 0.12931682E-01 0.12934871E-01 0.12924142E-01 0.12899697E-01
0001200 0.12863766E-01 0.12820732E-01 0.12776751E-01 0.12739155E-01 0.12715541E-01
0001300 0.12712594E-01 0.12734976E-01 0.12784045E-01 0.12856830E-01 0.12945231E-01
0001400 0.13035782E-01 0.13109822E-01 0.13144407E-01 0.13113853E-01 0.12991942E-01
0001500 0.12754630E-01 0.12382973E-01 0.11866126E-01 0.11203732E-01 0.10407452E-01
0001600 0.95008686E-02 0.85181221E-02 0.75005405E-02 0.64923875E-02 0.55360720E-02
0001700 0.46674833E-02 0.39088801E-02 0.32673974E-02 0.27402267E-02 0.23190717E-02
0001800 0.19934217E-02 0.17527407E-02 0.15878663E-02 0.14918137E-02 0.14603119E-02
EOF
q
redit pote21
LOADING POTE21
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26223981E 00-0.26222324E 00-0.26221085E 00-0.26221395E 00-0.26220846E 00
0000200-0.26222169E 00-0.26222318E 00-0.26221877E 00-0.26221871E 00-0.26220512E 00
0000300-0.26219875E 00-0.26217806E 00-0.26213944E 00-0.26212257E 00-0.26209295E 00
0000400-0.26207167E 00-0.26205438E 00-0.26204461E 00-0.26205438E 00-0.26207036E 00
0000500-0.26208991E 00-0.26211518E 00-0.26215017E 00-0.26218146E 00-0.26220584E 00
0000600-0.26223457E 00-0.26224858E 00-0.26224422E 00-0.26222908E 00-0.26221323E 00
0000700-0.26218235E 00-0.26215410E 00-0.26213056E 00-0.26211739E 00-0.26211786E 00
0000800-0.26213366E 00-0.26216590E 00-0.26221198E 00-0.26226836E 00-0.26232916E 00
0000900-0.26238841E 00-0.26243740E 00-0.26247227E 00-0.26248658E 00-0.26247841E 00
0001000-0.26244915E 00-0.26240087E 00-0.26234180E 00-0.26228094E 00-0.26222658E 00
0001100-0.26218927E 00-0.26217628E 00-0.26219261E 00-0.26224029E 00-0.26231664E 00
0001200-0.26241696E 00-0.26253456E 00-0.26266015E 00-0.26278347E 00-0.26289612E 00
0001300-0.26299107E 00-0.26306409E 00-0.26311785E 00-0.26315475E 00-0.26318055E 00
0001400-0.26319093E 00-0.26316661E 00-0.26305401E 00-0.26275802E 00-0.26212263E 00
0001500-0.26092255E 00-0.25885421E 00-0.25553250E 00-0.25049460E 00-0.24321204E 00
0001600-0.23311150E 00-0.21960623E 00-0.20213336E 00-0.18021256E 00-0.15338457E 00
0001700-0.12607360E 00-0.10266137E 00-0.82776845E-01-0.66239059E-01-0.52854825E-01
0001800-0.42462461E-01-0.34858637E-01-0.29847201E-01-0.26778318E-01-0.26197068E-01
EOF
q
```

MG NL a=5.0 DENS.

VEFF

```
redit pote22
LOADING POTE22
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12810133E-01 0.12809113E-01 0.12810476E-01 0.12814116E-01 0.12819629E-01
0000200 0.12826342E-01 0.12833450E-01 0.12839951E-01 0.12845065E-01 0.12848023E-01
0000300 0.12848403E-01 0.12846030E-01 0.12841117E-01 0.12834277E-01 0.12826364E-01
0000400 0.12818355E-01 0.12811381E-01 0.12806412E-01 0.12804244E-01 0.12805309E-01
0000500 0.12809612E-01 0.12816697E-01 0.12825772E-01 0.12835715E-01 0.12845192E-01
0000600 0.12852926E-01 0.12857739E-01 0.12858827E-01 0.12855824E-01 0.12848888E-01
0000700 0.12838759E-01 0.12826603E-01 0.12813970E-01 0.12802526E-01 0.12793932E-01
0000800 0.12789484E-01 0.12790065E-01 0.12795903E-01 0.12806501E-01 0.12820739E-01
0000900 0.12836929E-01 0.12852926E-01 0.12866590E-01 0.12875877E-01 0.12879200E-01
0001000 0.12875687E-01 0.12865376E-01 0.12849219E-01 0.12829062E-01 0.12807451E-01
0001100 0.12787335E-01 0.12771700E-01 0.12763172E-01 0.12763560E-01 0.12773596E-01
0001200 0.12792692E-01 0.12818899E-01 0.12849074E-01 0.12879167E-01 0.12904707E-01
0001300 0.12921467E-01 0.12925956E-01 0.12916230E-01 0.12892213E-01 0.12856018E-01
0001400 0.12812067E-01 0.12766656E-01 0.12727384E-01 0.12702249E-01 0.12698438E-01
0001500 0.12721099E-01 0.12771983E-01 0.12848448E-01 0.12942508E-01 0.13040468E-01
0001600 0.13123289E-01 0.13167374E-01 0.13146270E-01 0.13032895E-01 0.12802441E-01
0001700 0.12435425E-01 0.11920724E-01 0.11257701E-01 0.10457572E-01 0.95435455E-02
0001800 0.85492693E-02 0.75158365E-02 0.64875111E-02 0.55068545E-02 0.46101213E-02
0001900 0.38201269E-02 0.31447127E-02 0.25814176E-02 0.21216464E-02 0.17539670E-02
0002000 0.14663208E-02 0.12474118E-02 0.10875133E-02 0.97888103E-03 0.91592874E-03
0002100 0.89532905E-03 0.91592874E-03 0.97888103E-03 0.10875133E-02 0.12474118E-02
EOF
q
redit pote23
LOADING POTE23
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26224059E 00-0.26224267E 00-0.26224661E 00-0.26224202E 00-0.26223099E 00
0000200-0.26222342E 00-0.26221371E 00-0.26220196E 00-0.26218796E 00-0.26218975E 00
0000300-0.26219273E 00-0.26220036E 00-0.26221973E 00-0.26222634E 00-0.26225990E 00
0000400-0.26227456E 00-0.26228434E 00-0.26229721E 00-0.26229876E 00-0.26229805E 00
0000500-0.26228529E 00-0.26225561E 00-0.26224202E 00-0.26220971E 00-0.26218883E 00
0000600-0.26216793E 00-0.26215327E 00-0.26215738E 00-0.26216412E 00-0.26218170E 00
0000700-0.26219881E 00-0.26222938E 00-0.26225495E 00-0.26227558E 00-0.26229554E 00
0000800-0.26230413E 00-0.26229906E 00-0.26227802E 00-0.26225686E 00-0.26221514E 00
0000900-0.26217532E 00-0.26213866E 00-0.26211089E 00-0.26209623E 00-0.26209748E 00
0001000-0.26211572E 00-0.26214969E 00-0.26219672E 00-0.26225191E 00-0.26230776E 00
0001100-0.26235765E 00-0.26239562E 00-0.26241422E 00-0.26241040E 00-0.26238412E 00
0001200-0.26233518E 00-0.26226979E 00-0.26219565E 00-0.26212144E 00-0.26205629E 00
0001300-0.26200926E 00-0.26198709E 00-0.26199400E 00-0.26203227E 00-0.26210153E 00
0001400-0.26219904E 00-0.26232141E 00-0.26246274E 00-0.26261824E 00-0.26278323E 00
0001500-0.26295280E 00-0.26312608E 00-0.26329935E 00-0.26346797E 00-0.26361465E 00
0001600-0.26370311E 00-0.26366270E 00-0.26338142E 00-0.26268870E 00-0.26135290E 00
0001700-0.25906545E 00-0.25553590E 00-0.25040036E 00-0.24313325E 00-0.23317263E 00
0001800-0.21993333E 00-0.20284045E 00-0.18137896E 00-0.15505779E 00-0.12792379E 00
0001900-0.10399693E 00-0.83107412E-01-0.65211356E-01-0.50063781E-01-0.37502684E-01
0002000-0.27392715E-01-0.19605692E-01-0.13975468E-01-0.10317028E-01-0.81272833E-02
0002100-0.76946430E-02-0.81272833E-02-0.10317028E-01-0.13975468E-01-0.19605692E-01
EOF
q
```

MG NL a=6.0 DENS.

VEFF

```
redit pote24
LOADING POTE24
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12852442E-01 0.12856588E-01 0.12857497E-01 0.12854971E-01 0.12849208E-01
0000200 0.12840793E-01 0.12830775E-01 0.12820367E-01 0.12810875E-01 0.12803618E-01
0000300 0.12799583E-01 0.12799446E-01 0.12803346E-01 0.12810890E-01 0.12821224E-01
0000400 0.12833048E-01 0.12844846E-01 0.12854967E-01 0.12861978E-01 0.12864780E-01
0000500 0.12862753E-01 0.12855869E-01 0.12844831E-01 0.12830902E-01 0.12815781E-01
0000600 0.12801483E-01 0.12789991E-01 0.12782991E-01 0.12781717E-01 0.12786668E-01
0000700 0.12797549E-01 0.12813214E-01 0.12831848E-01 0.12851108E-01 0.12868375E-01
0000800 0.12881178E-01 0.12887467E-01 0.12885910E-01 0.12876220E-01 0.12859166E-01
0000900 0.12836579E-01 0.12811214E-01 0.12786403E-01 0.12765713E-01 0.12752373E-01
0001000 0.12748882E-01 0.12756605E-01 0.12775399E-01 0.12803610E-01 0.12838084E-01
0001100 0.12874495E-01 0.12907814E-01 0.12932982E-01 0.12945626E-01 0.12942702E-01
0001200 0.12923181E-01 0.12888398E-01 0.12842238E-01 0.12790881E-01 0.12742255E-01
0001300 0.12705069E-01 0.12687732E-01 0.12696877E-01 0.12736026E-01 0.12804225E-01
0001400 0.12895148E-01 0.12996536E-01 0.13090093E-01 0.13152394E-01 0.13156280E-01
0001500 0.13073105E-01 0.12875542E-01 0.12540843E-01 0.12054123E-01 0.11411268E-01
0001600 0.10620799E-01 0.97044818E-02 0.86959265E-02 0.76375082E-02 0.65758154E-02
0001700 0.55564009E-02 0.46183392E-02 0.37864535E-02 0.30694844E-02 0.24652204E-02
0001800 0.19649202E-02 0.15565935E-02 0.12272112E-02 0.96407044E-03 0.75555383E-03
0001900 0.59148017E-03 0.46319608E-03 0.36351895E-03 0.28659613E-03 0.22774015E-03
0002000 0.18325511E-03 0.15028381E-03 0.12667013E-03 0.11084935E-03 0.10176345E-03
0002100 0.98801567E-04 0.10176345E-03 0.11084935E-03 0.12667013E-03 0.15028381E-03
0002200///// BSN=2304, COMPLETE, 0000021,FSRRANTE.SNIDE
0002300
EOF
q
redit pote25
LOADING POTE25
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26224011E 00-0.26222289E 00-0.26221246E 00-0.26220679E 00-0.26221585E 00
0000200-0.26221746E 00-0.26224726E 00-0.26226097E 00-0.26227099E 00-0.26228213E 00
0000300-0.26228189E 00-0.26228166E 00-0.26226979E 00-0.26223677E 00-0.26221555E 00
0000400-0.26217568E 00-0.26214612E 00-0.26212084E 00-0.26209801E 00-0.26209569E 00
0000500-0.26210576E 00-0.26212364E 00-0.26214683E 00-0.26218170E 00-0.26221496E 00
0000600-0.26224309E 00-0.26227045E 00-0.26228541E 00-0.26228267E 00-0.26226324E 00
0000700-0.26223969E 00-0.26219273E 00-0.26214433E 00-0.26209760E 00-0.26206023E 00
0000800-0.26203710E 00-0.26203161E 00-0.26204681E 00-0.26208133E 00-0.26213181E 00
0000900-0.26219225E 00-0.26225632E 00-0.26231384E 00-0.26235884E 00-0.26238173E 00
0001000-0.26237923E 00-0.26235062E 00-0.26229644E 00-0.26222467E 00-0.26214546E 00
0001100-0.26206982E 00-0.26200891E 00-0.26197481E 00-0.26197445E 00-0.26201218E 00
0001200-0.26208794E 00-0.26219708E 00-0.26233315E 00-0.26248556E 00-0.26264292E 00
0001300-0.26279384E 00-0.26292759E 00-0.26303554E 00-0.26311725E 00-0.26317334E 00
0001400-0.26321059E 00-0.26322937E 00-0.26321977E 00-0.26314110E 00-0.26291186E 00
0001500-0.26239258E 00-0.26137316E 00-0.25956136E 00-0.25657910E 00-0.25196272E 00
0001600-0.24517393E 00-0.23561656E 00-0.22266793E 00-0.20571351E 00-0.18420315E 00
0001700-0.15759265E 00-0.13019687E 00-0.10626477E 00-0.85280836E-01-0.66904545E-01
0001800-0.50789643E-01-0.36632288E-01-0.24171535E-01-0.13183836E-01-0.34783466E-02
0001900 0.51066838E-02 0.12709886E-01 0.19454565E-01 0.25449496E-01 0.30797340E-01
0002000 0.35591800E-01 0.39897773E-01 0.43701958E-01 0.46835344E-01 0.48987284E-01
0002100 0.49733598E-01 0.48987284E-01 0.46835344E-01 0.43701958E-01 0.39897773E-01
EOF
q
```

MG NL a=10.0 DENS.

VEFF

```
redit pote26
LOADING POTE26
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.12851231E-01 0.12855671E-01 0.12856793E-01 0.12854349E-01 0.12848534E-01
0000200 0.12839992E-01 0.12829732E-01 0.12819003E-01 0.12809228E-01 0.12801636E-01
0000300 0.12797374E-01 0.12797065E-01 0.12800910E-01 0.12808498E-01 0.12819022E-01
0000400 0.12831088E-01 0.12843199E-01 0.12853652E-01 0.12860943E-01 0.12863919E-01
0000500 0.12861926E-01 0.12854982E-01 0.12843695E-01 0.12829401E-01 0.12813807E-01
0000600 0.12798958E-01 0.12786902E-01 0.12779403E-01 0.12777708E-01 0.12782406E-01
0000700 0.12793180E-01 0.12808934E-01 0.12827829E-01 0.12847457E-01 0.12865134E-01
0000800 0.12878347E-01 0.12884926E-01 0.12883540E-01 0.12873799E-01 0.12856450E-01
0000900 0.12833342E-01 0.12807287E-01 0.12781646E-01 0.12760088E-01 0.12745932E-01
0001000 0.12741808E-01 0.12749132E-01 0.12767870E-01 0.12796406E-01 0.12831561E-01
0001100 0.12868982E-01 0.12903575E-01 0.12930155E-01 0.12944203E-01 0.12942519E-01
0001200 0.12923978E-01 0.12889795E-01 0.12843754E-01 0.12792040E-01 0.12742575E-01
0001300 0.12704253E-01 0.12685541E-01 0.12693301E-01 0.12731250E-01 0.12798727E-01
0001400 0.12889579E-01 0.12991697E-01 0.13086911E-01 0.13151873E-01 0.13159323E-01
0001500 0.13080481E-01 0.12887776E-01 0.12558173E-01 0.12076367E-01 0.11437848E-01
0001600 0.10650828E-01 0.97366981E-02 0.87289102E-02 0.76979900E-02 0.66060349E-02
0001700 0.55834055E-02 0.46412908E-02 0.38048481E-02 0.30831003E-02 0.24740614E-02
0001800 0.19691510E-02 0.15564843E-02 0.12230899E-02 0.95627527E-03 0.74440218E-03
0001900 0.57723885E-03 0.44605648E-03 0.34357561E-03 0.26382506E-03 0.20197275E-03
0002000 0.15414915E-03 0.11728215E-03 0.88947752E-04 0.67243483E-04 0.50681003E-04
0002100 0.38098500E-04 0.28589275E-04 0.21445885E-04 0.16116872E-04 0.12174350E-04
0002200 0.92896898E-05 0.72148414E-05 0.57672460E-05 0.48175643E-05 0.42801576E-05
0002300 0.41062904E-05 0.42801576E-05 0.48175643E-05 0.57672460E-05 0.72148414E-05
EOF
q
```

MG NL a=15.0 DENS.

```
redit pote27
LOADING POTE27
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.26224059E 00-0.26222444E 00-0.26221293E 00-0.26221174E 00-0.26222444E 00
0000200-0.26222765E 00-0.26225930E 00-0.26227868E 00-0.26229024E 00-0.26230550E 00
0000300-0.26230943E 00-0.26230758E 00-0.26229388E 00-0.26225662E 00-0.26223540E 00
0000400-0.26219374E 00-0.26216203E 00-0.26213485E 00-0.26211107E 00-0.26211309E 00
0000500-0.26212299E 00-0.26214033E 00-0.26216626E 00-0.26220632E 00-0.26224411E 00
0000600-0.26227468E 00-0.26230103E 00-0.26231498E 00-0.26231158E 00-0.26228768E 00
0000700-0.26225835E 00-0.26220793E 00-0.26215565E 00-0.26210523E 00-0.26206470E 00
0000800-0.26203877E 00-0.26203161E 00-0.26204520E 00-0.26207936E 00-0.26213086E 00
0000900-0.26219237E 00-0.26225817E 00-0.26231748E 00-0.26236373E 00-0.26238728E 00
0001000-0.26238561E 00-0.26235604E 00-0.26230067E 00-0.26222724E 00-0.26214504E 00
0001100-0.26206660E 00-0.26200318E 00-0.26196694E 00-0.26196516E 00-0.26200259E 00
0001200-0.26207894E 00-0.26219070E 00-0.26233089E 00-0.26248819E 00-0.26265061E 00
0001300-0.26280785E 00-0.26294810E 00-0.26306188E 00-0.26314837E 00-0.26320809E 00
0001400-0.26324779E 00-0.26326841E 00-0.26326036E 00-0.26318330E 00-0.26295871E 00
0001500-0.26244783E 00-0.26144242E 00-0.25965232E 00-0.25670105E 00-0.25212675E 00
0001600-0.24539196E 00-0.23590207E 00-0.22303331E 00-0.20616961E 00-0.18475980E 00
0001700-0.15825737E 00-0.13097066E 00-0.10714281E 00-0.86254656E-01-0.67960083E-01
0001800-0.51906295E-01-0.37782717E-01-0.25319871E-01-0.14283057E-01-0.44673048E-02
0001900 0.43089353E-02 0.12210801E-01 0.19394230E-01 0.26015062E-01 0.32234516E-01
0002000 0.38226169E-01 0.44183251E-01 0.50311726E-01 0.56805439E-01 0.63798010E-01
0002100 0.71286261E-01 0.79048455E-01 0.86639941E-01 0.93511283E-01 0.99233568E-01
0002200 0.10367370E 00 0.10698223E 00 0.10940880E 00 0.11112362E 00 0.11217111E 00
0002300 0.11252528E 00 0.11217111E 00 0.11112362E 00 0.10940880E 00 0.10698223E 00
EOF
q
```

VEFF

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.10997508E-01 0.10997679E-01 0.10997918E-01 0.10998227E-01 0.10998592E-01
0000200 0.10999043E-01 0.10999553E-01 0.11000086E-01 0.11000648E-01 0.11001240E-01
0000300 0.11001840E-01 0.11002440E-01 0.11003006E-01 0.11003535E-01 0.11004012E-01
0000400 0.11004414E-01 0.11004731E-01 0.11004973E-01 0.11005115E-01 0.11005145E-01
0000500 0.11005078E-01 0.11004884E-01 0.11004586E-01 0.11004198E-01 0.11003722E-01
0000600 0.11003148E-01 0.11002526E-01 0.11001859E-01 0.11001125E-01 0.11000410E-01
0000700 0.10999717E-01 0.10999024E-01 0.10998409E-01 0.10997869E-01 0.10997396E-01
0000800 0.10997064E-01 0.10996860E-01 0.10996770E-01 0.10996848E-01 0.10997079E-01
0000900 0.10997448E-01 0.10997977E-01 0.10998636E-01 0.10999415E-01 0.11000324E-01
0001000 0.11001308E-01 0.11002336E-01 0.11003420E-01 0.11004500E-01 0.11005517E-01
0001100 0.11006486E-01 0.11007335E-01 0.11008050E-01 0.11008609E-01 0.11008959E-01
0001200 0.11009078E-01 0.11008974E-01 0.11008620E-01 0.11008009E-01 0.11007145E-01
0001300 0.11006042E-01 0.11004712E-01 0.11003181E-01 0.11001501E-01 0.10999695E-01
0001400 0.10997847E-01 0.10995969E-01 0.10994140E-01 0.10992464E-01 0.10990940E-01
0001500 0.10989677E-01 0.10988742E-01 0.10988176E-01 0.10988057E-01 0.10988396E-01
0001600 0.10989252E-01 0.10990657E-01 0.10992568E-01 0.10995034E-01 0.10997958E-01
0001700 0.11001319E-01 0.11005025E-01 0.11008993E-01 0.11013076E-01 0.11017140E-01
0001800 0.11021011E-01 0.11024456E-01 0.11027306E-01 0.11029311E-01 0.11030212E-01
0001900 0.11029728E-01 0.11027627E-01 0.11023611E-01 0.11017404E-01 0.11008769E-01
0002000 0.10997407E-01 0.10983091E-01 0.10965638E-01 0.10944858E-01 0.10920621E-01
0002100 0.10892816E-01 0.10861471E-01 0.10826539E-01 0.10788139E-01 0.10746427E-01
0002200 0.10701668E-01 0.10654144E-01 0.10604274E-01 0.10552559E-01 0.10499571E-01
0002300 0.10445956E-01 0.10392521E-01 0.10340024E-01 0.10289453E-01 0.10241799E-01
0002400 0.10198113E-01 0.10159563E-01 0.10127343E-01 0.10102727E-01 0.10086995E-01
0002500 0.10081626E-01 0.10086995E-01 0.10102727E-01 0.10127343E-01 0.10159563E-01
EOF
q
pedit pote3
LOADING POTE3
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.23670805E 00-0.23670721E 00-0.23670864E 00-0.23670757E 00-0.23670775E 00
0000200-0.23671585E 00-0.23671669E 00-0.23672116E 00-0.23672104E 00-0.23672324E 00
0000300-0.23672676E 00-0.23673248E 00-0.23672998E 00-0.23673320E 00-0.23673379E 00
0000400-0.23673457E 00-0.23673618E 00-0.23673284E 00-0.23673654E 00-0.23673606E 00
0000500-0.23673409E 00-0.23673326E 00-0.23673224E 00-0.23673135E 00-0.23673069E 00
0000600-0.23672915E 00-0.23672879E 00-0.23672801E 00-0.23672652E 00-0.23672479E 00
0000700-0.23672384E 00-0.23672265E 00-0.23672152E 00-0.23672032E 00-0.23671877E 00
0000800-0.23671758E 00-0.23671639E 00-0.23671502E 00-0.23671365E 00-0.23671198E 00
0000900-0.23671085E 00-0.23670983E 00-0.23670840E 00-0.23670769E 00-0.23670727E 00
0001000-0.23670715E 00-0.23670751E 00-0.23670787E 00-0.23670888E 00-0.23671007E 00
0001100-0.23671156E 00-0.23671275E 00-0.23671424E 00-0.23671621E 00-0.23671818E 00
0001200-0.23672062E 00-0.23672330E 00-0.23672509E 00-0.23672718E 00-0.23672909E 00
0001300-0.23673069E 00-0.23673135E 00-0.23673236E 00-0.23673213E 00-0.23673135E 00
0001400-0.23672992E 00-0.23672789E 00-0.23672527E 00-0.23672158E 00-0.23671770E 00
0001500-0.23671317E 00-0.23670816E 00-0.23670298E 00-0.23669738E 00-0.23669213E 00
0001600-0.23668706E 00-0.23668277E 00-0.23667896E 00-0.23667657E 00-0.23667568E 00
0001700-0.23667616E 00-0.23667848E 00-0.23668218E 00-0.23668760E 00-0.23669553E 00
0001800-0.23670477E 00-0.23671472E 00-0.23672581E 00-0.23673624E 00-0.23674506E 00
0001900-0.23675144E 00-0.23675358E 00-0.23674881E 00-0.23673475E 00-0.23670882E 00
0002000-0.23666763E 00-0.23660737E 00-0.23652405E 00-0.23641264E 00-0.23626792E 00
0002100-0.23608434E 00-0.23585588E 00-0.23557574E 00-0.23523664E 00-0.23483229E 00
0002200-0.23435432E 00-0.23379552E 00-0.23314840E 00-0.23240435E 00-0.23155737E 00
0002300-0.23059976E 00-0.22952527E 00-0.22832817E 00-0.22700429E 00-0.22554976E 00
0002400-0.22396225E 00-0.22224158E 00-0.22038829E 00-0.21851629E 00-0.21601820E 00
0002500-0.21556562E 00-0.21601820E 00-0.21851629E 00-0.22038829E 00-0.22224158E 00
EOF
-
```

MG+ LDA a=0.25 DENS.

VEFF

```
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
```

MG+ LDA a=0.5 DENS.

```
        TOP RECORD
0000100 0.10996781E-01 0.10997105E-01 0.10997996E-01 0.10999363E-01 0.11001091E-01
0000200 0.11003032E-01 0.11004910E-01 0.11006534E-01 0.11007563E-01 0.11008110E-01
0000300 0.11007808E-01 0.11006698E-01 0.11004847E-01 0.11002414E-01 0.10999657E-01
0000400 0.10996886E-01 0.10994449E-01 0.10992654E-01 0.10991793E-01 0.10992087E-01
0000500 0.10993600E-01 0.10996275E-01 0.10999884E-01 0.11004090E-01 0.11008412E-01
0000600 0.11012312E-01 0.11015251E-01 0.11016753E-01 0.11016384E-01 0.11013959E-01
0000700 0.11009544E-01 0.11003438E-01 0.10996196E-01 0.10988645E-01 0.10981768E-01
0000800 0.10976680E-01 0.10974396E-01 0.10975767E-01 0.10981359E-01 0.10991249E-01
0000900 0.11004861E-01 0.11020996E-01 0.11037640E-01 0.11052009E-01 0.11060718E-01
0001000 0.11059809E-01 0.11045001E-01 0.11012059E-01 0.10957018E-01 0.10876764E-01
0001100 0.10769300E-01 0.10634232E-01 0.10473110E-01 0.10289762E-01 0.10090433E-01
0001200 0.98838024E-02 0.96809976E-02 0.94952770E-02 0.93417615E-02 0.92368238E-02
0001300 0.92001818E-02 0.92368238E-02 0.93417615E-02 0.94952770E-02 0.96809976E-02
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670715E 00-0.23670352E 00-0.23671150E 00-0.23670834E 00-0.23670375E 00
0000200-0.23671132E 00-0.23671103E 00-0.23671097E 00-0.23671138E 00-0.23671155E 00
0000300-0.23671579E 00-0.23671639E 00-0.23671681E 00-0.23671681E 00-0.23671496E 00
0000400-0.23671240E 00-0.23670954E 00-0.23670530E 00-0.23670089E 00-0.23669583E 00
0000500-0.23669195E 00-0.23668939E 00-0.23668867E 00-0.23669034E 00-0.23669499E 00
0000600-0.23670137E 00-0.23671007E 00-0.23672009E 00-0.23673075E 00-0.23673993E 00
0000700-0.23674631E 00-0.23674899E 00-0.23674649E 00-0.23673886E 00-0.23672509E 00
0000800-0.23670751E 00-0.23668754E 00-0.23666823E 00-0.23665410E 00-0.23664856E 00
0000900-0.23665559E 00-0.23667783E 00-0.23671573E 00-0.23676455E 00-0.23681474E 00
0001000-0.23684961E 00-0.23684126E 00-0.23675174E 00-0.23652941E 00-0.23610854E 00
0001100-0.23540801E 00-0.23433304E 00-0.23277676E 00-0.23062503E 00-0.22775396E 00
0001200-0.22407115E 00-0.21946275E 00-0.21386373E 00-0.20763832E 00-0.19859272E 00
0001300-0.19680727E 00-0.19859272E 00-0.20763832E 00-0.21386373E 00-0.21946275E 00
EOF
q
```

```
dedit pote6
LOADING POTL6
REKEYED
EDIT
p99
```

MG+ LDA a=0.75

DENS.

```
        TOP RECORD
0000100 0.10995016E-01 0.10995068E-01 0.10995314E-01 0.10995787E-01 0.10996472E-01
0000200 0.10997370E-01 0.10998420E-01 0.10999635E-01 0.11000972E-01 0.11002410E-01
0000300 0.11003882E-01 0.11005379E-01 0.11006825E-01 0.11008156E-01 0.11009395E-01
0000400 0.11010472E-01 0.11011325E-01 0.11011921E-01 0.11012271E-01 0.11012338E-01
0000500 0.11012074E-01 0.11011511E-01 0.11010643E-01 0.11009466E-01 0.11008017E-01
0000600 0.11006340E-01 0.11004463E-01 0.11002425E-01 0.11000283E-01 0.10998104E-01
0000700 0.10995943E-01 0.10993876E-01 0.10991953E-01 0.10990266E-01 0.10988869E-01
0000800 0.10987770E-01 0.10987088E-01 0.10986816E-01 0.10986991E-01 0.10987643E-01
0000900 0.10988753E-01 0.10990329E-01 0.10992356E-01 0.10994762E-01 0.10997482E-01
0001000 0.11000507E-01 0.11003718E-01 0.11007015E-01 0.11010334E-01 0.11013556E-01
0001100 0.11016551E-01 0.11019252E-01 0.11021528E-01 0.11023276E-01 0.11024434E-01
0001200 0.11024911E-01 0.11024673E-01 0.11023641E-01 0.11021830E-01 0.11019245E-01
0001300 0.11015907E-01 0.11011869E-01 0.11007208E-01 0.11002049E-01 0.10996539E-01
0001400 0.10990798E-01 0.10985017E-01 0.10979392E-01 0.10974132E-01 0.10969404E-01
0001500 0.10965448E-01 0.10962468E-01 0.10960631E-01 0.10960121E-01 0.10961074E-01
0001600 0.10963608E-01 0.10967787E-01 0.10973614E-01 0.10981049E-01 0.10990020E-01
0001700 0.11000346E-01 0.11011805E-01 0.11024103E-01 0.11036839E-01 0.11049602E-01
0001800 0.11061866E-01 0.11073064E-01 0.11082549E-01 0.11089627E-01 0.11093564E-01
0001900 0.11093572E-01 0.11088904E-01 0.11078712E-01 0.11062238E-01 0.11038717E-01
0002000 0.11007424E-01 0.10967705E-01 0.10919012E-01 0.10860823E-01 0.10792848E-01
0002100 0.10714862E-01 0.10626793E-01 0.10528799E-01 0.10421157E-01 0.10304399E-01
0002200 0.10179222E-01 0.10046564E-01 0.99075548E-02 0.97635277E-02 0.96160695E-02
0002300 0.94669126E-02 0.93179680E-02 0.91713518E-02 0.90293065E-02 0.88942535E-02
0002400 0.87686889E-02 0.86552650E-02 0.85567161E-02 0.84758997E-02 0.84157176E-02
0002500 0.83786063E-02 0.83661228E-02 0.83786063E-02 0.84157176E-02 0.84758997E-02
EOF
q
```

```
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670810E 00-0.23670733E 00-0.23669964E 00-0.23669982E 00-0.23670930E 00
0000200-0.23670644E 00-0.23671085E 00-0.23670793E 00-0.23670805E 00-0.23671436E 00
0000300-0.23672259E 00-0.23672104E 00-0.23672199E 00-0.23672116E 00-0.23672068E 00
0000400-0.23672265E 00-0.23672271E 00-0.23672485E 00-0.23672444E 00-0.23672479E 00
0000500-0.23672533E 00-0.23672515E 00-0.23672616E 00-0.23672652E 00-0.23672640E 00
0000600-0.23672593E 00-0.23672640E 00-0.23672527E 00-0.23672348E 00-0.23672205E 00
0000700-0.23672056E 00-0.23671788E 00-0.23671591E 00-0.23671223E 00-0.23670965E 00
0000800-0.23670697E 00-0.23670316E 00-0.23669958E 00-0.23669600E 00-0.23669267E 00
0000900-0.23668993E 00-0.23668712E 00-0.23668563E 00-0.23668450E 00-0.23668426E 00
0001000-0.23668504E 00-0.23668671E 00-0.23668939E 00-0.23669285E 00-0.23669765E 00
0001100-0.23670292E 00-0.23670900E 00-0.23671591E 00-0.23672342E 00-0.23673081E 00
0001200-0.23673934E 00-0.23674667E 00-0.23675400E 00-0.23676091E 00-0.23676634E 00
0001300-0.23677081E 00-0.23677415E 00-0.23677486E 00-0.23677421E 00-0.23677188E 00
0001400-0.23676705E 00-0.23675972E 00-0.23675025E 00-0.23673880E 00-0.23672611E 00
0001500-0.23671097E 00-0.23669565E 00-0.23667967E 00-0.23666406E 00-0.23664868E 00
0001600-0.23663568E 00-0.23662496E 00-0.23661780E 00-0.23661482E 00-0.23661685E 00
0001700-0.23662400E 00-0.23663777E 00-0.23665738E 00-0.23668402E 00-0.23671621E 00
0001800-0.23675364E 00-0.23679560E 00-0.23683995E 00-0.23688340E 00-0.23692411E 00
0001900-0.23695731E 00-0.23697799E 00-0.23698044E 00-0.23695683E 00-0.23690009E 00
0002000-0.23680013E 00-0.23664612E 00-0.23642641E 00-0.23612720E 00-0.23573422E 00
0002100-0.23523122E 00-0.23460102E 00-0.23382539E 00-0.23288459E 00-0.23175901E 00
0002200-0.23042732E 00-0.22886896E 00-0.22706312E 00-0.22498870E 00-0.22262615E 00
0002300-0.21995634E 00-0.21696270E 00-0.21362978E 00-0.20994532E 00-0.20589966E 00
0002400-0.20148724E 00-0.19670534E 00-0.19155693E 00-0.18604845E 00-0.19137479E 00
0002500-0.17820662E 00-0.17776495E 00-0.17820662E 00-0.18137479E 00-0.18604845E 00
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.10992233E-01 0.10992125E-01 0.10993186E-01 0.10995362E-01 0.10998476E-01
0000200 0.11002243E-01 0.11006188E-01 0.11009898E-01 0.11012863E-01 0.11014674E-01
0000300 0.11014994E-01 0.11013683E-01 0.11010762E-01 0.11006426E-01 0.11001095E-01
0000400 0.10995362E-01 0.10989856E-01 0.10985333E-01 0.10982394E-01 0.10981604E-01
0000500 0.10983262E-01 0.10987390E-01 0.10993753E-01 0.11001747E-01 0.11010539E-01
0000600 0.11019118E-01 0.11026319E-01 0.11031065E-01 0.11032432E-01 0.11029795E-01
0000700 0.11022970E-01 0.11012290E-01 0.10998629E-01 0.10983404E-01 0.10968439E-01
0000800 0.10955885E-01 0.10947872E-01 0.10946427E-01 0.10953020E-01 0.10968339E-01
0000900 0.10991931E-01 0.11022165E-01 0.11055864E-01 0.11088379E-01 0.11113666E-01
0001000 0.11124548E-01 0.11113029E-01 0.11070881E-01 0.10990307E-01 0.10864723E-01
0001100 0.10689430E-01 0.10462601E-01 0.10185815E-01 0.98645352E-02 0.95084570E-02
0001200 0.91313533E-02 0.87506846E-02 0.83870701E-02 0.80634952E-02 0.78047775E-02
0001300 0.76362789E-02 0.75787939E-02 0.76362789E-02 0.78047775E-02 0.80634952E-02
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.23670810E 00-0.23670208E 00-0.23670423E 00-0.23669815E 00-0.23669267E 00
0000200-0.23670101E 00-0.23670328E 00-0.23670489E 00-0.23670727E 00-0.23671335E 00
0000300-0.23671675E 00-0.23672050E 00-0.23672342E 00-0.23672575E 00-0.23672462E 00
0000400-0.23672199E 00-0.23671633E 00-0.23670876E 00-0.23669940E 00-0.23668927E 00
0000500-0.23668021E 00-0.23667306E 00-0.23666930E 00-0.23666894E 00-0.23667544E 00
0000600-0.23668551E 00-0.23670089E 00-0.23671925E 00-0.23673975E 00-0.23675925E 00
0000700-0.23677528E 00-0.23678482E 00-0.23678553E 00-0.23677629E 00-0.23675585E 00
0000800-0.23672557E 00-0.23668903E 00-0.23665076E 00-0.23661762E 00-0.23659903E 00
0000900-0.23660129E 00-0.23663092E 00-0.23669267E 00-0.23678207E 00-0.23688811E 00
0001000-0.23698741E 00-0.23703980E 00-0.23698497E 00-0.23674083E 00-0.23619777E 00
0001100-0.23521739E 00-0.23363262E 00-0.23125052E 00-0.22785783E 00-0.22322893E 00
0001200-0.21714222E 00-0.20939451E 00-0.19982117E 00-0.18831682E 00-0.17517996E 00
0001300-0.16317582E 00-0.16141516E 00-0.16317582E 00-0.17517996E 00-0.18831682E 00
EOF
q
```

MG+ LDA a=1.0 DENS.

VEFF

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
```

MG⁺ LDA a=2.0 DENS.

```
        TOP RECORD
0000100 0.10985494E-01 0.10983102E-01 0.10982886E-01 0.10985024E-01 0.10989439E-01
0000200 0.10995731E-01 0.11003260E-01 0.11011187E-01 0.11018541E-01 0.11024401E-01
0000300 0.11027906E-01 0.11028439E-01 0.11025693E-01 0.11019725E-01 0.11010986E-01
0000400 0.11000384E-01 0.10989010E-01 0.10978252E-01 0.10969453E-01 0.10963965E-01
0000500 0.10962743E-01 0.10966387E-01 0.10974873E-01 0.10987651E-01 0.11003498E-01
0000600 0.11020727E-01 0.11037275E-01 0.11050947E-01 0.11059575E-01 0.11061437E-01
0000700 0.11055443E-01 0.11041317E-01 0.11019889E-01 0.10993004E-01 0.10963514E-01
0000800 0.10935068E-01 0.10911781E-01 0.10897812E-01 0.10896858E-01 0.10911480E-01
0000900 0.10942698E-01 0.10989413E-01 0.11047952E-01 0.11112001E-01 0.11172563E-01
0001000 0.11218153E-01 0.11235438E-01 0.11210036E-01 0.11127651E-01 0.10975253E-01
0001100 0.10742679E-01 0.10424003E-01 0.10018703E-01 0.95326081E-02 0.89783147E-02
0001200 0.83746985E-02 0.77460855E-02 0.71205124E-02 0.65279789E-02 0.59986301E-02
0001300 0.55611096E-02 0.52371435E-02 0.50388016E-02 0.49724951E-02 0.50388016E-02
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670810E 00-0.23669618E 00-0.23669159E 00-0.23668176E 00-0.23667353E 00
0000200-0.23667741E 00-0.23667759E 00-0.23668003E 00-0.23668605E 00-0.23669553E 00
0000300-0.23670453E 00-0.23671478E 00-0.23672426E 00-0.23673135E 00-0.23673356E 00
0000400-0.23673195E 00-0.23672462E 00-0.23671150E 00-0.23669404E 00-0.23667383E 00
0000500-0.23665321E 00-0.23663485E 00-0.23662090E 00-0.23661458E 00-0.23661792E 00
0000600-0.23663068E 00-0.23665333E 00-0.23668444E 00-0.23672152E 00-0.23675931E 00
0000700-0.23679286E 00-0.23681700E 00-0.23682588E 00-0.23681611E 00-0.23678422E 00
0000800-0.23673242E 00-0.23666406E 00-0.23658788E 00-0.23651689E 00-0.23646426E 00
0000900-0.23644722E 00-0.23648030E 00-0.23657417E 00-0.23673183E 00-0.23694342E 00
0001000-0.23718333E 00-0.23740184E 00-0.23752195E 00-0.23742980E 00-0.23697072E 00
0001100-0.23594397E 00-0.23409986E 00-0.23114008E 00-0.22672528E 00-0.22048455E 00
0001200-0.21203357E 00-0.20099872E 00-0.18704486E 00-0.16990739E 00-0.14942193E 00
0001300-0.12992805E 00-0.11621666E 00-0.10710311E 00-0.10550338E 00-0.10710311E 00
EOF
q
```

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p99
```

MG+ LDA a=30

DENS.

```
        TOP RECORD
0000100 0.11002377E-01 0.10997280E-01 0.10992348E-01 0.10988198E-01 0.10985386E-01
0000200 0.10984305E-01 0.10985237E-01 0.10988157E-01 0.10992855E-01 0.10998849E-01
0000300 0.11005506E-01 0.11012077E-01 0.11017762E-01 0.11021845E-01 0.11023745E-01
0000400 0.11023127E-01 0.11019908E-01 0.11014365E-01 0.11007044E-01 0.10998718E-01
0000500 0.10990366E-01 0.10982998E-01 0.10977600E-01 0.10974951E-01 0.10975543E-01
0000600 0.10979529E-01 0.10986648E-01 0.10996226E-01 0.11007234E-01 0.11018429E-01
0000700 0.11028443E-01 0.11035923E-01 0.11039749E-01 0.11039164E-01 0.11033867E-01
0000800 0.11024181E-01 0.11010874E-01 0.10995340E-01 0.10979321E-01 0.10964729E-01
0000900 0.10953564E-01 0.10947492E-01 0.10947749E-01 0.10954861E-01 0.10968618E-01
0001000 0.10987882E-01 0.11010759E-01 0.11034723E-01 0.11056781E-01 0.11073910E-01
0001100 0.11083327E-01 0.11082929E-01 0.11071626E-01 0.11049561E-01 0.11018336E-01
0001200 0.10980926E-01 0.10941599E-01 0.10905508E-01 0.10878216E-01 0.10865059E-01
0001300 0.10870393E-01 0.10896884E-01 0.10944802E-01 0.11011373E-01 0.11090472E-01
0001400 0.11172492E-01 0.11244409E-01 0.11290442E-01 0.11292860E-01 0.11233307E-01
0001500 0.11094313E-01 0.10861088E-01 0.10523424E-01 0.10077361E-01 0.95265955E-02
0001600 0.88831484E-02 0.81672035E-02 0.74059367E-02 0.66313893E-02 0.58776923E-02
0001700 0.51781833E-02 0.45623854E-02 0.40504076E-02 0.36513947E-02 0.33676694E-02
0001800 0.31983645E-02 0.31422819E-02 0.31983645E-02 0.33676694E-02 0.36513947E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670697E 00-0.23671144E 00-0.23671299E 00-0.23671389E 00-0.23671365E 00
0000200-0.23671180E 00-0.23671228E 00-0.23670918E 00-0.23670787E 00-0.23670727E 00
0000300-0.23671424E 00-0.23671544E 00-0.23671883E 00-0.23672265E 00-0.23672849E 00
0000400-0.23673737E 00-0.23673999E 00-0.03673999E 00-0.23674697E 00-0.23674309E 00
0000500-0.23673874E 00-0.23673737E 00-0.23672903E 00-0.23672491E 00-0.23671687E 00
0000600-0.23670739E 00-0.23671055E 00-0.23670483E 00-0.23670447E 00-0.23670727E 00
0000700-0.23671514E 00-0.23672336E 00-0.23673326E 00-0.23674303E 00-0.23675114E 00
0000800-0.23675334E 00-0.23675251E 00-0.23674601E 00-0.23673362E 00-0.23671603E 00
0000900-0.23669416E 00-0.23667115E 00-0.23664939E 00-0.23663235E 00-0.23662060E 00
0001000-0.23661798E 00-0.23662317E 00-0.23663813E 00-0.23666185E 00-0.23669302E 00
0001100-0.23672849E 00-0.23676461E 00-0.23679733E 00-0.23682255E 00-0.23683512E 00
0001200-0.23683190E 00-0.23681098E 00-0.23677313E 00-0.23672104E 00-0.23666286E 00
0001300-0.23660851E 00-0.23657054E 00-0.23656350E 00-0.23660141E 00-0.23669338E 00
0001400-0.23684150E 00-0.23703426E 00-0.23723859E 00-0.23739314E 00-0.23739791E 00
0001500-0.23710495E 00-0.23630744E 00-0.23473185E 00-0.23203123E 00-0.22778702E 00
0001600-0.22151351E 00-0.21267706E 00-0.20072246E 00-0.18510842E 00-0.16535270E 00
0001700-0.14113361E 00-0.11695099E 00-0.97267151E-01-0.81984282E-01-0.71191430E-01
0001800-0.64152181E-01-0.62716067E-01-0.64152181E-01-0.71191430E-01-0.81984282E-01
EOF
q
```

```
redit pote14
LOADING POTE14   MG+ LDA  a=5.0
REKEYED
EDIT             DENS.
p99
        TOP RECORD
0000100 0.11003751E-01 0.10995641E-01 0.10987889E-01 0.10981437E-01 0.10977089E-01
0000200 0.10975443E-01 0.10976780E-01 0.10981083E-01 0.10987956E-01 0.10996666E-01
0000300 0.11006251E-01 0.11015568E-01 0.11023514E-01 0.11029050E-01 0.11031378E-01
0000400 0.11030097E-01 0.11025149E-01 0.11016980E-01 0.11006407E-01 0.10994628E-01
0000500 0.10983039E-01 0.10973074E-01 0.10966081E-01 0.10963097E-01 0.10964762E-01
0000600 0.10971174E-01 0.10981839E-01 0.10995746E-01 0.11011370E-01 0.11026945E-01
0000700 0.11040520E-01 0.11050269E-01 0.11054706E-01 0.11052907E-01 0.11044610E-01
0000800 0.11030361E-01 0.11011463E-01 0.10989890E-01 0.10968130E-01 0.10948904E-01
0000900 0.10934789E-01 0.10927986E-01 0.10930032E-01 0.10941379E-01 0.10961488E-01
0001000 0.10988537E-01 0.11019766E-01 0.11051558E-01 0.11079852E-01 0.11100624E-01
0001100 0.11110313E-01 0.11106461E-01 0.11088017E-01 0.11055693E-01 0.11012144E-01
0001200 0.10961827E-01 0.10910816E-01 0.10866102E-01 0.10834981E-01 0.10824088E-01
0001300 0.10838505E-01 0.10880709E-01 0.10949738E-01 0.11040557E-01 0.11143766E-01
0001400 0.11245511E-01 0.11328023E-01 0.11370528E-01 0.11350710E-01 0.11246469E-01
0001500 0.11038173E-01 0.10710951E-01 0.10256886E-01 0.96769109E-02 0.89818127E-02
0001600 0.81922635E-02 0.73374435E-02 0.64526238E-02 0.55755526E-02 0.47425553E-02
0001700 0.39845593E-02 0.33210679E-02 0.27587432E-02 0.22956415E-02 0.19249821E-02
0001800 0.16379615E-02 0.14256127E-02 0.12800442E-02 0.11952084E-02 0.11673751E-02
EOF
q
redit pote15
LOADING POTE15
REKEYED          VEFF
EDIT
p99
        TOP RECORD
0000100-0.23670304E 00-0.23669118E 00-0.23668146E 00-0.23667341E 00-0.23666382E 00
0000200-0.23665816E 00-0.23665428E 00-0.23664868E 00-0.23664796E 00-0.23665702E 00
0000300-0.23666251E 00-0.23666906E 00-0.23667347E 00-0.23668277E 00-0.23669749E 00
0000400-0.23670793E 00-0.23671675E 00-0.23672825E 00-0.23673034E 00-0.23672903E 00
0000500-0.23673117E 00-0.23672283E 00-0.23672003E 00-0.23670888E 00-0.23669547E 00
0000600-0.23669487E 00-0.23668772E 00-0.23668474E 00-0.23668671E 00-0.23669535E 00
0000700-0.23670721E 00-0.23672265E 00-0.23674047E 00-0.23675787E 00-0.23677200E 00
0000800-0.23678088E 00-0.23678279E 00-0.23677564E 00-0.23675936E 00-0.23673475E 00
0000900-0.23670512E 00-0.23667341E 00-0.23664248E 00-0.23661715E 00-0.23660308E 00
0001000-0.23660010E 00-0.23661256E 00-0.23663944E 00-0.23667985E 00-0.23672938E 00
0001100-0.23678285E 00-0.23683393E 00-0.23687506E 00-0.23689818E 00-0.23689723E 00
0001200-0.23686820E 00-0.23681152E 00-0.23673111E 00-0.23663807E 00-0.23654735E 00
0001300-0.23647887E 00-0.23645371E 00-0.23649222E 00-0.23660946E 00-0.23681110E 00
0001400-0.23708767E 00-0.23740715E 00-0.23770863E 00-0.23789042E 00-0.23780090E 00
0001500-0.23722684E 00-0.23588425E 00-0.23341054E 00-0.22936368E 00-0.22322696E 00
0001600-0.21442163E 00-0.20233232E 00-0.18633658E 00-0.16584563E 00-0.14034343E 00
0001700-0.11399603E 00-0.91050446E-01-0.71200669E-01-0.54197378E-01-0.39782248E-01
0001800-0.27965825E-01-0.18705636E-01-0.12053769E-01-0.78246221E-02-0.67362823E-02
EOF
q
```

```
redit pote16
LOADING POTE16
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.11016943E-01 0.11007845E-01 0.10997567E-01 0.10987233E-01 0.10978028E-01
0000200 0.10971073E-01 0.10967206E-01 0.10967035E-01 0.10970648E-01 0.10977782E-01
0000300 0.10987647E-01 0.10999143E-01 0.11010896E-01 0.11021517E-01 0.11029605E-01
0000400 0.11034038E-01 0.11034094E-01 0.11029508E-01 0.11020605E-01 0.11008225E-01
0000500 0.10993715E-01 0.10978729E-01 0.10965057E-01 0.10954477E-01 0.10948498E-01
0000600 0.10948122E-01 0.10953791E-01 0.10965176E-01 0.10981299E-01 0.11000507E-01
0000700 0.11020709E-01 0.11039548E-01 0.11054654E-01 0.11064000E-01 0.11066101E-01
0000800 0.11060245E-01 0.11046685E-01 0.11026639E-01 0.11002135E-01 0.10976028E-01
0000900 0.10951474E-01 0.10931768E-01 0.10919824E-01 0.10917827E-01 0.10926973E-01
0001000 0.10947090E-01 0.10976639E-01 0.11012789E-01 0.11051573E-01 0.11088308E-01
0001100 0.11118080E-01 0.11136375E-01 0.11139609E-01 0.11125736E-01 0.11094671E-01
0001200 0.11048570E-01 0.10991767E-01 0.10930590E-01 0.10872882E-01 0.10827042E-01
0001300 0.10801241E-01 0.10802232E-01 0.10834180E-01 0.10897730E-01 0.10989133E-01
0001400 0.11099745E-01 0.11215933E-01 0.11319466E-01 0.11388425E-01 0.11398673E-01
0001500 0.11325788E-01 0.11147466E-01 0.10846000E-01 0.10410886E-01 0.98408684E-02
0001600 0.91452375E-02 0.83440468E-02 0.74667297E-02 0.65495707E-02 0.56319386E-02
0001700 0.47520176E-02 0.39424747E-02 0.32241826E-02 0.26047712E-02 0.20826100E-02
0001800 0.16504603E-02 0.12982087E-02 0.10147258E-02 0.78905118E-03 0.61108172E-03
0001900 0.47189952E-03 0.36388356E-03 0.28067618E-03 0.21708236E-03 0.16893036E-03
0002000 0.13292859E-03 0.10652885E-03 0.87807974E-04 0.75369811E-04 0.68269976E-04
0002100 0.65962900E-04 0.68269976E-04 0.75369811E-04 0.87807974E-04 0.10652885E-03
EOF
q
redit pote17
LOADING POTE17
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.23670805E 00-0.23670077E 00-0.23669064E 00-0.23667842E 00-0.23666221E 00
0000200-0.23664433E 00-0.23662740E 00-0.23660761E 00-0.23659259E 00-0.23657846E 00
0000300-0.23657930E 00-0.23657477E 00-0.23657554E 00-0.23657513E 00-0.23657978E 00
0000400-0.23659641E 00-0.23660189E 00-0.23660845E 00-0.23662174E 00-0.23662192E 00
0000500-0.23661560E 00-0.23661852E 00-0.23660421E 00-0.23659617E 00-0.23657757E 00
0000600-0.23656189E 00-0.23656172E 00-0.23655421E 00-0.23655576E 00-0.23656505E 00
0000700-0.23658299E 00-0.23660868E 00-0.23663980E 00-0.23667467E 00-0.23670989E 00
0000800-0.23674166E 00-0.23676687E 00-0.23678261E 00-0.23678619E 00-0.23677713E 00
0000900-0.23675680E 00-0.23672730E 00-0.23669410E 00-0.23666072E 00-0.23663354E 00
0001000-0.23662013E 00-0.23662168E 00-0.23664248E 00-0.23668331E 00-0.23674238E 00
0001100-0.23681414E 00-0.23689151E 00-0.23696470E 00-0.23702413E 00-0.23705667E 00
0001200-0.23705310E 00-0.23700714E 00-0.23691732E 00-0.23678875E 00-0.23663670E 00
0001300-0.23648161E 00-0.23635072E 00-0.23627508E 00-0.23628259E 00-0.23639524E 00
0001400-0.23662180E 00-0.23695576E 00-0.23736250E 00-0.23777938E 00-0.23810041E 00
0001500-0.23816949E 00-0.23777026E 00-0.23661536E 00-0.23434240E 00-0.23051292E 00
0001600-0.22461861E 00-0.21609694E 00-0.20435166E 00-0.18877912E 00-0.16880429E 00
0001700-0.14391035E 00-0.11800998E 00-0.95066965E-01-0.74713767E-01-0.56615412E-01
0001800-0.40462226E-01-0.25992852E-01-0.12981787E-01-0.12398593E-02 0.93895085E-02
0001900 0.19033168E-01 0.27790427E-01 0.35735045E-01 0.42915002E-01 0.49351126E-01
0002000 0.55032957E-01 0.59915110E-01 0.63911736E-01 0.66908002E-01 0.68788528E-01
0002100 0.69410145E-01 0.68788528E-01 0.66908002E-01 0.63911736E-01 0.59915110E-01
EOF
q
```

MG+ LDA a=10.0 DENS.

VEFF

```
redit pote18
LOADING POTE18
REKEYED
EDIT
p99
```

MG+LDA a=15.0
DENS.

```
        TOP RECORD
0000100 0.11013214E-01 0.11005037E-01 0.10995746E-01 0.10986429E-01 0.10978226E-01
0000200 0.10972232E-01 0.10969277E-01 0.10969937E-01 0.10974310E-01 0.10982111E-01
0000300 0.10992590E-01 0.11004627E-01 0.11016876E-01 0.11027891E-01 0.11036348E-01
0000400 0.11041064E-01 0.11041313E-01 0.11036858E-01 0.11028003E-01 0.11015587E-01
0000500 0.11000942E-01 0.10985747E-01 0.10971799E-01 0.10960869E-01 0.10954484E-01
0000600 0.10953650E-01 0.10958843E-01 0.10969732E-01 0.10985311E-01 0.11003997E-01
0000700 0.11023689E-01 0.11041962E-01 0.11056550E-01 0.11065338E-01 0.11066835E-01
0000800 0.11060368E-01 0.11046134E-01 0.11025310E-01 0.10999996E-01 0.10972966E-01
0000900 0.10947440E-01 0.10926697E-01 0.10913689E-01 0.10910671E-01 0.10918800E-01
0001000 0.10938048E-01 0.10966890E-01 0.11002559E-01 0.11041109E-01 0.11077907E-01
0001100 0.11108063E-01 0.11127017E-01 0.11131175E-01 0.11118457E-01 0.11088699E-01
0001200 0.11043943E-01 0.10988437E-01 0.10928426E-01 0.10871638E-01 0.10826435E-01
0001300 0.10800947E-01 0.10801915E-01 0.10833595E-01 0.10896690E-01 0.10987554E-01
0001400 0.11097692E-01 0.11213578E-01 0.11317126E-01 0.11386514E-01 0.11397682E-01
0001500 0.11326239E-01 0.11149827E-01 0.10850642E-01 0.10417990E-01 0.98503940E-02
0001600 0.91568977E-02 0.83572455E-02 0.74807815E-02 0.65636747E-02 0.56453645E-02
0001700 0.47641806E-02 0.39530136E-02 0.32329326E-02 0.26116688E-02 0.20876527E-02
0001800 0.16536813E-02 0.12996572E-02 0.10144582E-02 0.78712730E-03 0.60755038E-03
0001900 0.46679145E-03 0.35719573E-03 0.27236133E-03 0.20702690E-03 0.15693509E-03
0002000 0.11868200E-03 0.89572059E-04 0.67489440E-04 0.50785296E-04 0.38182930E-04
0002100 0.28699345E-04 0.21581422E-04 0.16255231E-04 0.12285267E-04 0.93431045E-05
0002200 0.71828281E-05 0.56222216E-05 0.45286261E-05 0.38084827E-05 0.33998494E-05
0002300 0.32674543E-05 0.33998494E-05 0.38084827E-05 0.45286261E-05 0.56222216E-05
EOF
q
redit pote19
LOADING POTE19
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670805E 00-0.23672730E 00-0.23674184E 00-0.23674673E 00-0.23674887E 00
0000200-0.23674583E 00-0.23674524E 00-0.23673850E 00-0.23673028E 00-0.23672444E 00
0000300-0.23672885E 00-0.23672831E 00-0.23672861E 00-0.23672891E 00-0.23673910E 00
0000400-0.23675448E 00-0.23676234E 00-0.23677188E 00-0.23678505E 00-0.23679298E 00
0000500-0.23679125E 00-0.23679221E 00-0.23678082E 00-0.23677677E 00-0.23675859E 00
0000600-0.23673999E 00-0.23673356E 00-0.23671901E 00-0.23671001E 00-0.23670620E 00
0000700-0.23671198E 00-0.23672122E 00-0.23673719E 00-0.23675692E 00-0.23677850E 00
0000800-0.23679811E 00-0.23681337E 00-0.23682052E 00-0.23681694E 00-0.23680168E 00
0000900-0.23677510E 00-0.23673892E 00-0.23669630E 00-0.23665172E 00-0.23661101E 00
0001000-0.23658127E 00-0.23656535E 00-0.23656839E 00-0.23659217E 00-0.23663598E 00
0001100-0.23669648E 00-0.23676783E 00-0.23684168E 00-0.23690826E 00-0.23695600E 00
0001200-0.23697406E 00-0.23695523E 00-0.23689544E 00-0.23679841E 00-0.23667467E 00
0001300-0.23654306E 00-0.23642850E 00-0.23636007E 00-0.23636562E 00-0.23646694E 00
0001400-0.23667538E 00-0.23698527E 00-0.23736686E 00-0.23775804E 00-0.23805791E 00
0001500-0.23811477E 00-0.23771483E 00-0.23657495E 00-0.23433399E 00-0.23055303E 00
0001600-0.22472107E 00-0.21626770E 00-0.20458722E 00-0.18906486E 00-0.16911232E 00
0001700-0.14419949E 00-0.11828220E 00-0.95367908E-01-0.75079143E-01-0.57066765E-01
0001800-0.41014694E-01-0.26649680E-01-0.13736833E-01-0.20771702E-02 0.84968507E-02
0001900 0.18125217E-01 0.26924223E-01 0.34990776E-01 0.42405490E-01 0.49236055E-01
0002000 0.55538874E-01 0.61361164E-01 0.66742539E-01 0.71719348E-01 0.76319098E-01
0002100 0.80566466E-01 0.84479809E-01 0.88073730E-01 0.91355383E-01 0.94324708E-01
0002200 0.96969724E-01 0.99263608E-01 0.10116053E 00 0.10259652E 00 0.10349983E 00
0002300 0.10380816E 00 0.10349983E 00 0.10259652E 00 0.10116053E 00 0.99263608E-01
EOF
q
```

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
```

MG+ NL a=0.25 DENS.

```
        TOP RECORD
0000100 0.10998525E-01 0.10998655E-01 0.10998849E-01 0.10999117E-01 0.10999426E-01
0000200 0.10999810E-01 0.11000231E-01 0.11000682E-01 0.11001162E-01 0.11001680E-01
0000300 0.11002198E-01 0.11002708E-01 0.11003181E-01 0.11003643E-01 0.11004053E-01
0000400 0.11004400E-01 0.11004671E-01 0.11004888E-01 0.11005010E-01 0.11005048E-01
0000500 0.11004988E-01 0.11004854E-01 0.11004638E-01 0.11004314E-01 0.11003930E-01
0000600 0.11003472E-01 0.11002954E-01 0.11002399E-01 0.11001803E-01 0.11001196E-01
0000700 0.11000603E-01 0.11000033E-01 0.10999497E-01 0.10999013E-01 0.10998599E-01
0000800 0.10998279E-01 0.10998059E-01 0.10997925E-01 0.10997940E-01 0.10998052E-01
0000900 0.10998312E-01 0.10998677E-01 0.10999136E-01 0.10999713E-01 0.11000376E-01
0001000 0.11001110E-01 0.11001870E-01 0.11002682E-01 0.11003487E-01 0.11004254E-01
0001100 0.11004962E-01 0.11005618E-01 0.11006147E-01 0.11006553E-01 0.11006795E-01
0001200 0.11006873E-01 0.11006776E-01 0.11006456E-01 0.11005983E-01 0.11005297E-01
0001300 0.11004429E-01 0.11003409E-01 0.11002246E-01 0.11000987E-01 0.10999676E-01
0001400 0.10998294E-01 0.10996964E-01 0.10995712E-01 0.10994580E-01 0.10993626E-01
0001500 0.10992896E-01 0.10992434E-01 0.10992322E-01 0.10992587E-01 0.10993231E-01
0001600 0.10994282E-01 0.10995764E-01 0.10997649E-01 0.10999937E-01 0.11002559E-01
0001700 0.11005480E-01 0.11008602E-01 0.11011824E-01 0.11015005E-01 0.11018045E-01
0001800 0.11020739E-01 0.11022933E-01 0.11024404E-01 0.11024967E-01 0.11024375E-01
0001900 0.11022378E-01 0.11018753E-01 0.11013236E-01 0.11005644E-01 0.10995679E-01
0002000 0.10983158E-01 0.10967877E-01 0.10949656E-01 0.10928351E-01 0.10903869E-01
0002100 0.10876171E-01 0.10845222E-01 0.10811076E-01 0.10773811E-01 0.10733642E-01
0002200 0.10690775E-01 0.10645520E-01 0.10598280E-01 0.10549504E-01 0.10499731E-01
0002300 0.10449570E-01 0.10399714E-01 0.10350935E-01 0.10304037E-01 0.10259960E-01
0002400 0.10219663E-01 0.10184165E-01 0.10154556E-01 0.10131981E-01 0.10117553E-01
0002500 0.10112651E-01 0.10117553E-01 0.10131981E-01 0.10154556E-01 0.10184165E-01
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670882E 00-0.23670113E 00-0.23670846E 00-0.23670661E 00-0.23670465E 00
0000200-0.23671728E 00-0.23670918E 00-0.23671818E 00-0.23671961E 00-0.23672235E 00
0000300-0.23672664E 00-0.23673230E 00-0.23672962E 00-0.23673034E 00-0.23672938E 00
0000400-0.23672825E 00-0.23672819E 00-0.23672825E 00-0.23672873E 00-0.23672789E 00
0000500-0.23672771E 00-0.23672974E 00-0.23672950E 00-0.23672980E 00-0.23672992E 00
0000600-0.23673081E 00-0.23673242E 00-0.23673296E 00-0.23673308E 00-0.23673290E 00
0000700-0.23673278E 00-0.23673445E 00-0.23673338E 00-0.23673236E 00-0.23673189E 00
0000800-0.23673213E 00-0.23673040E 00-0.23672801E 00-0.23672676E 00-0.23672485E 00
0000900-0.23672247E 00-0.23671967E 00-0.23671639E 00-0.23671502E 00-0.23671228E 00
0001000-0.23670816E 00-0.23670685E 00-0.23670495E 00-0.23670143E 00-0.23669952E 00
0001100-0.23669869E 00-0.23669702E 00-0.23669666E 00-0.23669595E 00-0.23669529E 00
0001200-0.23669714E 00-0.23669922E 00-0.23669994E 00-0.23670244E 00-0.23670524E 00
0001300-0.23670721E 00-0.23671108E 00-0.23671502E 00-0.23671794E 00-0.23672092E 00
0001400-0.23672462E 00-0.23672909E 00-0.23673224E 00-0.23673475E 00-0.23673803E 00
0001500-0.23674065E 00-0.23674273E 00-0.23674530E 00-0.23674589E 00-0.23674738E 00
0001600-0.23674875E 00-0.23674977E 00-0.23675030E 00-0.23675209E 00-0.23675311E 00
0001700-0.23675328E 00-0.23675501E 00-0.23675692E 00-0.23675644E 00-0.23675770E 00
0001800-0.23675781E 00-0.23675531E 00-0.23675269E 00-0.23674732E 00-0.23673600E 00
0001900-0.23672116E 00-0.23669976E 00-0.23666906E 00-0.23662639E 00-0.23657060E 00
0002000-0.23649830E 00-0.23640615E 00-0.23629135E 00-0.23614860E 00-0.23597342E 00
0002100-0.23576140E 00-0.23550743E 00-0.23520809E 00-0.23485416E 00-0.23444074E 00
0002200-0.23396367E 00-0.23341525E 00-0.23278934E 00-0.23208064E 00-0.23128229E 00
0002300-0.23038918E 00-0.22939736E 00-0.22830075E 00-0.22709507E 00-0.22577870E 00
0002400-0.22434902E 00-0.22280586E 00-0.22114354E 00-0.21948802E 00-0.21722895E 00
0002500-0.21685219E 00-0.21722895E 00-0.21948802E 00-0.22114354E 00-0.22280586E 00
EOF
```

```
q
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.10997035E-01 0.10997206E-01 0.10997891E-01 0.10998975E-01 0.11000428E-01
0000200 0.11002049E-01 0.11003643E-01 0.11005029E-01 0.11006024E-01 0.11006471E-01
0000300 0.11006281E-01 0.11005428E-01 0.11003979E-01 0.11002034E-01 0.10999806E-01
0000400 0.10997571E-01 0.10995589E-01 0.10994133E-01 0.10993436E-01 0.10993682E-01
0000500 0.10994945E-01 0.10997139E-01 0.11000108E-01 0.11003532E-01 0.11007089E-01
0000600 0.11010267E-01 0.11012651E-01 0.11013858E-01 0.11013549E-01 0.11011627E-01
0000700 0.11008110E-01 0.11003327E-01 0.10997724E-01 0.10992035E-01 0.10987073E-01
0000800 0.10983743E-01 0.10982838E-01 0.10985021E-01 0.10990631E-01 0.10999590E-01
0000900 0.11011258E-01 0.11024345E-01 0.11036959E-01 0.11046503E-01 0.11049785E-01
0001000 0.11043247E-01 0.11023052E-01 0.10985449E-01 0.10926988E-01 0.10845080E-01
0001100 0.10738116E-01 0.10606030E-01 0.10450564E-01 0.10275409E-01 0.10086499E-01
0001200 0.98919086E-02 0.97018741E-02 0.95285513E-02 0.93857422E-02 0.92882700E-02
0001300 0.92543140E-02 0.92882700E-02 0.93857422E-02 0.95285513E-02 0.97018741E-02
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.23670769E 00-0.23669964E 00-0.23670524E 00-0.23670024E 00-0.23669511E 00
0000200-0.23670286E 00-0.23669785E 00-0.23669481E 00-0.23669350E 00-0.23669434E 00
0000300-0.23669612E 00-0.23669899E 00-0.23670352E 00-0.23670852E 00-0.23671299E 00
0000400-0.23671722E 00-0.23672044E 00-0.23672134E 00-0.23671991E 00-0.23671716E 00
0000500-0.23671240E 00-0.23670673E 00-0.23670024E 00-0.23669386E 00-0.23668963E 00
0000600-0.23668706E 00-0.23668730E 00-0.23669100E 00-0.23669875E 00-0.23670870E 00
0000700-0.23672092E 00-0.23673433E 00-0.23674780E 00-0.23676032E 00-0.23676991E 00
0000800-0.23677719E 00-0.23678184E 00-0.23678374E 00-0.23678529E 00-0.23678684E 00
0000900-0.23679036E 00-0.23679537E 00-0.23680097E 00-0.23680180E 00-0.23678732E 00
0001000-0.23674214E 00-0.23663950E 00-0.23644567E 00-0.23611408E 00-0.23558646E 00
0001100-0.23479259E 00-0.23365092E 00-0.23207164E 00-0.22995913E 00-0.22721708E 00
0001200-0.22375435E 00-0.21949196E 00-0.21435606E 00-0.20875299E 00-0.20044196E 00
0001300-0.19892579E 00-0.20044196E 00-0.20875299E 00-0.21435606E 00-0.21949196E 00
EOF
```

MG+ NL a=0.5
DENS.

VEFF

```
redit pote6
LOADING POTE6
REKEYED
EDIT
p99
```

MG+ NL a=0.75 DENS.

```
        TOP RECORD
0000100 0.10995276E-01 0.10995328E-01 0.10995548E-01 0.10995962E-01 0.10996532E-01
0000200 0.10997288E-01 0.10998186E-01 0.10999206E-01 0.11000346E-01 0.11001535E-01
0000300 0.11002772E-01 0.11004012E-01 0.11005212E-01 0.11006340E-01 0.11007369E-01
0000400 0.11008270E-01 0.11008982E-01 0.11009507E-01 0.11009820E-01 0.11009891E-01
0000500 0.11009719E-01 0.11009298E-01 0.11008620E-01 0.11007711E-01 0.11006586E-01
0000600 0.11005253E-01 0.11003755E-01 0.11002146E-01 0.11000425E-01 0.10998685E-01
0000700 0.10996964E-01 0.10995302E-01 0.10993768E-01 0.10992397E-01 0.10991238E-01
0000800 0.10990363E-01 0.10989778E-01 0.10989539E-01 0.10989636E-01 0.10990120E-01
0000900 0.10990981E-01 0.10992181E-01 0.10993738E-01 0.10995589E-01 0.10997705E-01
0001000 0.11000030E-01 0.11002533E-01 0.11005061E-01 0.11007626E-01 0.11010095E-01
0001100 0.11012390E-01 0.11014443E-01 0.11016171E-01 0.11017483E-01 0.11018343E-01
0001200 0.11018671E-01 0.11018444E-01 0.11017617E-01 0.11016190E-01 0.11014186E-01
0001300 0.11011619E-01 0.11008564E-01 0.11005092E-01 0.11001263E-01 0.10997240E-01
0001400 0.10993119E-01 0.10989048E-01 0.10985166E-01 0.10981664E-01 0.10978706E-01
0001500 0.10976408E-01 0.10974981E-01 0.10974523E-01 0.10975171E-01 0.10977007E-01
0001600 0.10980107E-01 0.10984492E-01 0.10990128E-01 0.10996982E-01 0.11004895E-01
0001700 0.11013716E-01 0.11023168E-01 0.11033002E-01 0.11042856E-01 0.11052269E-01
0001800 0.11060808E-01 0.11067893E-01 0.11072978E-01 0.11075445E-01 0.11074588E-01
0001900 0.11069782E-01 0.11060294E-01 0.11045437E-01 0.11024527E-01 0.10996908E-01
0002000 0.10962006E-01 0.10919224E-01 0.10868147E-01 0.10808375E-01 0.10739654E-01
0002100 0.10661863E-01 0.10575026E-01 0.10479297E-01 0.10375042E-01 0.10262746E-01
0002200 0.10143105E-01 0.10017011E-01 0.98855160E-02 0.97498707E-02 0.96115135E-02
0002300 0.94720051E-02 0.93331374E-02 0.91967918E-02 0.90649985E-02 0.89399219E-02
0002400 0.88238269E-02 0.87191202E-02 0.86282641E-02 0.85538216E-02 0.84984079E-02
0002500 0.84642619E-02 0.84527843E-02 0.84642619E-02 0.84984079E-02 0.85538216E-02
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670912E 00-0.23671359E 00-0.23670936E 00-0.23670769E 00-0.23671830E 00
0000200-0.23671401E 00-0.23672169E 00-0.23671842E 00-0.23671710E 00-0.23671865E 00
0000300-0.23672616E 00-0.23671997E 00-0.23671657E 00-0.23671252E 00-0.23670930E 00
0000400-0.23670715E 00-0.23670453E 00-0.23670304E 00-0.23670280E 00-0.23670220E 00
0000500-0.23670232E 00-0.23670268E 00-0.23670524E 00-0.23670840E 00-0.23671073E 00
0000600-0.23671299E 00-0.23671681E 00-0.23672086E 00-0.23672390E 00-0.23672724E 00
0000700-0.23673093E 00-0.23673362E 00-0.23673558E 00-0.23673689E 00-0.23673880E 00
0000800-0.23673838E 00-0.23673630E 00-0.23673505E 00-0.23673296E 00-0.23672986E 00
0000900-0.23672485E 00-0.23672014E 00-0.23671567E 00-0.23670852E 00-0.23670232E 00
0001000-0.23669612E 00-0.23668885E 00-0.23668391E 00-0.23667890E 00-0.23667324E 00
0001100-0.23666859E 00-0.23666632E 00-0.23666346E 00-0.23666334E 00-0.23666483E 00
0001200-0.23666680E 00-0.23667079E 00-0.23667657E 00-0.23668289E 00-0.23669028E 00
0001300-0.23670006E 00-0.23671019E 00-0.23672080E 00-0.23673207E 00-0.23674333E 00
0001400-0.23675680E 00-0.23676813E 00-0.23677903E 00-0.23679137E 00-0.23680252E 00
0001500-0.23681062E 00-0.23682028E 00-0.23682874E 00-0.23683661E 00-0.23684371E 00
0001600-0.23684901E 00-0.23685527E 00-0.23686296E 00-0.23686880E 00-0.23687434E 00
0001700-0.23688042E 00-0.23688871E 00-0.23689574E 00-0.23690259E 00-0.23690897E 00
0001800-0.23691237E 00-0.23691392E 00-0.23691100E 00-0.23689914E 00-0.23687810E 00
0001900-0.23684263E 00-0.23678887E 00-0.23671091E 00-0.23660177E 00-0.23645532E 00
0002000-0.23626256E 00-0.23601419E 00-0.23570061E 00-0.23530936E 00-0.23482758E 00
0002100-0.23424202E 00-0.23353899E 00-0.23270398E 00-0.23171800E 00-0.23056602E 00
0002200-0.22923416E 00-0.22770238E 00-0.22595531E 00-0.22397685E 00-0.22175020E 00
0002300-0.21926135E 00-0.21649736E 00-0.21344525E 00-0.21009278E 00-0.20643371E 00
0002400-0.20246047E 00-0.19816816E 00-0.19356048E 00-0.18862200E 00-0.18446410E 00
0002500-0.18160969E 00-0.18125755E 00-0.18160969E 00-0.18446410E 00-0.18862200E 00
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.10993227E-01 0.10993116E-01 0.10994006E-01 0.10995846E-01 0.10998461E-01
0000200 0.11001606E-01 0.11004921E-01 0.11008017E-01 0.11010490E-01 0.11012048E-01
0000300 0.11012401E-01 0.11011429E-01 0.11009131E-01 0.11005707E-01 0.11001464E-01
0000400 0.10996893E-01 0.10992512E-01 0.10988872E-01 0.10986511E-01 0.10985848E-01
0000500 0.10987099E-01 0.10990318E-01 0.10995265E-01 0.11001479E-01 0.11008296E-01
0000600 0.11014901E-01 0.11020396E-01 0.11023972E-01 0.11024881E-01 0.11022720E-01
0000700 0.11017434E-01 0.11009328E-01 0.10999180E-01 0.10988191E-01 0.10977879E-01
0000800 0.10969937E-01 0.10966089E-01 0.10967769E-01 0.10975957E-01 0.10990399E-01
0000900 0.11011869E-01 0.11037003E-01 0.11063140E-01 0.11085390E-01 0.11099659E-01
0001000 0.11097938E-01 0.11073649E-01 0.11019606E-01 0.10929164E-01 0.10796864E-01
0001100 0.10619126E-01 0.10394923E-01 0.10126345E-01 0.96189525E-02 0.94819553E-02
0001200 0.91280863E-02 0.87732561E-02 0.84360428E-02 0.81370957E-02 0.78986585E-02
0001300 0.77435635E-02 0.76907575E-02 0.77435635E-02 0.78986585E-02 0.81370957E-02
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.23670852E 00-0.23670489E 00-0.23671395E 00-0.23670870E 00-0.23670375E 00
0000200-0.23670888E 00-0.23670208E 00-0.23669535E 00-0.23669136E 00-0.23668897E 00
0000300-0.23669082E 00-0.23669499E 00-0.23670238E 00-0.23671228E 00-0.23672193E 00
0000400-0.23673201E 00-0.23674023E 00-0.23674482E 00-0.23674476E 00-0.23674089E 00
0000500-0.23673165E 00-0.23671877E 00-0.23670262E 00-0.23668557E 00-0.23666966E 00
0000600-0.23665565E 00-0.23664731E 00-0.23664582E 00-0.23665226E 00-0.23666614E 00
0000700-0.23668724E 00-0.23671341E 00-0.23674393E 00-0.23677635E 00-0.23680764E 00
0000800-0.23683655E 00-0.23686177E 00-0.23688245E 00-0.23690045E 00-0.23691690E 00
0000900-0.23693377E 00-0.23695201E 00-0.23697126E 00-0.23698467E 00-0.23697853E 00
0001000-0.23692912E 00-0.23679566E 00-0.23652345E 00-0.23603586E 00-0.23523420E 00
0001100-0.23399788E 00-0.23218602E 00-0.22964078E 00-0.22619319E 00-0.22166967E 00
0001200-0.21590543E 00-0.20875078E 00-0.20006361E 00-0.18982154E 00-0.17821574E 00
0001300-0.16750461E 00-0.16614795E 00-0.16750461E 00-0.17821574E 00-0.18982154E 00
EOF
q
```

MG+ NL a=1.0 DENS.

VEFF

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
```

MG+ NL a=2.0 DENS.

```
        TOP RECORD
0000100 0.10987069E-01 0.10985091E-01 0.10984931E-01 0.10986727E-01 0.10990381E-01
0000200 0.10995578E-01 0.11001788E-01 0.11008300E-01 0.11014383E-01 0.11019237E-01
0000300 0.11022199E-01 0.11022743E-01 0.11020660E-01 0.11015963E-01 0.11009045E-01
0000400 0.11000592E-01 0.10991525E-01 0.10982912E-01 0.10975868E-01 0.10971427E-01
0000500 0.10970380E-01 0.10973141E-01 0.10979731E-01 0.10989670E-01 0.11002004E-01
0000600 0.11015393E-01 0.11028197E-01 0.11038695E-01 0.11045232E-01 0.11046525E-01
0000700 0.11041801E-01 0.11031020E-01 0.11014920E-01 0.10995157E-01 0.10974064E-01
0000800 0.10954697E-01 0.10940295E-01 0.10934066E-01 0.10938738E-01 0.10955941E-01
0000900 0.10985926E-01 0.11026997E-01 0.11075269E-01 0.11124596E-01 0.11166442E-01
0001000 0.11190332E-01 0.11184290E-01 0.11135604E-01 0.11031881E-01 0.10862198E-01
0001100 0.10618351E-01 0.10296080E-01 0.98960809E-02 0.94247721E-02 0.88943392E-02
0001200 0.83224960E-02 0.77313967E-02 0.71463808E-02 0.65943301E-02 0.61022155E-02
0001300 0.56958757E-02 0.53950511E-02 0.52108355E-02 0.51492751E-02 0.52108355E-02
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670870E 00-0.23671484E 00-0.23672342E 00-0.23671627E 00-0.23670405E 00
0000200-0.23670369E 00-0.23668671E 00-0.23667181E 00-0.23665899E 00-0.23664957E 00
0000300-0.23664701E 00-0.23664963E 00-0.23665881E 00-0.23667336E 00-0.23669147E 00
0000400-0.23671192E 00-0.23673075E 00-0.23674595E 00-0.23675406E 00-0.23675472E 00
0000500-0.23674554E 00-0.23672765E 00-0.23670125E 00-0.23666936E 00-0.23663557E 00
0000600-0.23660338E 00-0.23657823E 00-0.23656255E 00-0.23656094E 00-0.23657370E 00
0000700-0.23660123E 00-0.23664254E 00-0.23669553E 00-0.23675555E 00-0.23681742E 00
0000800-0.23687899E 00-0.23693550E 00-0.23698443E 00-0.23702639E 00-0.23706239E 00
0000900-0.23709673E 00-0.23713225E 00-0.23717439E 00-0.23722100E 00-0.23726147E 00
0001000-0.23727161E 00-0.23720437E 00-0.23698705E 00-0.23651284E 00-0.23563731E 00
0001100-0.23417711E 00-0.23190743E 00-0.22856951E 00-0.22387761E 00-0.21753234E 00
0001200-0.20923704E 00-0.19871789E 00-0.18574369E 00-0.17015713E 00-0.15178591E 00
0001300-0.13457865E 00-0.12269694E 00-0.11473399E 00-0.11354125E 00-0.11473399E 00
EOF
q
```

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.11002447E-01 0.10998353E-01 0.10994371E-01 0.10990970E-01 0.10988630E-01
0000200 0.10987658E-01 0.10988310E-01 0.10990571E-01 0.10994244E-01 0.10999016E-01
0000300 0.11004366E-01 0.11009667E-01 0.11014290E-01 0.11017673E-01 0.11019330E-01
0000400 0.11019003E-01 0.11016600E-01 0.11012323E-01 0.11006590E-01 0.11000045E-01
0000500 0.10993406E-01 0.10987557E-01 0.10983251E-01 0.10981079E-01 0.10981496E-01
0000600 0.10984611E-01 0.10990229E-01 0.10997780E-01 0.11006508E-01 0.11015378E-01
0000700 0.11023287E-01 0.11029221E-01 0.11032246E-01 0.11031754E-01 0.11027511E-01
0000800 0.11019755E-01 0.11009146E-01 0.10996722E-01 0.10983925E-01 0.10972276E-01
0000900 0.10963324E-01 0.10958407E-01 0.10958496E-01 0.10964010E-01 0.10974742E-01
0001000 0.10989778E-01 0.11007596E-01 0.11026144E-01 0.11043105E-01 0.11056080E-01
0001100 0.11062920E-01 0.11062093E-01 0.11052843E-01 0.11035543E-01 0.11011612E-01
0001200 0.10983739E-01 0.10955520E-01 0.10931224E-01 0.10915343E-01 0.10912046E-01
0001300 0.10924470E-01 0.10954183E-01 0.11000477E-01 0.11059955E-01 0.11126190E-01
0001400 0.11189651E-01 0.11237949E-01 0.11256374E-01 0.11228822E-01 0.11138938E-01
0001500 0.10971684E-01 0.10714941E-01 0.10361128E-01 0.99086687E-02 0.93630254E-02
0001600 0.87370202E-02 0.80503859E-02 0.73285177E-02 0.66003948E-02 0.58962703E-02
0001700 0.52451752E-02 0.46728253E-02 0.41968971E-02 0.38255949E-02 0.35612327E-02
0001800 0.34032986E-02 0.33509717E-02 0.34032986E-02 0.35612327E-02 0.38255949E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.23670828E 00-0.23672342E 00-0.23673761E 00-0.23674524E 00-0.23675197E 00
0000200-0.23675495E 00-0.23675305E 00-0.23674518E 00-0.23673123E 00-0.23671901E 00
0000300-0.23671085E 00-0.23669624E 00-0.23668343E 00-0.23667526E 00-0.23667306E 00
0000400-0.23668575E 00-0.23669219E 00-0.23670328E 00-0.23672980E 00-0.23674369E 00
0000500-0.23675835E 00-0.23678023E 00-0.23678577E 00-0.23679578E 00-0.23678637E 00
0000600-0.23677057E 00-0.23676229E 00-0.23673797E 00-0.23671198E 00-0.23668760E 00
0000700-0.23666680E 00-0.23665410E 00-0.23664916E 00-0.23665392E 00-0.23666739E 00
0000800-0.23668814E 00-0.23671454E 00-0.23674202E 00-0.23676682E 00-0.23678559E 00
0000900-0.23679519E 00-0.23679185E 00-0.23677617E 00-0.23674643E 00-0.23670614E 00
0001000-0.23665929E 00-0.23660988E 00-0.23656493E 00-0.23653024E 00-0.23651081E 00
0001100-0.23651022E 00-0.23653018E 00-0.23657072E 00-0.23663127E 00-0.23670644E 00
0001200-0.23679107E 00-0.23688000E 00-0.23696709E 00-0.23704743E 00-0.23711860E 00
0001300-0.23717940E 00-0.23723209E 00-0.23728204E 00-0.23733550E 00-0.23739564E 00
0001400-0.23745912E 00-0.23750782E 00-0.23750043E 00-0.23736584E 00-0.23699212E 00
0001500-0.23622304E 00-0.23484850E 00-0.23260719E 00-0.22914493E 00-0.22422540E 00
0001600-0.21734285E 00-0.20814073E 00-0.19623899E 00-0.18130273E 00-0.16308415E 00
0001700-0.14135385E 00-0.12006181E 00-0.10309583E 00-0.90203106E-01-0.81371188E-01
0001800-0.75612485E-01-0.74648559E-01-0.75612485E-01-0.81371188E-01-0.90203106E-01
EOF
q
```

MG+ NL a=3.0 DENS.

VEFF

```
redit pote14
LOADING POTE14
REKEYED
EDIT
p99
```

MG+ NL a=5.0 DENS.

```
        TOP RECORD
0000100 0.11003785E-01 0.10997564E-01 0.10991581E-01 0.10986499E-01 0.10983046E-01
0000200 0.10981698E-01 0.10982700E-01 0.10986090E-01 0.10991566E-01 0.10998599E-01
0000300 0.11006381E-01 0.11014055E-01 0.11020679E-01 0.11025421E-01 0.11027634E-01
0000400 0.11026908E-01 0.11023253E-01 0.11016909E-01 0.11008535E-01 0.10999106E-01
0000500 0.10989685E-01 0.10981470E-01 0.10975547E-01 0.10972757E-01 0.10973707E-01
0000600 0.10978453E-01 0.10986656E-01 0.10997519E-01 0.11009883E-01 0.11022270E-01
0000700 0.11033148E-01 0.11041023E-01 0.11044718E-01 0.11043422E-01 0.11036880E-01
0000800 0.11025533E-01 0.11010375E-01 0.10992978E-01 0.10975361E-01 0.10959636E-01
0000900 0.10947946E-01 0.10942049E-01 0.10943171E-01 0.10951720E-01 0.10967195E-01
0001000 0.10988232E-01 0.11012580E-01 0.11037383E-01 0.11059429E-01 0.11075523E-01
0001100 0.11082936E-01 0.11079829E-01 0.11065491E-01 0.11040770E-01 0.11008009E-01
0001200 0.10971025E-01 0.10934878E-01 0.10905296E-01 0.10888148E-01 0.10888517E-01
0001300 0.10910008E-01 0.10953784E-01 0.11017963E-01 0.11096969E-01 0.11181351E-01
0001400 0.11257790E-01 0.11309646E-01 0.11317808E-01 0.11262182E-01 0.11123236E-01
0001500 0.10884177E-01 0.10532990E-01 0.10064345E-01 0.94811544E-02 0.87952614E-02
0001600 0.80271885E-02 0.72046183E-02 0.63600652E-02 0.55275746E-02 0.47394335E-02
0001700 0.40228702E-02 0.33949539E-02 0.28614735E-02 0.24206748E-02 0.20665398E-02
0001800 0.17712288E-02 0.15867711E-02 0.14461614E-02 0.13640169E-02 0.13370381E-02
EOF
q
redit pote15
LOADING POTE15
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670781E 00-0.23672658E 00-0.23674405E 00-0.23675585E 00-0.23676270E 00
0000200-0.23676473E 00-0.23675781E 00-0.23674673E 00-0.23673040E 00-0.23671961E 00
0000300-0.23669857E 00-0.23667914E 00-0.23666352E 00-0.23665434E 00-0.23666084E 00
0000400-0.23666638E 00-0.23668122E 00-0.23671114E 00-0.23673505E 00-0.23675758E 00
0000500-0.23679280E 00-0.23681128E 00-0.23682970E 00-0.23682892E 00-0.23681879E 00
0000600-0.23681056E 00-0.23678088E 00-0.23674691E 00-0.23671108E 00-0.23667777E 00
0000700-0.23665136E 00-0.23663431E 00-0.23662996E 00-0.23663807E 00-0.23665875E 00
0000800-0.23668981E 00-0.23672712E 00-0.23676634E 00-0.23680151E 00-0.23682797E 00
0000900-0.23684001E 00-0.23683596E 00-0.23681217E 00-0.23677099E 00-0.23671603E 00
0001000-0.23665100E 00-0.23658562E 00-0.23652661E 00-0.23648220E 00-0.23645890E 00
0001100-0.23646104E 00-0.23649120E 00-0.23654884E 00-0.23663014E 00-0.23673040E 00
0001200-0.23684299E 00-0.23695999E 00-0.23707461E 00-0.23718035E 00-0.23727316E 00
0001300-0.23735261E 00-0.23742288E 00-0.23749179E 00-0.23756623E 00-0.23765063E 00
0001400-0.23773748E 00-0.23779619E 00-0.23776740E 00-0.23754638E 00-0.23697811E 00
0001500-0.23584759E 00-0.23387402E 00-0.23071176E 00-0.22595698E 00-0.21915501E 00
0001600-0.20982373E 00-0.19747597E 00-0.18165189E 00-0.16196704E 00-0.13805270E 00
0001700-0.11372977E 00-0.92788100E-01-0.74932694E-01-0.60027715E-01-0.47922455E-01
0001800-0.38488824E-01-0.31554595E-01-0.26957620E-01-0.24131183E-01-0.23584105E-01
EOF
q
```

```
redit pote16
LOADING POTE16
REKEYED
EDIT
p99
```

MG+ NL a=10.0 DENS.

```
        TOP RECORD
0000100 0.11017725E-01 0.11010971E-01 0.11003003E-01 0.10994714E-01 0.10987133E-01
0000200 0.10981232E-01 0.10977797E-01 0.10977376E-01 0.10980181E-01 0.10986019E-01
0000300 0.10994337E-01 0.11004273E-01 0.11014685E-01 0.11024378E-01 0.11032160E-01
0000400 0.11036988E-01 0.11038151E-01 0.11035357E-01 0.11028741E-01 0.11018947E-01
0000500 0.11007003E-01 0.10994274E-01 0.10982260E-01 0.10972440E-01 0.10966141E-01
0000600 0.10964327E-01 0.10967482E-01 0.10975458E-01 0.10987516E-01 0.11002406E-01
0000700 0.11018444E-01 0.11033691E-01 0.11046141E-01 0.11054069E-01 0.11056121E-01
0000800 0.11051610E-01 0.11040591E-01 0.11023972E-01 0.11003315E-01 0.10980923E-01
0000900 0.10959376E-01 0.10941397E-01 0.10929491E-01 0.10925572E-01 0.10930695E-01
0001000 0.10944936E-01 0.10967191E-01 0.10995232E-01 0.11025932E-01 0.11055555E-01
0001100 0.11080146E-01 0.11096019E-01 0.11100288E-01 0.11091299E-01 0.11069011E-01
0001200 0.11035241E-01 0.10993566E-01 0.10949284E-01 0.10908723E-01 0.10878801E-01
0001300 0.10866020E-01 0.10875590E-01 0.10910410E-01 0.10970224E-01 0.11050813E-01
0001400 0.11143692E-01 0.11235960E-01 0.11310622E-01 0.11347607E-01 0.11324987E-01
0001500 0.11220865E-01 0.11015486E-01 0.10693606E-01 0.10246728E-01 0.96749514E-02
0001600 0.89879818E-02 0.82052164E-02 0.73544383E-02 0.64693503E-02 0.55861175E-02
0001700 0.47396831E-02 0.39598458E-02 0.32656756E-02 0.26641814E-02 0.21539817E-02
0001800 0.17285699E-02 0.13787777E-02 0.10944647E-02 0.86559588E-03 0.68286969E-03
0001900 0.53803250E-03 0.42398623E-03 0.33477298E-03 0.26548817E-03 0.21216522E-03
0002000 0.17164885E-03 0.14147996E-03 0.11978993E-03 0.10521449E-03 0.96826741E-04
0002100 0.94089555E-04 0.96826741E-04 0.10521449E-03 0.11978993E-03 0.14147996E-03
EOF
q
redit pote17
LOADING POTE17
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.23670858E 00-0.23672277E 00-0.23674232E 00-0.23676115E 00-0.23677385E 00
0000200-0.23678344E 00-0.23678988E 00-0.23678499E 00-0.23677236E 00-0.23675078E 00
0000300-0.23673689E 00-0.23670816E 00-0.23668116E 00-0.23665798E 00-0.23664206E 00
0000400-0.23664558E 00-0.23664212E 00-0.23664892E 00-0.23667687E 00-0.23670506E 00
0000500-0.23673284E 00-0.23677206E 00-0.23679590E 00-0.23682553E 00-0.23682940E 00
0000600-0.23681957E 00-0.23681355E 00-0.23677909E 00-0.23673689E 00-0.23669046E 00
0000700-0.23664343E 00-0.23660266E 00-0.23657095E 00-0.23655379E 00-0.23655266E 00
0000800-0.23656744E 00-0.23659760E 00-0.23663944E 00-0.23668671E 00-0.23673356E 00
0000900-0.23677421E 00-0.23680067E 00-0.23680913E 00-0.23679447E 00-0.23675734E 00
0001000-0.23670089E 00-0.23662835E 00-0.23654890E 00-0.23647237E 00-0.23640853E 00
0001100-0.23636657E 00-0.23635310E 00-0.23637158E 00-0.23642480E 00-0.23650914E 00
0001200-0.23661911E 00-0.23674947E 00-0.23688960E 00-0.23703039E 00-0.23716456E 00
0001300-0.23728424E 00-0.23738581E 00-0.23747075E 00-0.23754543E 00-0.23761839E 00
0001400-0.23769802E 00-0.23778510E 00-0.23785889E 00-0.23787296E 00-0.23773646E 00
0001500-0.23730636E 00-0.23637944E 00-0.23468292E 00-0.23187375E 00-0.22754318E 00
0001600-0.22122377E 00-0.21240962E 00-0.20057750E 00-0.18521833E 00-0.16588306E 00
0001700-0.14212632E 00-0.11766076E 00-0.96150517E-01-0.77169776E-01-0.60441151E-01
0001800-0.45678075E-01-0.32630887E-01-0.21080501E-01-0.10838505E-01-0.17429953E-02
0001900 0.63476302E-02 0.13555665E-01 0.19990645E-01 0.25757115E-01 0.30952871E-01
0002000 0.35665683E-01 0.39950542E-01 0.43774743E-01 0.46942938E-01 0.49120739E-01
0002100 0.49878486E-01 0.49120739E-01 0.46942938E-01 0.43774743E-01 0.39950542E-01
EOF
q
```

```
redit pote18
LOADING POTE18
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.11014421E-01 0.11007659E-01 0.10999572E-01 0.10991182E-01 0.10983460E-01
0000200 0.10977414E-01 0.10973863E-01 0.10973405E-01 0.10976192E-01 0.10982122E-01
0000300 0.10990579E-01 0.11000685E-01 0.11011284E-01 0.11021148E-01 0.11029031E-01
0000400 0.11033978E-01 0.11035156E-01 0.11032294E-01 0.11025541E-01 0.11015486E-01
0000500 0.11003215E-01 0.10990139E-01 0.10977797E-01 0.10967728E-01 0.10961305E-01
0000600 0.10959510E-01 0.10962866E-01 0.10971218E-01 0.10983855E-01 0.10999467E-01
0000700 0.11016339E-01 0.11032462E-01 0.11045806E-01 0.11054527E-01 0.11057273E-01
0000800 0.11053275E-01 0.11042595E-01 0.11026070E-01 0.11005353E-01 0.10982722E-01
0000900 0.10960899E-01 0.10942597E-01 0.10930415E-01 0.10926336E-01 0.10931496E-01
0001000 0.10945998E-01 0.10968715E-01 0.10997456E-01 0.11029057E-01 0.11059687E-01
0001100 0.11085290E-01 0.11102114E-01 0.11107154E-01 0.11098664E-01 0.11076536E-01
0001200 0.11042498E-01 0.11000164E-01 0.10954794E-01 0.10912847E-01 0.10881267E-01
0001300 0.10866739E-01 0.10874595E-01 0.10907911E-01 0.10966551E-01 0.11046488E-01
0001400 0.11139326E-01 0.11232190E-01 0.11308189E-01 0.11347178E-01 0.11327162E-01
0001500 0.11226110E-01 0.11024054E-01 0.10705531E-01 0.10261804E-01 0.96926913E-02
0001600 0.90076774E-02 0.82259849E-02 0.73752888E-02 0.64892769E-02 0.56042150E-02
0001700 0.47551915E-02 0.39722510E-02 0.32746647E-02 0.26696261E-02 0.21558946E-02
0001800 0.17270700E-02 0.13740472E-02 0.10867203E-02 0.85505540E-03 0.66973176E-03
0001900 0.52245148E-03 0.40605408E-03 0.31450135E-03 0.24278564E-03 0.18681448E-03
0002000 0.14327954E-03 0.10952870E-03 0.83451290E-04 0.63376123E-04 0.47984970E-04
0002100 0.36240264E-04 0.27326038E-04 0.20601306E-04 0.15563302E-04 0.11820276E-04
0002200 0.90702124E-05 0.70844972E-05 0.56943427E-05 0.47798230E-05 0.42613101E-05
0002300 0.40933855E-05 0.42613101E-05 0.47798230E-05 0.56943427E-05 0.70844972E-05
EOF
q
redit pote19
LOADING POTE19
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.23670864E 00-0.23673111E 00-0.23675781E 00-0.23678339E 00-0.23680198E 00
0000200-0.23681504E 00-0.23681861E 00-0.23681235E 00-0.23680049E 00-0.23677981E 00
0000300-0.23676360E 00-0.23673290E 00-0.23670179E 00-0.23667502E 00-0.23665231E 00
0000400-0.23665208E 00-0.23665005E 00-0.23666334E 00-0.23669767E 00-0.23672342E 00
0000500-0.23675406E 00-0.23679525E 00-0.23682421E 00-0.23685467E 00-0.23686320E 00
0000600-0.23685730E 00-0.23685318E 00-0.23682290E 00-0.23678350E 00-0.23673987E 00
0000700-0.23669553E 00-0.23665768E 00-0.23662961E 00-0.23661649E 00-0.23661953E 00
0000800-0.23663926E 00-0.23667544E 00-0.23672324E 00-0.23677695E 00-0.23683029E 00
0000900-0.23687708E 00-0.23690939E 00-0.23692250E 00-0.23691159E 00-0.23687690E 00
0001000-0.23682094E 00-0.23674721E 00-0.23666626E 00-0.23658639E 00-0.23651868E 00
0001100-0.23647189E 00-0.23645353E 00-0.23646796E 00-0.23651695E 00-0.23659784E 00
0001200-0.23670530E 00-0.23683298E 00-0.23697108E 00-0.23711020E 00-0.23724192E 00
0001300-0.23735881E 00-0.23745584E 00-0.23753470E 00-0.23760170E 00-0.23766506E 00
0001400-0.23773366E 00-0.23780876E 00-0.23787159E 00-0.23787588E 00-0.23773271E 00
0001500-0.23730242E 00-0.23638207E 00-0.23470086E 00-0.23191768E 00-0.22762442E 00
0001600-0.22135448E 00-0.21260035E 00-0.20083845E 00-0.18555737E 00-0.16630429E 00
0001700-0.14262962E 00-0.11824876E 00-0.96821964E-01-0.77919781E-01-0.61259035E-01
0001800-0.46546958E-01-0.33526190E-01-0.21969657E-01-0.11677671E-01-0.24739236E-02
0001900 0.57998747E-02 0.13291482E-01 0.20143338E-01 0.26499920E-01 0.32513253E-01
0002000 0.38350109E-01 0.44192377E-01 0.50225511E-01 0.56614831E-01 0.63449800E-01
0002100 0.70680737E-01 0.78059375E-01 0.85160196E-01 0.91507077E-01 0.96762896E-01
0002200 0.10085684E 00 0.10394382E 00 0.10623819E 00 0.10787427E 00 0.10887730E 00
0002300 0.10921651E 00 0.10887730E 00 0.10787427E 00 0.10623819E 00 0.10394382E 00
EOF
q
```

MG+ NL a=150 DENS.

VEFF

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p 99
        TOP RECORD
0000100 0.37572079E-02 0.37572342E-02 0.37572805E-02 0.37573494E-02 0.37574403E-02
0000200 0.37575511E-02 0.37576859E-02 0.37578414E-02 0.37580160E-02 0.37582100E-02
0000300 0.37584221E-02 0.37586479E-02 0.37588878E-02 0.37591357E-02 0.37593897E-02
0000400 0.37596498E-02 0.37599083E-02 0.37601625E-02 0.37604088E-02 0.37606426E-02
0000500 0.37608615E-02 0.37610591E-02 0.37612324E-02 0.37613788E-02 0.37614917E-02
0000600 0.37615716E-02 0.37616116E-02 0.37616126E-02 0.37615690E-02 0.37614820E-02
0000700 0.37613502E-02 0.37611723E-02 0.37609490E-02 0.37606787E-02 0.37603660E-02
0000800 0.37600105E-02 0.37596168E-02 0.37591886E-02 0.37587280E-02 0.37582435E-02
0000900 0.37577390E-02 0.37572221E-02 0.37566985E-02 0.37561757E-02 0.37556617E-02
0001000 0.37551669E-02 0.37546984E-02 0.37542665E-02 0.37538775E-02 0.37535427E-02
0001100 0.37532691E-02 0.37530661E-02 0.37529415E-02 0.37529024E-02 0.37529559E-02
0001200 0.37531101E-02 0.37533653E-02 0.37537292E-02 0.37542046E-02 0.37547913E-02
0001300 0.37554891E-02 0.37562968E-02 0.37572095E-02 0.37582256E-02 0.37593336E-02
0001400 0.37605269E-02 0.37617923E-02 0.37631195E-02 0.37644918E-02 0.37658908E-02
0001500 0.37672983E-02 0.37686930E-02 0.37700536E-02 0.37713528E-02 0.37725666E-02
0001600 0.37736660E-02 0.37746213E-02 0.37754031E-02 0.37759822E-02 0.37763240E-02
0001700 0.37763964E-02 0.37761678E-02 0.37756059E-02 0.37746765E-02 0.37733510E-02
0001800 0.37715985E-02 0.37693889E-02 0.37666971E-02 0.37634983E-02 0.37597697E-02
0001900 0.37554915E-02 0.37506532E-02 0.37452376E-02 0.37392385E-02 0.37326547E-02
0002000 0.37254887E-02 0.37177473E-02 0.37094462E-02 0.37006021E-02 0.36912453E-02
0002100 0.36814036E-02 0.36711222E-02 0.36604456E-02 0.36494322E-02 0.36381409E-02
0002200 0.36266467E-02 0.36150243E-02 0.36033622E-02 0.35917542E-02 0.35803043E-02
0002300 0.35691222E-02 0.35583272E-02 0.35480433E-02 0.35384046E-02 0.35295482E-02
0002400 0.35216194E-02 0.35147702E-02 0.35091590E-02 0.35049480E-02 0.35023014E-02
0002500 0.35014029E-02 0.35023014E-02 0.35049480E-02 0.35091590E-02 0.35147702E-02
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p 99
        TOP RECORD
0000100-0.11567652E 00-0.11567611E 00-0.11567622E 00-0.11567616E 00-0.11567599E 00
0000200-0.11567533E 00-0.11567611E 00-0.11567563E 00-0.11567551E 00-0.11567497E 00
0000300-0.11567456E 00-0.11567485E 00-0.11567426E 00-0.11567467E 00-0.11567426E 00
0000400-0.11567450E 00-0.11567485E 00-0.11567408E 00-0.11567497E 00-0.11567533E 00
0000500-0.11567503E 00-0.11567545E 00-0.11567551E 00-0.11567605E 00-0.11567611E 00
0000600-0.11567[illegible]E 00-0.11567694E 00-0.11567670E 00-0.11567718E 00-0.11567694E 00
0000700-0.11567[illegible]E 00-0.11567670E 00-0.11567670E 00-0.11567640E 00-0.11567593E 00
0000800-0.11567503E 00-0.11567444E 00-0.11567330E 00-0.11567175E 00-0.11566979E 00
0000900-0.11566800E 00-0.11566585E 00-0.11566311E 00-0.11566079E 00-0.11565822E 00
0001000-0.11565536E 00-0.11565179E 00-0.11564869E 00-0.11564517E 00-0.11564183E 00
0001100-0.11563867E 00-0.11563522E 00-0.11563241E 00-0.11562943E 00-0.11562669E 00
0001200-0.11562407E 00-0.11562234E 00-0.11562079E 00-0.11562020E 00-0.11562002E 00
0001300-0.11562037E 00-0.11562210E 00-0.11562431E 00-0.11562771E 00-0.11563206E 00
0001400-0.11563742E 00-0.11564398E 00-0.11565161E 00-0.11566067E 00-0.11567098E 00
0001500-0.11568236E 00-0.11569458E 00-0.11570835E 00-0.11572313E 00-0.11573893E 00
0001600-0.11575496E 00-0.11577195E 00-0.11578929E 00-0.11580694E 00-0.11582452E 00
0001700-0.11584193E 00-0.11585873E 00-0.11587435E 00-0.11588836E 00-0.11590058E 00
0001800-0.11590999E 00-0.11591637E 00-0.11591858E 00-0.11591595E 00-0.11590785E 00
0001900-0.11589307E 00-0.11587071E 00-0.11583972E 00-0.11579895E 00-0.11574745E 00
0002000-0.11568284E 00-0.11560464E 00-0.11551142E 00-0.11540115E 00-0.11527222E 00
0002100-0.11512357E 00-0.11495274E 00-0.11475837E 00-0.11453933E 00-0.11429244E 00
0002200-0.11401749E 00-0.11371189E 00-0.11337423E 00-0.11300361E 00-0.11259860E 00
0002300-0.11215752E 00-0.11167997E 00-0.11116469E 00-0.11061209E 00-0.11002135E 00
0002400-0.10939342E 00-0.10872877E 00-0.10802811E 00-0.10733324E 00-0.10642576E 00
0002500-0.10626221E 00-0.10642576E 00-0.10733324E 00-0.10802811E 00-0.10872877E 00
EOF
```

NA LDA a=0.25 DENS.

VEFF

```
q
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
```

NA LDA a=0.5 DENS.

```
        TOP RECORD
0000100 0.37551771E-02 0.37552225E-02 0.37554663E-02 0.37559131E-02 0.37565546E-02
0000200 0.37573678E-02 0.37583173E-02 0.37593590E-02 0.37604365E-02 0.37614873E-02
0000300 0.37624440E-02 0.37632391E-02 0.37638061E-02 0.37640894E-02 0.37640401E-02
0000400 0.37636296E-02 0.37628438E-02 0.37616910E-02 0.37602051E-02 0.37584426E-02
0000500 0.37564833E-02 0.37544291E-02 0.37524011E-02 0.37505361E-02 0.37489741E-02
0000600 0.37478604E-02 0.37473333E-02 0.37475163E-02 0.37485065E-02 0.37503701E-02
0000700 0.37531303E-02 0.37567618E-02 0.37611825E-02 0.37662503E-02 0.37717610E-02
0000800 0.37774420E-02 0.37829622E-02 0.37879320E-02 0.37919111E-02 0.37944182E-02
0000900 0.37949472E-02 0.37929851E-02 0.37880228E-02 0.37795873E-02 0.37672557E-02
0001000 0.37506879E-02 0.37296470E-02 0.37040215E-02 0.36738645E-02 0.36393979E-02
0001100 0.36010463E-02 0.35594420E-02 0.35154433E-02 0.34701356E-02 0.34248289E-02
0001200 0.33810565E-02 0.33405575E-02 0.33052624E-02 0.32772701E-02 0.32587876E-02
0001300 0.32524082E-02 0.32587876E-02 0.32772701E-02 0.33052624E-02 0.33405575E-02
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.11567611E 00-0.11567384E 00-0.11567241E 00-0.11567134E 00-0.11567086E 00
0000200-0.11567110E 00-0.11567134E 00-0.11567241E 00-0.11567390E 00-0.11567736E 00
0000300-0.11567998E 00-0.11568385E 00-0.11568707E 00-0.11569107E 00-0.11569411E 00
0000400-0.11569697E 00-0.11569905E 00-0.11569893E 00-0.11569732E 00-0.11569291E 00
0000500-0.11568701E 00-0.11567903E 00-0.11566949E 00-0.11565793E 00-0.11564565E 00
0000600-0.11563289E 00-0.11562121E 00-0.11561114E 00-0.11560416E 00-0.11560112E 00
0000700-0.11560392E 00-0.11561340E 00-0.11563087E 00-0.11565709E 00-0.11569521E 00
0000800-0.11573827E 00-0.11579281E 00-0.11585575E 00-0.11592507E 00-0.11599767E 00
0000900-0.11607009E 00-0.11613619E 00-0.11618912E 00-0.11621976E 00-0.11621714E 00
0001000-0.11616778E 00-0.11605579E 00-0.11586225E 00-0.11556679E 00-0.11514604E 00
0001100-0.11457449E 00-0.11382520E 00-0.11287194E 00-0.11168730E 00-0.11024719E 00
0001200-0.10853088E 00-0.10652429E 00-0.10422057E 00-0.10177046E 00-0.98374546E-01
0001300-0.97712398E-01-0.98374546E-01-0.10177046E 00-0.10422057E 00-0.10652429E 00
EOF
q
```

```
redit pote6
LOADING POTE6
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.37530579E-02 0.37530260E-02 0.37530642E-02 0.37531781E-02 0.37533664E-02
0000200 0.37536330E-02 0.37539757E-02 0.37543934E-02 0.37548831E-02 0.37554398E-02
0000300 0.37560589E-02 0.37567345E-02 0.37574589E-02 0.37582242E-02 0.37590198E-02
0000400 0.37598347E-02 0.37606598E-02 0.37614817E-02 0.37622862E-02 0.37630638E-02
0000500 0.37638003E-02 0.37644817E-02 0.37650976E-02 0.37656333E-02 0.37660762E-02
0000600 0.37664184E-02 0.37666475E-02 0.37667572E-02 0.37667367E-02 0.37665816E-02
0000700 0.37662876E-02 0.37658508E-02 0.37652727E-02 0.37645530E-02 0.37636959E-02
0000800 0.37627071E-02 0.37615960E-02 0.37603730E-02 0.37590468E-02 0.37576391E-02
0000900 0.37561632E-02 0.37546400E-02 0.37530884E-02 0.37515324E-02 0.37499955E-02
0001000 0.37485028E-02 0.37470814E-02 0.37457603E-02 0.37445636E-02 0.37435209E-02
0001100 0.37426576E-02 0.37420024E-02 0.37415784E-02 0.37414096E-02 0.37415167E-02
0001200 0.37419188E-02 0.37426315E-02 0.37436693E-02 0.37450399E-02 0.37467475E-02
0001300 0.37487962E-02 0.37511785E-02 0.37538847E-02 0.37569015E-02 0.37602081E-02
0001400 0.37637791E-02 0.37675819E-02 0.37715782E-02 0.37757230E-02 0.37799680E-02
0001500 0.37842561E-02 0.37885255E-02 0.37927108E-02 0.37967372E-02 0.38005284E-02
0001600 0.38040024E-02 0.38070739E-02 0.38096521E-02 0.38116460E-02 0.38129620E-02
0001700 0.38135021E-02 0.38131734E-02 0.38118779E-02 0.38095238E-02 0.38060187E-02
0001800 0.38012755E-02 0.37952070E-02 0.37877406E-02 0.37788013E-02 0.37683302E-02
0001900 0.37562707E-02 0.37425826E-02 0.37272323E-02 0.37102017E-02 0.36914859E-02
0002000 0.36710959E-02 0.36490590E-02 0.36254169E-02 0.36002309E-02 0.35735788E-02
0002100 0.35455604E-02 0.35162922E-02 0.34859113E-02 0.34545744E-02 0.34224566E-02
0002200 0.33897527E-02 0.33566791E-02 0.33234705E-02 0.32903752E-02 0.32576644E-02
0002300 0.32256213E-02 0.31945521E-02 0.31647694E-02 0.31366029E-02 0.31103985E-02
0002400 0.30865110E-02 0.30653076E-02 0.30471699E-02 0.30324913E-02 0.30216696E-02
0002500 0.30150372E-02 0.30128132E-02 0.30150372E-02 0.30216696E-02 0.30324913E-02
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.11567646E 00-0.11567497E 00-0.11567360E 00-0.11567253E 00-0.11567122E 00
0000200-0.11567146E 00-0.11567044E 00-0.11566943E 00-0.11566931E 00-0.11566895E 00
0000300-0.11566931E 00-0.11566901E 00-0.11566985E 00-0.11566979E 00-0.11567080E 00
0000400-0.11567229E 00-0.11567372E 00-0.11567616E 00-0.11567783E 00-0.11567968E 00
0000500-0.11568213E 00-0.11568469E 00-0.11568791E 00-0.11569041E 00-0.11569315E 00
0000600-0.11569691E 00-0.11569983E 00-0.11570275E 00-0.11570489E 00-0.11570793E 00
0000700-0.11570960E 00-0.11571169E 00-0.11571360E 00-0.11571431E 00-0.11571473E 00
0000800-0.11571431E 00-0.11571354E 00-0.11571127E 00-0.11570859E 00-0.11570495E 00
0000900-0.11570096E 00-0.11569571E 00-0.11569023E 00-0.11568379E 00-0.11567640E 00
0001000-0.11566842E 00-0.11566031E 00-0.11565131E 00-0.11564225E 00-0.11563313E 00
0001100-0.11562335E 00-0.11561435E 00-0.11560553E 00-0.11559719E 00-0.11558938E 00
0001200-0.11558324E 00-0.11557770E 00-0.11557370E 00-0.11557156E 00-0.11557084E 00
0001300-0.11557305E 00-0.11557722E 00-0.11558402E 00-0.11559379E 00-0.11560625E 00
0001400-0.11562198E 00-0.11564118E 00-0.11566401E 00-0.11569083E 00-0.11572009E 00
0001500-0.11575341E 00-0.11579025E 00-0.11583060E 00-0.11587399E 00-0.11592031E 00
0001600-0.11596918E 00-0.11602026E 00-0.11607355E 00-0.11612737E 00-0.11618227E 00
0001700-0.11623675E 00-0.11628938E 00-0.11633986E 00-0.11638635E 00-0.11642796E 00
0001800-0.11646241E 00-0.11648840E 00-0.11650360E 00-0.11650574E 00-0.11649209E 00
0001900-0.11646104E 00-0.11640823E 00-0.11633199E 00-0.11622763E 00-0.11609203E 00
0002000-0.11592108E 00-0.11571127E 00-0.11545753E 00-0.11515588E 00-0.11480135E 00
0002100-0.11438924E 00-0.11391443E 00-0.11337185E 00-0.11275697E 00-0.11206400E 00
0002200-0.11128843E 00-0.11042565E 00-0.10947114E 00-0.10842001E 00-0.10726911E 00
0002300-0.10601491E 00-0.10465485E 00-0.10318673E 00-0.10160923E 00-0.99922299E-01
0002400-0.98126471E-01-0.96223354E-01-0.94215572E-01-0.92107594E-01-0.90336859E-01
0002500-0.89135289E-01-0.88966966E-01-0.89135289E-01-0.90336859E-01-0.92107594E-01
EOF
q
```

NA LDA a=0.75 DENS.

VEFF

```
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
```

NA LDA a=1.0 DENS.

```
        TOP RECORD
0000100 0.37518309E-02 0.37516037E-02 0.37517741E-02 0.37523662E-02 0.37533771E-02
0000200 0.37547799E-02 0.37565175E-02 0.37585131E-02 0.37606638E-02 0.37628494E-02
0000300 0.37649353E-02 0.37667837E-02 0.37682543E-02 0.37692168E-02 0.37695621E-02
0000400 0.37692073E-02 0.37681018E-02 0.37662364E-02 0.37636482E-02 0.37604210E-02
0000500 0.37566924E-02 0.37526416E-02 0.37484919E-02 0.37445019E-02 0.37409503E-02
0000600 0.37381325E-02 0.37363356E-02 0.37358257E-02 0.37368308E-02 0.37395270E-02
0000700 0.37440085E-02 0.37502816E-02 0.37582549E-02 0.37677127E-02 0.37783196E-02
0000800 0.37896109E-02 0.38009982E-02 0.38117697E-02 0.38211080E-02 0.38281111E-02
0000900 0.38318075E-02 0.38311952E-02 0.38252755E-02 0.38130886E-02 0.37937709E-02
0001000 0.37665935E-02 0.37310147E-02 0.36867298E-02 0.36337222E-02 0.35722950E-02
0001100 0.35031126E-02 0.34272198E-02 0.33460492E-02 0.32614239E-02 0.31755324E-02
0001200 0.30909057E-02 0.30103792E-02 0.29370449E-02 0.28742224E-02 0.28254276E-02
0001300 0.27942557E-02 0.27836689E-02 0.27942557E-02 0.28254276E-02 0.28742224E-02
EOF
q
```

```
reditkpote9
LOADING POTE9
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.11567646E 00-0.11566991E 00-0.11566401E 00-0.11565942E 00-0.11565516E 00
0000200-0.11565316E 00-0.11565262E 00-0.11565369E 00-0.11565644E 00-0.11566210E 00
0000300-0.11566806E 00-0.11567599E 00-0.11568445E 00-0.11569351E 00-0.11570209E 00
0000400-0.11570948E 00-0.11571574E 00-0.11571854E 00-0.11571866E 00-0.11571467E 00
0000500-0.11570603E 00-0.11569327E 00-0.11567664E 00-0.11565590E 00-0.11563283E 00
0000600-0.11560845E 00-0.11558449E 00-0.11556202E 00-0.11554460E 00-0.11553419E 00
0000700-0.11553288E 00-0.11554354E 00-0.11556870E 00-0.11560984E 00-0.11567014E 00
0000800-0.11574817E 00-0.11584574E 00-0.11596102E 00-0.11609179E 00-0.11623317E 00
0000900-0.11637968E 00-0.11652219E 00-0.11664903E 00-0.11674432E 00-0.11679089E 00
0001000-0.11676359E 00-0.11663544E 00-0.11637282E 00-0.11593625E 00-0.11526073E 00
0001100-0.11437720E 00-0.11315256E 00-0.11136231E 00-0.10955364E 00-0.10707575E 00
0001200-0.10408437E 00-0.10054421E 00-0.96433282E-01-0.91746569E-01-0.86625397E-01
0001300-0.82037032E-01-0.81361949E-01-0.82037032E-01-0.86625397E-01-0.91746569E-01
EOF
q
```

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
```

NA LDA a=2.0 DENS.

```
        TOP RECORD
0000100 0.37461643E-02 0.37447631E-02 0.37440872E-02 0.37442304E-02 0.37452441E-02
0000200 0.37471277E-02 0.37498283E-02 0.37532363E-02 0.37571911E-02 0.37614868E-02
0000300 0.37658773E-02 0.37700930E-02 0.37738469E-02 0.37768595E-02 0.37788702E-02
0000400 0.37796525E-02 0.37790379E-02 0.37769238E-02 0.37732888E-02 0.37682087E-02
0000500 0.37618512E-02 0.37544859E-02 0.37464700E-02 0.37382499E-02 0.37303346E-02
0000600 0.37232814E-02 0.37176684E-02 0.37140590E-02 0.37129805E-02 0.37148774E-02
0000700 0.37200816E-02 0.37287842E-02 0.37409936E-02 0.37565166E-02 0.37749368E-02
0000800 0.37955951E-02 0.38175939E-02 0.38397883E-02 0.38608143E-02 0.38791087E-02
0000900 0.38929482E-02 0.39005016E-02 0.38998902E-02 0.38892629E-02 0.38668867E-02
0001000 0.38312299E-02 0.37810595E-02 0.37155414E-02 0.36343271E-02 0.35376318E-02
0001100 0.34262938E-02 0.33018007E-02 0.31662993E-02 0.30225564E-02 0.28738871E-02
0001200 0.27240661E-02 0.25771942E-02 0.24375843E-02 0.23096330E-02 0.21977539E-02
0001300 0.21062689E-02 0.20387231E-02 0.19973582E-02 0.19834985E-02 0.19973582E-02
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.11567646E 00-0.11565548E 00-0.11563671E 00-0.11562049E 00-0.11560667E 00
0000200-0.11559683E 00-0.11559033E 00-0.11558789E 00-0.11558998E 00-0.11559749E 00
0000300-0.11560756E 00-0.11562252E 00-0.11563957E 00-0.11565948E 00-0.11567992E 00
0000400-0.11569971E 00-0.11571783E 00-0.11573148E 00-0.11574024E 00-0.11574137E 00
0000500-0.11573547E 00-0.11572099E 00-0.11569715E 00-0.11566466E 00-0.11562502E 00
0000600-0.11557955E 00-0.11553144E 00-0.11548269E 00-0.11543870E 00-0.11540288E 00
0000700-0.11538041E 00-0.11537623E 00-0.11539501E 00-0.11544192E 00-0.11552113E 00
0000800-0.11563492E 00-0.11578602E 00-0.11597395E 00-0.11619717E 00-0.11645144E 00
0000900-0.11672896E 00-0.11701763E 00-0.11730206E 00-0.11755949E 00-0.11776245E 00
0001000-0.11787426E 00-0.11785191E 00-0.11764252E 00-0.11718416E 00-0.11640620E 00
0001100-0.11522355E 00-0.11356539E 00-0.11132264E 00-0.10840458E 00-0.10471606E 00
0001200-0.10010617E 00-0.94682515E-01-0.88198364E-01-0.80679297E-01-0.72120011E-01
0001300-0.64134538E-01-0.58499152E-01-0.54743566E-01-0.54083120E-01-0.54743566E-01
EOF
q
```

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.37508809E-02 0.37526868E-02 0.37550044E-02 0.37577252E-02 0.37607211E-02
0000200 0.37638347E-02 0.37668964E-02 0.37697295E-02 0.37721021E-02 0.37740348E-02
0000300 0.37752092E-02 0.37755826E-02 0.37750890E-02 0.37737123E-02 0.37714832E-02
0000400 0.37684832E-02 0.37648436E-02 0.37607423E-02 0.37563897E-02 0.37520300E-02
0000500 0.37479138E-02 0.37442998E-02 0.37414299E-02 0.37395188E-02 0.37387363E-02
0000600 0.37391982E-02 0.37409519E-02 0.37439719E-02 0.37481504E-02 0.37533222E-02
0000700 0.37592165E-02 0.37655204E-02 0.37718692E-02 0.37778607E-02 0.37830836E-02
0000800 0.37871334E-02 0.37896505E-02 0.37903248E-02 0.37889367E-02 0.37853706E-02
0000900 0.37796332E-02 0.37718650E-02 0.37623430E-02 0.37514854E-02 0.37398410E-02
0001000 0.37280682E-02 0.37169158E-02 0.37071847E-02 0.36996901E-02 0.36952266E-02
0001100 0.36945103E-02 0.36981269E-02 0.37064988E-02 0.37198255E-02 0.37380408E-02
0001200 0.37607914E-02 0.37874000E-02 0.38168498E-02 0.38477948E-02 0.38785583E-02
0001300 0.39071627E-02 0.39313845E-02 0.39488301E-02 0.39569549E-02 0.39532259E-02
0001400 0.39352067E-02 0.39006749E-02 0.38477399E-02 0.37750194E-02 0.36817323E-02
0001500 0.35678199E-02 0.34340248E-02 0.32819479E-02 0.31140514E-02 0.29336037E-02
0001600 0.27445806E-02 0.25515084E-02 0.23592664E-02 0.21728738E-02 0.19972795E-02
0001700 0.18371809E-02 0.16968586E-02 0.15795629E-02 0.14872288E-02 0.14208704E-02
0001800 0.13809328E-02 0.13676342E-02 0.13809328E-02 0.14208704E-02 0.14872288E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.11567611E 00-0.11568344E 00-0.11569118E 00-0.11569792E 00-0.11570549E 00
0000200-0.11571223E 00-0.11571896E 00-0.11572558E 00-0.11573249E 00-0.11573905E 00
0000300-0.11574513E 00-0.11575013E 00-0.11575371E 00-0.11575574E 00-0.11575651E 00
0000400-0.11575359E 00-0.11574924E 00-0.11574167E 00-0.11573148E 00-0.11571872E 00
0000500-0.11570352E 00-0.11568636E 00-0.11566889E 00-0.11564982E 00-0.11563253E 00
0000600-0.11561626E 00-0.11560333E 00-0.11559319E 00-0.11558706E 00-0.11558592E 00
0000700-0.11559081E 00-0.11559969E 00-0.11561471E 00-0.11563307E 00-0.11565548E 00
0000800-0.11567938E 00-0.11570436E 00-0.11572838E 00-0.11574829E 00-0.11576325E 00
0000900-0.11576986E 00-0.11576802E 00-0.11575538E 00-0.11573094E 00-0.11569458E 00
0001000-0.11564690E 00-0.11558878E 00-0.11552435E 00-0.11545533E 00-0.11538845E 00
0001100-0.11532855E 00-0.11528230E 00-0.11525631E 00-0.11525798E 00-0.11529458E 00
0001200-0.11537200E 00-0.11549473E 00-0.11566657E 00-0.11588925E 00-0.11616117E 00
0001300-0.11647916E 00-0.11683547E 00-0.11721826E 00-0.11761045E 00-0.11798930E 00
0001400-0.11832404E 00-0.11857575E 00-0.11869508E 00-0.11862159E 00-0.11828333E 00
0001500-0.11759531E 00-0.11645907E 00-0.11476505E 00-0.11239141E 00-0.10920817E 00
0001600-0.10508037E 00-0.99874437E-01-0.93463600E-01-0.85738897E-01-0.76616406E-01
0001700-0.66056371E-01-0.55698171E-01-0.47176257E-01-0.40511187E-01-0.35784200E-01
0001800-0.32692980E-01-0.32063767E-01-0.32692980E-01-0.35784200E-01-0.40511187E-01
EOF
q
```

NA LDA a=3.0 DENS.

VEFF

```
redit pote14
LOADING POTE14
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.3745766lE-02 0.37484306E-02 0.37518672E-02 0.37559271E-02 0.37604072E-02
0000200 0.37650773E-02 0.37696811E-02 0.37739577E-02 0.37776453E-02 0.37805056E-02
0000300 0.37823331E-02 0.37829753E-02 0.37823336E-02 0.37803815E-02 0.37771654E-02
0000400 0.37728092E-02 0.37675060E-02 0.37615162E-02 0.37551520E-02 0.37487664E-02
0000500 0.3742739lE-02 0.37374403E-02 0.37332242E-02 0.37304049E-02 0.37292265E-02
0000600 0.37298545E-02 0.37323595E-02 0.37366950E-02 0.37427144E-02 0.37501482E-02
0000700 0.37586277E-02 0.37676967E-02 0.37768206E-02 0.37854267E-02 0.37929225E-02
0000800 0.37987395E-02 0.38023610E-02 0.38033554E-02 0.38014217E-02 0.37964038E-02
0000900 0.37883248E-02 0.37773966E-02 0.37640270E-02 0.37488211E-02 0.37325590E-02
0001000 0.37161750E-02 0.37007157E-02 0.36873003E-02 0.36770601E-02 0.36710764E-02
0001100 0.36703185E-02 0.36755702E-02 0.36873729E-02 0.37059544E-02 0.37311872E-02
0001200 0.37625341E-02 0.37990222E-02 0.38392374E-02 0.38813076E-02 0.39229356E-02
0001300 0.39614514E-02 0.39938726E-02 0.40170066E-02 0.40275082E-02 0.40220954E-02
0001400 0.39976314E-02 0.39513595E-02 0.38810349E-02 0.37851119E-02 0.36629287E-02
0001500 0.35148223E-02 0.33422275E-02 0.31476950E-02 0.29348577E-02 0.27082954E-02
0001600 0.24733334E-02 0.22357553E-02 0.20014800E-02 0.17762133E-02 0.15651349E-02
0001700 0.13725872E-02 0.12014704E-02 0.10530469E-02 0.92739379E-03 0.82384679E-03
0001800 0.74135046E-03 0.67873043E-03 0.63489052E-03 0.60895737E-03 0.60038199E-03
EOF
q
redit pote15
LOADING POTE15
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.11567438E 00-0.11568481E 00-0.11569482E 00-0.11570555E 00-0.11571521E 00
0000200-0.11572611E 00-0.11573678E 00-0.11574757E 00-0.11575872E 00-0.11576957E 00
0000300-0.11577952E 00-0.11578876E 00-0.11579508E 00-0.11580074E 00-0.11580199E 00
0000400-0.11580116E 00-0.11579686E 00-0.11578810E 00-0.11577564E 00-0.11575907E 00
0000500-0.11573911E 00-0.11571599E 00-0.11569250E 00-0.11566818E 00-0.11564350E 00
0000600-0.11562115E 00-0.11560202E 00-0.11558670E 00-0.11557674E 00-0.11557454E 00
0000700-0.11557776E 00-0.11558843E 00-0.11560494E 00-0.11562836E 00-0.11565542E 00
0000800-0.11568493E 00-0.11571616E 00-0.11574453E 00-0.11576903E 00-0.11578536E 00
0000900-0.11579263E 00-0.11578792E 00-0.11576951E 00-0.11573666E 00-0.11568928E 00
0001000-0.11562860E 00-0.11555743E 00-0.11547810E 00-0.11539668E 00-0.11531919E 00
0001100-0.11525238E 00-0.11520487E 00-0.11518443E 00-0.11519969E 00-0.11525851E 00
0001200-0.11536688E 00-0.11553210E 00-0.11575764E 00-0.11604470E 00-0.11639345E 00
0001300-0.11679894E 00-0.11725408E 00-0.11774367E 00-0.11824811E 00-0.11873871E 00
0001400-0.11917621E 00-0.11951083E 00-0.11967814E 00-0.11959851E 00-0.11917698E 00
0001500-0.11830062E 00-0.11683965E 00-0.11464602E 00-0.11155921E 00-0.10740602E 00
0001600-0.10200816E 00-0.95187366E-01-0.86776018E-01-0.76626062E-01-0.64618289E-01
0001700-0.52334554E-01-0.41378163E-01-0.31702969E-01-0.23276471E-01-0.16066171E-01
0001800-0.10106418E-01-0.54170266E-02-0.20507479E-02 0.91477457E-04 0.63618855E-03
EOF
q
```

NA LDA a=5.0 DENS.

VEFF

```
redit pote16
LOADING POTE16
REKEYED
EDIT
p 99
```

NA LDA a=100 DENS.

```
      TOP RECORD
0000100 0.37391149E-02 0.37407726E-02 0.37436332E-02 0.37475941E-02 0.37524900E-02
0000200 0.37580692E-02 0.37641085E-02 0.37702296E-02 0.37761079E-02 0.37814016E-02
0000300 0.37857734E-02 0.37889290E-02 0.37906272E-02 0.37906975E-02 0.37890507E-02
0000400 0.37856959E-02 0.37807394E-02 0.37743840E-02 0.37669269E-02 0.37587434E-02
0000500 0.37502742E-02 0.37420031E-02 0.37344242E-02 0.37280254E-02 0.37232526E-02
0000600 0.37204344E-02 0.37200029E-02 0.37219771E-02 0.37264379E-02 0.37332757E-02
0000700 0.37422273E-02 0.37528977E-02 0.37647465E-02 0.37771391E-02 0.37893527E-02
0000800 0.38006220E-02 0.38101824E-02 0.38173052E-02 0.38213448E-02 0.38217902E-02
0000900 0.38182982E-02 0.38107331E-02 0.37991826E-02 0.37839918E-02 0.37657518E-02
0001000 0.37452949E-02 0.37236731E-02 0.37021181E-02 0.36819843E-02 0.36647006E-02
0001100 0.36516800E-02 0.36442569E-02 0.36435891E-02 0.36505917E-02 0.36658503E-02
0001200 0.36895492E-02 0.37214197E-02 0.37606829E-02 0.38060353E-02 0.38556198E-02
0001300 0.39070509E-02 0.39574355E-02 0.40034987E-02 0.40415637E-02 0.40677711E-02
0001400 0.40781461E-02 0.40688515E-02 0.40363520E-02 0.39776154E-02 0.38904026E-02
0001500 0.37733612E-02 0.36263489E-02 0.34504784E-02 0.32482073E-02 0.30232931E-02
0001600 0.27606617E-02 0.25261578E-02 0.22662194E-02 0.20074651E-02 0.17562793E-02
0001700 0.15184041E-02 0.12985661E-02 0.10998612E-02 0.92358678E-03 0.76967711E-03
0001800 0.63712336E-03 0.52432227E-03 0.42934413E-03 0.35013468E-03 0.28465339E-03
0001900 0.23096937E-03 0.18731330E-03 0.15211180E-03 0.12399507E-03 0.10179674E-03
0002000 0.84544241E-04 0.71445989E-04 0.61877538E-04 0.55368786E-04 0.51592113E-04
0002100 0.50354443E-04 0.51592113E-04 0.55368786E-04 0.61877538E-04 0.71445989E-04
EOF
q
redit pote17
LOADING POTE17
REKEYED
EDIT
p 99
```

VEFF

```
      TOP RECORD
0000100-0.11567634E 00-0.11568356E 00-0.11569071E 00-0.11569738E 00-0.11570549E 00
0000200-0.11571348E 00-0.11572260E 00-0.11573344E 00-0.11574566E 00-0.11575919E 00
0000300-0.11577308E 00-0.11578721E 00-0.11580080E 00-0.11581260E 00-0.11582261E 00
0000400-0.11582851E 00-0.11583114E 00-0.11582851E 00-0.11581987E 00-0.11580610E 00
0000500-0.11578637E 00-0.11576110E 00-0.11573160E 00-0.11569899E 00-0.11566520E 00
0000600-0.11563116E 00-0.11559963E 00-0.11557233E 00-0.11555111E 00-0.11553758E 00
0000700-0.11553419E 00-0.11554015E 00-0.11555707E 00-0.11558378E 00-0.11562103E 00
0000800-0.11566657E 00-0.11571801E 00-0.11577362E 00-0.11582834E 00-0.11588013E 00
0000900-0.11592352E 00-0.11595494E 00-0.11596996E 00-0.11596447E 00-0.11593562E 00
0001000-0.11588126E 00-0.11580098E 00-0.11569685E 00-0.11557120E 00-0.11543089E 00
0001100-0.11528313E 00-0.11513716E 00-0.11500460E 00-0.11489707E 00-0.11482757E 00
0001200-0.11480868E 00-0.11485189E 00-0.11496753E 00-0.11516476E 00-0.11544883E 00
0001300-0.11582345E 00-0.11628765E 00-0.11683547E 00-0.11745507E 00-0.11812592E 00
0001400-0.11881757E 00-0.11948830E 00-0.12008148E 00-0.12052709E 00-0.12073678E 00
0001500-0.12060511E 00-0.12000996E 00-0.11881226E 00-0.11685902E 00-0.11396488E 00
0001600-0.11001786E 00-0.10478246E 00-0.98108113E-01-0.89832604E-01-0.79809666E-01
0001700-0.67914367E-01-0.55559203E-01-0.44166304E-01-0.33652950E-01-0.23939215E-01
0001800-0.14951598E-01-0.66244267E-02 0.10995422E-02 0.82687996E-02 0.14923058E-01
0001900 0.21092523E-01 0.26797973E-01 0.32049496E-01 0.36845386E-01 0.41170336E-01
0002000 0.44993453E-01 0.48267361E-01 0.50929278E-01 0.52904438E-01 0.54134224E-01
0002100 0.54535687E-01 0.54134224E-01 0.52904438E-01 0.50929278E-01 0.48267361E-01
EOF
q
```

```
redit pote18
LOADING POTE18
REKEYED
EDIT
p99
```

NA LDA a=15.0 DENS.

```
        TOP RECORD
0000100 0.37378436E-02 0.37395358E-02 0.37424597E-02 0.37465137E-02 0.37515266E-02
0000200 0.37572614E-02 0.37634315E-02 0.37697088E-02 0.37757461E-02 0.37811834E-02
0000300 0.37856803E-02 0.37889355E-02 0.37906966E-02 0.37907863E-02 0.37891129E-02
0000400 0.37856796E-02 0.37805941E-02 0.37740637E-02 0.37663870E-02 0.37579490E-02
0000500 0.37491997E-02 0.37406341E-02 0.37327614E-02 0.37260819E-02 0.37210595E-02
0000600 0.37180816E-02 0.37174474E-02 0.37193329E-02 0.37237797E-02 0.37306859E-02
0000700 0.37397912E-02 0.37506917E-02 0.37628522E-02 0.37756243E-02 0.37882708E-02
0000800 0.38000157E-02 0.38100712E-02 0.38176884E-02 0.38221984E-02 0.38230694E-02
0000900 0.38199327E-02 0.38126293E-02 0.38012362E-02 0.37860763E-02 0.37677358E-02
0001000 0.37470434E-02 0.37250551E-02 0.37030084E-02 0.36822818E-02 0.36643203E-02
0001100 0.36505710E-02 0.36424010E-02 0.36410086E-02 0.36473484E-02 0.36620416E-02
0001200 0.36853179E-02 0.37169356E-02 0.37561539E-02 0.38016806E-02 0.38516836E-02
0001300 0.39037829E-02 0.39550774E-02 0.40022656E-02 0.40416569E-02 0.40693507E-02
0001400 0.40813126E-02 0.40736571E-02 0.40427595E-02 0.39855428E-02 0.38996788E-02
0001500 0.37837664E-02 0.36376072E-02 0.34622783E-02 0.32602136E-02 0.30351714E-02
0001600 0.27920860E-02 0.25368347E-02 0.22758911E-02 0.20159194E-02 0.17633531E-02
0001700 0.15239783E-02 0.13025638E-02 0.11022484E-02 0.92437235E-03 0.76890877E-03
0001800 0.63487538E-03 0.52068685E-03 0.42441906E-03 0.34400891E-03 0.27740118E-03
0001900 0.22263697E-03 0.17791272E-03 0.14161142E-03 0.11231091E-03 0.88781890E-04
0002000 0.69976144E-04 0.55010882E-04 0.43150081E-04 0.33785822E-04 0.26420108E-04
0002100 0.20647974E-04 0.16142658E-04 0.12642047E-04 0.99376512E-05 0.78648918E-05
0002200 0.62951876E-05 0.51295156E-05 0.42932634E-05 0.37322407E-05 0.34097602E-05
0002300 0.33045817E-05 0.34097602E-05 0.37322407E-05 0.42932634E-05 0.51295156E-05
EOF
q
redit pote19
LOADING POTE19
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.11567646E 00-0.11568224E 00-0.11568862E 00-0.11569470E 00-0.11570227E 00
0000200-0.11570960E 00-0.11571801E 00-0.11572927E 00-0.11574137E 00-0.11575550E 00
0000300-0.11577004E 00-0.11578536E 00-0.11579961E 00-0.11581230E 00-0.11582363E 00
0000400-0.11583048E 00-0.11583340E 00-0.11583078E 00-0.11582220E 00-0.11580706E 00
0000500-0.11578625E 00-0.11575919E 00-0.11572802E 00-0.11569256E 00-0.11565596E 00
0000600-0.11561942E 00-0.11558539E 00-0.11555541E 00-0.11553198E 00-0.11551672E 00
0000700-0.11551249E 00-0.11551815E 00-0.11553627E 00-0.11556530E 00-0.11560547E 00
0000800-0.11565560E 00-0.11571312E 00-0.11577576E 00-0.11583847E 00-0.11589956E 00
0000900-0.11595207E 00-0.11599332E 00-0.11601776E 00-0.11602098E 00-0.11599904E 00
0001000-0.11594951E 00-0.11587173E 00-0.11576706E 00-0.11563748E 00-0.11548948E 00
0001100-0.11533034E 00-0.11517018E 00-0.11502099E 00-0.11489558E 00-0.11480761E 00
0001200-0.11477095E 00-0.11479717E 00-0.11489892E 00-0.11508572E 00-0.11536336E 00
0001300-0.11573672E 00-0.11620468E 00-0.11676192E 00-0.11739576E 00-0.11808556E 00
0001400-0.11879981E 00-0.11949617E 00-0.12011802E 00-0.12059265E 00-0.12083107E 00
0001500-0.12072700E 00-0.12015712E 00-0.11898237E 00-0.11705023E 00-0.11419690E 00
0001600-0.11025321E 00-0.10504752E 00-0.98412693E-01-0.90191126E-01-0.80241024E-01
0001700-0.68440259E-01-0.56174815E-01-0.44839501E-01-0.34352321E-01-0.24633795E-01
0001800-0.15610274E-01-0.72148517E-02 0.61221770E-03 0.79236291E-02 0.14765520E-01
0001900 0.21177862E-01 0.27195439E-01 0.32847889E-01 0.38161017E-01 0.43156940E-01
0002000 0.47854859E-01 0.52271143E-01 0.56419946E-01 0.60313173E-01 0.63959181E-01
0002100 0.67368388E-01 0.70543587E-01 0.73485851E-01 0.76192200E-01 0.78651786E-01
0002200 0.80845475E-01 0.82744002E-01 0.84305763E-01 0.85479200E-01 0.86212158E-01
0002300 0.86460412E-01 0.86212158E-01 0.85479200E-01 0.84305763E-01 0.82744002E-01
EOF
q
```

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
```

NA NL a=0.25
DENS.

```
        TOP RECORD
0000100 0.37563927E-02 0.37564647E-02 0.37565569E-02 0.37566698E-02 0.37568053E-02
0000200 0.37569632E-02 0.37571415E-02 0.37573408E-02 0.37575625E-02 0.37578009E-02
0000300 0.37580566E-02 0.37583283E-02 0.37586114E-02 0.37589066E-02 0.37592088E-02
0000400 0.37595145E-02 0.37598240E-02 0.37601271E-02 0.37604258E-02 0.37607157E-02
0000500 0.37609919E-02 0.37612508E-02 0.37614882E-02 0.37617031E-02 0.37618896E-02
0000600 0.37620468E-02 0.37621709E-02 0.37622587E-02 0.37623104E-02 0.37623236E-02
0000700 0.37622976E-02 0.37622303E-02 0.37621229E-02 0.37619765E-02 0.37617914E-02
0000800 0.37615688E-02 0.37613134E-02 0.37610263E-02 0.37607111E-02 0.37603735E-02
0000900 0.37600184E-02 0.37596496E-02 0.37592757E-02 0.37589003E-02 0.37585320E-02
0001000 0.37581755E-02 0.37578391E-02 0.37575308E-02 0.37572565E-02 0.37570246E-02
0001100 0.37568421E-02 0.37567150E-02 0.37566507E-02 0.37566544E-02 0.37567304E-02
0001200 0.37568852E-02 0.37571196E-02 0.37574410E-02 0.37578440E-02 0.37583339E-02
0001300 0.37589094E-02 0.37595665E-02 0.37603036E-02 0.37611125E-02 0.37619872E-02
0001400 0.37629174E-02 0.37638955E-02 0.37649060E-02 0.37659386E-02 0.37669726E-02
0001500 0.37679938E-02 0.37689814E-02 0.37699144E-02 0.37707724E-02 0.37715307E-02
0001600 0.37721631E-02 0.37726439E-02 0.37729493E-02 0.37730485E-02 0.37729135E-02
0001700 0.37725167E-02 0.37718283E-02 0.37708231E-02 0.37694699E-02 0.37677430E-02
0001800 0.37656180E-02 0.37630699E-02 0.37600761E-02 0.37566172E-02 0.37526758E-02
0001900 0.37482360E-02 0.37432900E-02 0.37378266E-02 0.37318433E-02 0.37253422E-02
0002000 0.37183282E-02 0.37108124E-02 0.37028079E-02 0.36943390E-02 0.36854323E-02
0002100 0.36761204E-02 0.36664433E-02 0.36564448E-02 0.36461784E-02 0.36357041E-02
0002200 0.36250856E-02 0.36143954E-02 0.36037122E-02 0.35931203E-02 0.35827111E-02
0002300 0.35725823E-02 0.35628362E-02 0.35535835E-02 0.35449381E-02 0.35370195E-02
0002400 0.35299510E-02 0.35238620E-02 0.35188855E-02 0.35151597E-02 0.35128233E-02
0002500 0.35120347E-02 0.35128233E-02 0.35151597E-02 0.35188855E-02 0.35238620E-02
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.11567807E 00-0.11568063E 00-0.11568075E 00-0.11568016E 00-0.11568063E 00
0000200-0.11568075E 00-0.11568207E 00-0.11568284E 00-0.11568350E 00-0.11568463E 00
0000300-0.11568540E 00-0.11568719E 00-0.11568832E 00-0.11569041E 00-0.11569154E 00
0000400-0.11569333E 00-0.11569464E 00-0.11569649E 00-0.11569852E 00-0.11570066E 00
0000500-0.11570239E 00-0.11570418E 00-0.11570603E 00-0.11570847E 00-0.11570978E 00
0000600-0.11571115E 00-0.11571360E 00-0.11571479E 00-0.11571687E 00-0.11571860E 00
0000700-0.11572027E 00-0.11572158E 00-0.11572301E 00-0.11572438E 00-0.11572558E 00
0000800-0.11572629E 00-0.11572707E 00-0.11572796E 00-0.11572862E 00-0.11572844E 00
0000900-0.11572826E 00-0.11572874E 00-0.11572754E 00-0.11572760E 00-0.11572719E 00
0001000-0.11572599E 00-0.11572444E 00-0.11572331E 00-0.11572140E 00-0.11572033E 00
0001100-0.11571848E 00-0.11571604E 00-0.11571532E 00-0.11571348E 00-0.11571109E 00
0001200-0.11570925E 00-0.11570823E 00-0.11570686E 00-0.11570579E 00-0.11570483E 00
0001300-0.11570400E 00-0.11570466E 00-0.11570531E 00-0.11570609E 00-0.11570817E 00
0001400-0.11571068E 00-0.11571330E 00-0.11571717E 00-0.11572224E 00-0.11572748E 00
0001500-0.11573380E 00-0.11574078E 00-0.11574852E 00-0.11575681E 00-0.11576593E 00
0001600-0.11577427E 00-0.11578351E 00-0.11579299E 00-0.11580193E 00-0.11581022E 00
0001700-0.11581826E 00-0.11582494E 00-0.11582989E 00-0.11583263E 00-0.11583346E 00
0001800-0.11583108E 00-0.11582452E 00-0.11581409E 00-0.11579812E 00-0.11577630E 00
0001900-0.11574811E 00-0.11571205E 00-0.11566734E 00-0.11561280E 00-0.11554754E 00
0002000-0.11547101E 00-0.11538142E 00-0.11527783E 00-0.11515880E 00-0.11502355E 00
0002100-0.11487067E 00-0.11469883E 00-0.11450720E 00-0.11429423E 00-0.11405873E 00
0002200-0.11380011E 00-0.11351675E 00-0.11320817E 00-0.11287320E 00-0.11251074E 00
0002300-0.11212087E 00-0.11170298E 00-0.11125547E 00-0.11077946E 00-0.11027473E 00
0002400-0.10974115E 00-0.10917920E 00-0.10858876E 00-0.10801387E 00-0.10723960E 00
0002500-0.10711581E 00-0.10723960E 00-0.10801387E 00-0.10858876E 00-0.10917920E 00
EOF
```

```
q
redit pote4
LOADING POTL4
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.40802285E-02 0.40799230E-02 0.40797889E-02 0.40798485E-02 0.40801056E-02
0000200 0.40805675E-02 0.40812194E-02 0.40820315E-02 0.40829591E-02 0.40839687E-02
0000300 0.40849820E-02 0.40859357E-02 0.40867701E-02 0.40874295E-02 0.40878318E-02
0000400 0.40879399E-02 0.40877163E-02 0.40871538E-02 0.40862523E-02 0.40850453E-02
0000500 0.40835775E-02 0.40819459E-02 0.40802397E-02 0.40785670E-02 0.40770881E-02
0000600 0.40759146E-02 0.40752031E-02 0.40750690E-02 0.40756389E-02 0.40769912E-02
0000700 0.40791593E-02 0.40821694E-02 0.40859357E-02 0.40903576E-02 0.40952452E-02
0000800 0.41003413E-02 0.41053221E-02 0.41097999E-02 0.41133277E-02 0.41154176E-02
0000900 0.41155256E-02 0.41131116E-02 0.41076504E-02 0.40985905E-02 0.40855184E-02
0001000 0.40680319E-02 0.40458739E-02 0.40189214E-02 0.39872117E-02 0.39509907E-02
0001100 0.39107054E-02 0.38670227E-02 0.38208587E-02 0.37733638E-02 0.37259227E-02
0001200 0.36801444E-02 0.36378473E-02 0.36010379E-02 0.35718849E-02 0.35526517E-02
0001300 0.35460249E-02 0.35526517E-02 0.35718849E-02 0.36010379E-02 0.36378473E-02
EOF
q
redit pote5
LOADING POTL5
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.12224805E 00-0.12224662E 00-0.12224376E 00-0.12224013E 00-0.12223750E 00
0000200-0.12223548E 00-0.12223321E 00-0.12223154E 00-0.12223053E 00-0.12223011E 00
0000300-0.12222993E 00-0.12223136E 00-0.12223291E 00-0.12223554E 00-0.12223923E 00
0000400-0.12224311E 00-0.12224782E 00-0.12225205E 00-0.12225670E 00-0.12226003E 00
0000500-0.12226290E 00-0.12226534E 00-0.12226605E 00-0.12226552E 00-0.12226439E 00
0000600-0.12226111E 00-0.12225854E 00-0.12225461E 00-0.12225223E 00-0.12225145E 00
0000700-0.12225211E 00-0.12225711E 00-0.12226701E 00-0.12228251E 00-0.12230480E 00
0000800-0.12233365E 00-0.12236989E 00-0.12241256E 00-0.12246013E 00-0.12250972E 00
0000900-0.12255728E 00-0.12259728E 00-0.12262291E 00-0.12262422E 00-0.12259024E 00
0001000-0.12250721E 00-0.12235945E 00-0.12212837E 00-0.12179542E 00-0.12133831E 00
0001100-0.12073499E 00-0.11990228E 00-0.11899793E 00-0.11781996E 00-0.11640930E 00
0001200-0.11475044E 00-0.11283219E 00-0.11064398E 00-0.10836053E 00-0.10512543E 00
0001300-0.10454768E 00-0.10512543E 00-0.10836053E 00-0.11064398E 00-0.11283219E 00
...
q
```

NA+ NL a=0.5 DENS.

VEFF

```
redit pote6
LOADING POTE6
REKEYED
EDIT
p99
```

NA NL a=0.75
DENS.

```
        TOP RECORD
0000100 0.37539406E-02 0.37539476E-02 0.37540162E-02 0.37541431E-02 0.37543359E-02
0000200 0.37545916E-02 0.37549103E-02 0.37552898E-02 0.37557303E-02 0.37562230E-02
0000300 0.37567685E-02 0.37573602E-02 0.37579893E-02 0.37586517E-02 0.37593390E-02
0000400 0.37600431E-02 0.37607553E-02 0.37614664E-02 0.37621621E-02 0.37628391E-02
0000500 0.37634831E-02 0.37640836E-02 0.37646326E-02 0.37651197E-02 0.37655334E-02
0000600 0.37658685E-02 0.37661144E-02 0.37662669E-02 0.37663174E-02 0.37662629E-02
0000700 0.37661023E-02 0.37658294E-02 0.37654496E-02 0.37649598E-02 0.37643663E-02
0000800 0.37636722E-02 0.37628848E-02 0.37620147E-02 0.37610694E-02 0.37600657E-02
0000900 0.37590147E-02 0.37579320E-02 0.37568356E-02 0.37557457E-02 0.37546768E-02
0001000 0.37536547E-02 0.37526994E-02 0.37518304E-02 0.37510714E-02 0.37504407E-02
0001100 0.37499627E-02 0.37496560E-02 0.37495412E-02 0.37496365E-02 0.37499564E-02
0001200 0.37505140E-02 0.37513243E-02 0.37523904E-02 0.37537212E-02 0.37553154E-02
0001300 0.37571713E-02 0.37592833E-02 0.37616375E-02 0.37642210E-02 0.37670124E-02
0001400 0.37699861E-02 0.37731112E-02 0.37763526E-02 0.37796665E-02 0.37830099E-02
0001500 0.37863266E-02 0.37895632E-02 0.37926596E-02 0.37955465E-02 0.37981579E-02
0001600 0.38004154E-02 0.38022466E-02 0.38035703E-02 0.38043025E-02 0.38043596E-02
0001700 0.38036609E-02 0.38021207E-02 0.37996531E-02 0.37961798E-02 0.37916136E-02
0001800 0.37858980E-02 0.37789417E-02 0.37706897E-02 0.37610803E-02 0.37500674E-02
0001900 0.37376059E-02 0.37236658E-02 0.37082271E-02 0.36912796E-02 0.36726289E-02
0002000 0.36528902E-02 0.36315001E-02 0.36087045E-02 0.35845670E-02 0.35591675E-02
0002100 0.35326020E-02 0.35049852E-02 0.34764460E-02 0.34471327E-02 0.34172066E-02
0002200 0.33868530E-02 0.33562628E-02 0.33256509E-02 0.32952419E-02 0.32652770E-02
0002300 0.32360097E-02 0.32077057E-02 0.31806406E-02 0.31551183E-02 0.31314211E-02
0002400 0.31098644E-02 0.30907707E-02 0.30744676E-02 0.30612934E-02 0.30515946E-02
0002500 0.30456539E-02 0.30436618E-02 0.30456539E-02 0.30515946E-02 0.30612934E-02
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.11567819E 00-0.11568576E 00-0.11568695E 00-0.11568719E 00-0.11568743E 00
0000200-0.11568791E 00-0.11568815E 00-0.11568791E 00-0.11568767E 00-0.11568731E 00
0000300-0.11568701E 00-0.11568594E 00-0.11568534E 00-0.11568427E 00-0.11568350E 00
0000400-0.11568320E 00-0.11568254E 00-0.11568224E 00-0.11568260E 00-0.11568242E 00
0000500-0.11568266E 00-0.11568326E 00-0.11568433E 00-0.11568481E 00-0.11568594E 00
0000600-0.11568856E 00-0.11568987E 00-0.11569238E 00-0.11569464E 00-0.11569786E 00
0000700-0.11570013E 00-0.11570400E 00-0.11570740E 00-0.11571050E 00-0.11571401E 00
0000800-0.11571753E 00-0.11572111E 00-0.11572427E 00-0.11572742E 00-0.11573046E 00
0000900-0.11573344E 00-0.11573535E 00-0.11573809E 00-0.11574012E 00-0.11574137E 00
0001000-0.11574227E 00-0.11574334E 00-0.11574334E 00-0.11574328E 00-0.11574262E 00
0001100-0.11574167E 00-0.11574095E 00-0.11573964E 00-0.11573899E 00-0.11573714E 00
0001200-0.11573654E 00-0.11573595E 00-0.11573547E 00-0.11573637E 00-0.11573738E 00
0001300-0.11573958E 00-0.11574310E 00-0.11574781E 00-0.11575437E 00-0.11576176E 00
0001400-0.11577177E 00-0.11578393E 00-0.11579782E 00-0.11581463E 00-0.11583281E 00
0001500-0.11585379E 00-0.11587685E 00-0.11590171E 00-0.11592942E 00-0.11595845E 00
0001600-0.11598867E 00-0.11602074E 00-0.11605304E 00-0.11608499E 00-0.11611652E 00
0001700-0.11614674E 00-0.11617428E 00-0.11619765E 00-0.11621648E 00-0.11622852E 00
0001800-0.11623222E 00-0.11622655E 00-0.11620867E 00-0.11617661E 00-0.11612839E 00
0001900-0.11606127E 00-0.11597264E 00-0.11585945E 00-0.11571884E 00-0.11554813E 00
0002000-0.11534333E 00-0.11510164E 00-0.11481965E 00-0.11449331E 00-0.11411893E 00
0002100-0.11369383E 00-0.11321318E 00-0.11267465E 00-0.11207396E 00-0.11140722E 00
0002200-0.11067188E 00-0.10986471E 00-0.10898280E 00-0.10802364E 00-0.10698438E 00
0002300-0.10586345E 00-0.10465854E 00-0.10336936E 00-0.10199451E 00-0.10053366E 00
0002400-0.98987818E-01-0.97357035E-01-0.95645666E-01-0.93848348E-01-0.92350304E-01
0002500-0.91320038E-01-0.91193199E-01-0.91320038E-01-0.92350304E-01-0.93848348E-01
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.37529357E-02 0.37528623E-02 0.37531224E-02 0.37537219E-02 0.37546572E-02
0000200 0.37558945E-02 0.37573867E-02 0.37590675E-02 0.37608529E-02 0.37626494E-02
0000300 0.37643490E-02 0.37658464E-02 0.37670373E-02 0.37678254E-02 0.37681300E-02
0000400 0.37678960E-02 0.37670902E-02 0.37657171E-02 0.37638184E-02 0.37614689E-02
0000500 0.37587844E-02 0.37559199E-02 0.37530509E-02 0.37503922E-02 0.37481615E-02
0000600 0.37465906E-02 0.37458979E-02 0.37462830E-02 0.37479100E-02 0.37508891E-02
0000700 0.37552665E-02 0.37610093E-02 0.37679907E-02 0.37759873E-02 0.37846682E-02
0000800 0.37935884E-02 0.38022005E-02 0.38098563E-02 0.38158144E-02 0.38192668E-02
0000900 0.38193541E-02 0.38152011E-02 0.38059433E-02 0.37907718E-02 0.37689705E-02
0001000 0.37399668E-02 0.37033677E-02 0.36590023E-02 0.36069686E-02 0.35476563E-02
0001100 0.34817732E-02 0.34103538E-02 0.33347660E-02 0.32566926E-02 0.31781110E-02
0001200 0.31012665E-02 0.30286305E-02 0.29628731E-02 0.29068273E-02 0.28634786E-02
0001300 0.28358577E-02 0.28264986E-02 0.28358577E-02 0.28634786E-02 0.29068273E-02
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.11567724E 00-0.11568445E 00-0.11568797E 00-0.11569011E 00-0.11569101E 00
0000200-0.11569089E 00-0.11568946E 00-0.11568773E 00-0.11568552E 00-0.11568421E 00
0000300-0.11568248E 00-0.11568248E 00-0.11568266E 00-0.11568511E 00-0.11568856E 00
0000400-0.11569315E 00-0.11569959E 00-0.11570597E 00-0.11571312E 00-0.11571974E 00
0000500-0.11572695E 00-0.11573291E 00-0.11573774E 00-0.11574113E 00-0.11574334E 00
0000600-0.11574423E 00-0.11574483E 00-0.11574477E 00-0.11574686E 00-0.11575097E 00
0000700-0.11575902E 00-0.11577314E 00-0.11579478E 00-0.11582524E 00-0.11586767E 00
0000800-0.11592084E 00-0.11598647E 00-0.11606270E 00-0.11614704E 00-0.11623490E 00
0000900-0.11631936E 00-0.11639118E 00-0.11643827E 00-0.11644423E 00-0.11639047E 00
0001000-0.11625451E 00-0.11601013E 00-0.11562890E 00-0.11507845E 00-0.11432582E 00
0001100-0.11333579E 00-0.11207300E 00-0.11050355E 00-0.10859460E 00-0.10631764E 00
0001200-0.10364801E 00-0.10056669E 00-0.97062945E-01-0.93134463E-01-0.88896632E-01
0001300-0.85047245E-01-0.84577203E-01-0.85047245E-01-0.88896632E-01-0.93134463E-01
EOF
q
```

NA NL -a=1.0 DENS.

VEFF

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.37483547E-02 0.37474730E-02 0.37471955E-02 0.37475803E-02 0.37486472E-02
0000200 0.37503813E-02 0.37527275E-02 0.37555879E-02 0.37588351E-02 0.37622962E-02
0000300 0.37657858E-02 0.37690918E-02 0.37719989E-02 0.37742970E-02 0.37757964E-02
0000400 0.37763370E-02 0.37758048E-02 0.37741426E-02 0.37713544E-02 0.37675216E-02
0000500 0.37628005E-02 0.37574212E-02 0.37516837E-02 0.37459552E-02 0.37406415E-02
0000600 0.37361870E-02 0.37330415E-02 0.37316347E-02 0.37323623E-02 0.37355337E-02
0000700 0.37413673E-02 0.37499487E-02 0.37612068E-02 0.37748930E-02 0.37905672E-02
0000800 0.38075803E-02 0.38250787E-02 0.38419978E-02 0.38570957E-02 0.38689554E-02
0000900 0.38760433E-02 0.38767431E-02 0.38694220E-02 0.38524978E-02 0.38245150E-02
0001000 0.37842300E-02 0.37307013E-02 0.36633583E-02 0.35820892E-02 0.34872950E-02
0001100 0.33799284E-02 0.32615042E-02 0.31340891E-02 0.30002573E-02 0.28630137E-02
0001200 0.27257085E-02 0.25919287E-02 0.24653969E-02 0.23498896E-02 0.22491764E-02
0001300 0.21669683E-02 0.21063276E-02 0.20691971E-02 0.20567651E-02 0.20691971E-02
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.11567706E 00-0.11568767E 00-0.11569417E 00-0.11569798E 00-0.11569875E 00
0000200-0.11569625E 00-0.11569166E 00-0.11568546E 00-0.11567754E 00-0.11567038E 00
0000300-0.11566317E 00-0.11565799E 00-0.11565375E 00-0.11565298E 00-0.11565489E 00
0000400-0.11565989E 00-0.11566824E 00-0.11567813E 00-0.11569095E 00-0.11570376E 00
0000500-0.11571789E 00-0.11573166E 00-0.11574388E 00-0.11575460E 00-0.11576223E 00
0000600-0.11576772E 00-0.11577141E 00-0.11577272E 00-0.11577451E 00-0.11577827E 00
0000700-0.11578596E 00-0.11580086E 00-0.11582649E 00-0.11586018E 00-0.11592478E 00
0000800-0.11600375E 00-0.11610681E 00-0.11623406E 00-0.11638373E 00-0.11655188E 00
0000900-0.11673027E 00-0.11690640E 00-0.11706239E 00-0.11717510E 00-0.11721414E 00
0001000-0.11714363E 00-0.11692047E 00-0.11649543E 00-0.11581320E 00-0.11481456E 00
0001100-0.11343592E 00-0.11161327E 00-0.10928237E 00-0.10636255E 00-0.10285819E 00
0001200-0.98661184E-01-0.93753278E-01-0.88106573E-01-0.81712604E-01-0.74539423E-01
0001300-0.67933321E-01-0.63336551E-01-0.60222350E-01-0.59765786E-01-0.60222350E-01
EOF
q
```

NA NL a=2.0

DENS

VEFF

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p99
```

NA NL a=3.0

DENS.

```
        TOP RECORD
0000100 0.37510919E-02 0.37521918E-02 0.37536938E-02 0.37555259E-02 0.37575953E-02
0000200 0.37597795E-02 0.37619537E-02 0.37639861E-02 0.37657435E-02 0.37671006E-02
0000300 0.37679514E-02 0.37682119E-02 0.37678340E-02 0.37667952E-02 0.37651153E-02
0000400 0.37628573E-02 0.37601150E-02 0.37570193E-02 0.37537329E-02 0.37504302E-02
0000500 0.37473063E-02 0.37445584E-02 0.37423645E-02 0.37408876E-02 0.37402580E-02
0000600 0.37405593E-02 0.37418292E-02 0.37440446E-02 0.37471282E-02 0.37509392E-02
0000700 0.37552894E-02 0.37599311E-02 0.37645893E-02 0.37689607E-02 0.37727412E-02
0000800 0.37756290E-02 0.37773584E-02 0.37777086E-02 0.37765279E-02 0.37737507E-02
0000900 0.37694019E-02 0.37636207E-02 0.37566468E-02 0.37488327E-02 0.37406264E-02
0001000 0.37325616E-02 0.37252388E-02 0.37192882E-02 0.37153498E-02 0.37140292E-02
0001100 0.37158602E-02 0.37212628E-02 0.37305071E-02 0.37436632E-02 0.37605865E-02
0001200 0.37808660E-02 0.38038180E-02 0.38284718E-02 0.38535642E-02 0.38775515E-02
0001300 0.38986446E-02 0.39148331E-02 0.39239712E-02 0.39238259E-02 0.39121695E-02
0001400 0.38868915E-02 0.38461136E-02 0.37883068E-02 0.37124060E-02 0.36179344E-02
0001500 0.35050712E-02 0.33747393E-02 0.32286188E-02 0.30691295E-02 0.28993674E-02
0001600 0.27229954E-02 0.25440855E-02 0.23669505E-02 0.21959636E-02 0.20353887E-02
0001700 0.18892530E-02 0.17612458E-02 0.16542068E-02 0.15698771E-02 0.15092127E-02
0001800 0.14726724E-02 0.14605038E-02 0.14726724E-02 0.15092127E-02 0.15698771E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.11567682E 00-0.11566985E 00-0.11566091E 00-0.11565018E 00-0.11564010E 00
0000200-0.11562908E 00-0.11561882E 00-0.11561042E 00-0.11560363E 00-0.11559922E 00
0000300-0.11559701E 00-0.11559725E 00-0.11560023E 00-0.11560535E 00-0.11561334E 00
0000400-0.11562228E 00-0.11563265E 00-0.11564314E 00-0.11565298E 00-0.11566114E 00
0000500-0.11566710E 00-0.11567014E 00-0.11567068E 00-0.11566609E 00-0.11565816E 00
0000600-0.11564600E 00-0.11563057E 00-0.11561209E 00-0.11559081E 00-0.11556882E 00
0000700-0.11554718E 00-0.11552620E 00-0.11550850E 00-0.11549342E 00-0.11548328E 00
0000800-0.11547858E 00-0.11547923E 00-0.11548620E 00-0.11549747E 00-0.11551404E 00
0000900-0.11553323E 00-0.11555570E 00-0.11557877E 00-0.11560179E 00-0.11562347E 00
0001000-0.11564267E 00-0.11565864E 00-0.11567156E 00-0.11568129E 00-0.11568969E 00
0001100-0.11569726E 00-0.11570752E 00-0.11572397E 00-0.11575049E 00-0.11579317E 00
0001200-0.11585671E 00-0.11594552E 00-0.11606622E 00-0.11622125E 00-0.11641127E 00
0001300-0.11663485E 00-0.11688572E 00-0.11715150E 00-0.11741447E 00-0.11764902E 00
0001400-0.11782116E 00-0.11788845E 00-0.11779881E 00-0.11749023E 00-0.11689240E 00
0001500-0.11592692E 00-0.11450863E 00-0.11254817E 00-0.10995424E 00-0.10663607E 00
0001600-0.10251552E 00-0.97512662E-01-0.91568232E-01-0.84637165E-01-0.76699138E-01
0001700-0.67718387E-01-0.59055630E-01-0.52048437E-01-0.46639394E-01-0.42675938E-01
0001800-0.40384483E-01-0.39962791E-01-0.40384483E-01-0.42675938E-01-0.46639394E-01
EOF
q
```

```
redit pote14
LOADING POTE14
KEKEYED
EDIT
p99
        TOP RECORD
0000100 0.37462031E-02 0.37480243E-02 0.37505042E-02 0.37535299E-02 0.37569515E-02
0000200 0.37605935E-02 0.37642536E-02 0.37677260E-02 0.37708106E-02 0.37733116E-02
0000300 0.37750653E-02 0.37759410E-02 0.37758581E-02 0.37747857E-02 0.37727482E-02
0000400 0.37698343E-02 0.37661844E-02 0.37619951E-02 0.37575001E-02 0.37529718E-02
0000500 0.37486933E-02 0.37449528E-02 0.37420273E-02 0.37401502E-02 0.37395135E-02
0000600 0.37402457E-02 0.37424006E-02 0.37459424E-02 0.37507499E-02 0.37566172E-02
0000700 0.37632566E-02 0.37703095E-02 0.37773638E-02 0.37839739E-02 0.37896831E-02
0000800 0.37940561E-02 0.37967006E-02 0.37972974E-02 0.37956261E-02 0.37915909E-02
0000900 0.37852351E-02 0.37767568E-02 0.37665132E-02 0.37550100E-02 0.37428997E-02
0001000 0.37309506E-02 0.37200178E-02 0.37110050E-02 0.37048184E-02 0.37023094E-02
0001100 0.37042252E-02 0.37111451E-02 0.37234304E-02 0.37411726E-02 0.37641369E-02
0001200 0.37917364E-02 0.38229998E-02 0.38565616E-02 0.38906587E-02 0.39231591E-02
0001300 0.39516054E-02 0.39732717E-02 0.39852634E-02 0.39845817E-02 0.39683171E-02
0001400 0.39337501E-02 0.38785418E-02 0.38008669E-02 0.36996186E-02 0.35745173E-02
0001500 0.34262245E-02 0.32563983E-02 0.30676883E-02 0.28636570E-02 0.26486320E-02
0001600 0.24274902E-02 0.22053968E-02 0.19875190E-02 0.17787484E-02 0.15834542E-02
0001700 0.14052771E-02 0.12466568E-02 0.11086834E-02 0.99147297E-03 0.89451927E-03
0001800 0.81698759E-03 0.75793196E-03 0.71647158E-03 0.69189351E-03 0.68375934E-03
EOF
q
redit pote15
LOADING POTE15
KEKEYED
EDIT
p99
        TOP RECORD
0000100-0.11567676E 00-0.11567491E 00-0.11567092E 00-0.11566526E 00-0.11565769E 00
0000200-0.11564928E 00-0.11564213E 00-0.11563641E 00-0.11563283E 00-0.11563247E 00
0000300-0.11563605E 00-0.11564350E 00-0.11565471E 00-0.11567056E 00-0.11568874E 00
0000400-0.11571068E 00-0.11573428E 00-0.11575854E 00-0.11578232E 00-0.11580420E 00
0000500-0.11582327E 00-0.11583900E 00-0.11584884E 00-0.11585367E 00-0.11585188E 00
0000600-0.11584377E 00-0.11582977E 00-0.11581039E 00-0.11578661E 00-0.11576104E 00
0000700-0.11573315E 00-0.11570680E 00-0.11568153E 00-0.11566144E 00-0.11564654E 00
0000800-0.11563772E 00-0.11563653E 00-0.11564177E 00-0.11565381E 00-0.11567110E 00
0000900-0.11569417E 00-0.11571997E 00-0.11574697E 00-0.11577421E 00-0.11579901E 00
0001000-0.11582035E 00-0.11583829E 00-0.11585051E 00-0.11585844E 00-0.11586279E 00
0001100-0.11586529E 00-0.11586940E 00-0.11588001E 00-0.11590272E 00-0.11594546E 00
0001200-0.11601400E 00-0.11611789E 00-0.11626405E 00-0.11645716E 00-0.11670113E 00
0001300-0.11699313E 00-0.11732388E 00-0.11767918E 00-0.11803490E 00-0.11835611E 00
0001400-0.11859721E 00-0.11869997E 00-0.11859441E 00-0.11819744E 00-0.11741376E 00
0001500-0.11613828E 00-0.11425650E 00-0.11164939E 00-0.10819626E 00-0.10377777E 00
0001600-0.98283768E-01-0.91616154E-01-0.83693564E-01-0.74465692E-01-0.63870609E-01
0001700-0.53242851E-01-0.43899115E-01-0.35782546E-01-0.28882999E-01-0.23170188E-01
0001800-0.18607613E-01-0.15146177E-01-0.12762904E-01-0.11243306E-01-0.10931905E-01
EOF
q
```

NA NL a=5.0 DENS.

VEFF

```
redit pote16
LOADING POTE16
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.37391635E-02 0.37396424E-02 0.37411670E-02 0.37436765E-02 0.37470555E-02
0000200 0.37511317E-02 0.37556882E-02 0.37604708E-02 0.37652014E-02 0.37695917E-02
0000300 0.37733591E-02 0.37762532E-02 0.37780530E-02 0.37785952E-02 0.37777857E-02
0000400 0.37756020E-02 0.37721021E-02 0.37674236E-02 0.37617877E-02 0.37554754E-02
0000500 0.37488281E-02 0.37422257E-02 0.37360666E-02 0.37307427E-02 0.37266242E-02
0000600 0.37240260E-02 0.37231960E-02 0.37242912E-02 0.37273597E-02 0.37323390E-02
0000700 0.37390452E-02 0.37471768E-02 0.37563315E-02 0.37660133E-02 0.37756586E-02
0000800 0.37846675E-02 0.37924305E-02 0.37983728E-02 0.38019801E-02 0.38028455E-02
0000900 0.38006974E-02 0.37954245E-02 0.37871122E-02 0.37760364E-02 0.37626836E-02
0001000 0.37477359E-02 0.37320505E-02 0.37166346E-02 0.37025928E-02 0.36910861E-02
0001100 0.36832597E-02 0.36801840E-02 0.36827801E-02 0.36917522E-02 0.37075144E-02
0001200 0.37301336E-02 0.37592705E-02 0.37941474E-02 0.38335123E-02 0.38756316E-02
0001300 0.39182864E-02 0.39588772E-02 0.39943606E-02 0.40214323E-02 0.40366126E-02
0001400 0.40363520E-02 0.40172487E-02 0.39761923E-02 0.39105825E-02 0.38185145E-02
0001500 0.36989953E-02 0.35520715E-02 0.33789431E-02 0.31820126E-02 0.29648261E-02
0001600 0.27319370E-02 0.24886869E-02 0.22408969E-02 0.19945137E-02 0.17552495E-02
0001700 0.15282370E-02 0.13177162E-02 0.11264971E-02 0.95580518E-03 0.80566620E-03
0001800 0.67525893E-03 0.56322664E-03 0.46790554E-03 0.38750446E-03 0.32022758E-03
0001900 0.26435894E-03 0.21831525E-03 0.18067537E-03 0.15019372E-03 0.12560003E-03
0002000 0.10659535E-03 0.91842041E-04 0.80954313E-04 0.73487550E-04 0.69130314E-04
0002100 0.67698260E-04 0.69130314E-04 0.73487550E-04 0.80954313E-04 0.91842041E-04
EOF
q
redit pote17
LOADING POTE17
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.11567712E 00-0.11567378E 00-0.11566490E 00-0.11565107E 00-0.11563486E 00
0000200-0.11561537E 00-0.11559451E 00-0.11557472E 00-0.11555654E 00-0.11554062E 00
0000300-0.11552900E 00-0.11552197E 00-0.11552036E 00-0.11552465E 00-0.11553490E 00
0000400-0.11554956E 00-0.11556941E 00-0.11559266E 00-0.11561793E 00-0.11564380E 00
0000500-0.11566865E 00-0.11569053E 00-0.11570841E 00-0.11571980E 00-0.11572486E 00
0000600-0.11572200E 00-0.11571044E 00-0.11569118E 00-0.11566412E 00-0.11563081E 00
0000700-0.11559391E 00-0.11555403E 00-0.11551470E 00-0.11547768E 00-0.11544639E 00
0000800-0.11542249E 00-0.11540765E 00-0.11540329E 00-0.11540920E 00-0.11542648E 00
0000900-0.11545312E 00-0.11548913E 00-0.11553150E 00-0.11557806E 00-0.11562657E 00
0001000-0.11567450E 00-0.11571872E 00-0.11575794E 00-0.11578953E 00-0.11581409E 00
0001100-0.11583042E 00-0.11583942E 00-0.11584342E 00-0.11584646E 00-0.11585456E 00
0001200-0.11587560E 00-0.11591709E 00-0.11599147E 00-0.11610818E 00-0.11627638E 00
0001300-0.11650521E 00-0.11679798E 00-0.11715198E 00-0.11755866E 00-0.11800116E 00
0001400-0.11844879E 00-0.11886156E 00-0.11918604E 00-0.11935055E 00-0.11927176E 00
0001500-0.11885130E 00-0.11797440E 00-0.11651504E 00-0.11433828E 00-0.11130196E 00
0001600-0.10726142E 00-0.10207659E 00-0.95614254E-01-0.87755799E-01-0.78406513E-01
0001700-0.67461610E-01-0.56212101E-01-0.45925193E-01-0.36493428E-01-0.27858835E-01
0001800-0.19951481E-01-0.12707524E-01-0.60653128E-02 0.33809643E-04 0.56437515E-02
0001900 0.10819249E-01 0.15615024E-01 0.20082589E-01 0.24273127E-01 0.28226096E-01
0002000 0.31951886E-01 0.35408411E-01 0.38474679E-01 0.40943269E-01 0.42578712E-01
0002100 0.43134015E-01 0.42578712E-01 0.40943269E-01 0.38474679E-01 0.35408411E-01
EOF
q
```

NA NL a=100
DENS.

VEFF

```
redit pote18
LOADING PUTE18
REKEYED
EDIT
p99
```

NA NL a=15.0 DENS.

```
        TOP RECORD
0000100 0.37377463E-02 0.37383973E-02 0.37401551E-02 0.37429568E-02 0.37466763E-02
0000200 0.37511319E-02 0.37560931E-02 0.37612962E-02 0.37664492E-02 0.37712483E-02
0000300 0.37754024E-02 0.37786446E-02 0.37807440E-02 0.37815308E-02 0.37809026E-02
0000400 0.37788341E-02 0.37753836E-02 0.37706937E-02 0.37649865E-02 0.37585557E-02
0000500 0.37517552E-02 0.37449775E-02 0.37386352E-02 0.37331376E-02 0.37288694E-02
0000600 0.37261618E-02 0.37252728E-02 0.37263688E-02 0.37295045E-02 0.37346189E-02
0000700 0.37415284E-02 0.37499245E-02 0.37593944E-02 0.37694282E-02 0.37794455E-02
0000800 0.37888288E-02 0.37969470E-02 0.38032045E-02 0.38070614E-02 0.38080961E-02
0000900 0.38060122E-02 0.38006944E-02 0.37922096E-02 0.37808323E-02 0.37670494E-02
0001000 0.37515485E-02 0.37352012E-02 0.37190309E-02 0.37041679E-02 0.36917981E-02
0001100 0.36831028E-02 0.36791842E-02 0.36809952E-02 0.36892770E-02 0.37044750E-02
0001200 0.37266850E-02 0.37555962E-02 0.37904503E-02 0.38300101E-02 0.38725506E-02
0001300 0.39158538E-02 0.39573126E-02 0.39938800E-02 0.40222183E-02 0.40388107E-02
0001400 0.40400773E-02 0.40225647E-02 0.39831027E-02 0.39190315E-02 0.38283879E-02
0001500 0.37100941E-02 0.35641396E-02 0.33916696E-02 0.31950355E-02 0.29777563E-02
0001600 0.27443743E-02 0.25002407E-02 0.22512050E-02 0.20032662E-02 0.17621997E-02
0001700 0.15332084E-02 0.13206033E-02 0.11272610E-02 0.95446012E-03 0.80226478E-03
0001800 0.66988310E-03 0.55597303E-03 0.45887288E-03 0.37678308E-03 0.30788896E-03
0001900 0.25044545E-03 0.20283172E-03 0.16357870E-03 0.13138168E-03 0.10509910E-03
0002000 0.83745210E-04 0.66477558E-04 0.52581629E-04 0.41455947E-04 0.32596188E-04
0002100 0.25581336E-04 0.20061358E-04 0.15746788E-04 0.12399970E-04 0.98282017E-05
0002200 0.78776047E-05 0.64277874E-05 0.53871472E-05 0.46887981E-05 0.42873044E-05
0002300 0.41563499E-05 0.42873044E-05 0.46887981E-05 0.53871472E-05 0.64277874E-05
EOF
q
redit pote19
LOADING PUTE19
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.11567688E 00-0.11567837E 00-0.11567473E 00-0.11566627E 00-0.11565441E 00
0000200-0.11563885E 00-0.11562175E 00-0.11560541E 00-0.11559063E 00-0.11557847E 00
0000300-0.11557025E 00-0.11556673E 00-0.11556906E 00-0.11557704E 00-0.11559153E 00
0000400-0.11561060E 00-0.11563480E 00-0.11566240E 00-0.11569226E 00-0.11572254E 00
0000500-0.11575133E 00-0.11577719E 00-0.11579883E 00-0.11581361E 00-0.11582136E 00
0000600-0.11582059E 00-0.11581099E 00-0.11579287E 00-0.11576656E 00-0.11573333E 00
0000700-0.11569607E 00-0.11565542E 00-0.11561477E 00-0.11557633E 00-0.11554301E 00
0000800-0.11551690E 00-0.11550033E 00-0.11549437E 00-0.11549836E 00-0.11551452E 00
0000900-0.11553985E 00-0.11557454E 00-0.11561626E 00-0.11566198E 00-0.11570960E 00
0001000-0.11575615E 00-0.11579889E 00-0.11583650E 00-0.11586565E 00-0.11588645E 00
0001100-0.11589843E 00-0.11590189E 00-0.11589885E 00-0.11589390E 00-0.11589217E 00
0001200-0.11590242E 00-0.11593252E 00-0.11599386E 00-0.11609769E 00-0.11625266E 00
0001300-0.11646932E 00-0.11675149E 00-0.11709654E 00-0.11749727E 00-0.11793637E 00
0001400-0.11838609E 00-0.11880636E 00-0.11914265E 00-0.11932588E 00-0.11927265E 00
0001500-0.11888438E 00-0.11804748E 00-0.11663496E 00-0.11451197E 00-0.11153501E 00
0001600-0.10756016E 00-0.10244465E 00-0.96055031E-01-0.88269889E-01-0.78993261E-01
0001700-0.68118274E-01-0.56930661E-01-0.46693899E-01-0.37297525E-01-0.28679404E-01
0001800-0.20766739E-01-0.13489299E-01-0.67797750E-02-0.57324371E-03 0.51954277E-02
0001900 0.10593642E-01 0.15691731E-01 0.20565681E-01 0.25301632E-01 0.29991493E-01
0002000 0.34730513E-01 0.39608110E-01 0.44689506E-01 0.49990032E-01 0.55448975E-01
0002100 0.60916591E-01 0.66171169E-01 0.70976138E-01 0.75149894E-01 0.78622341E-01
0002200 0.81431389E-01 0.83666503E-01 0.85403562E-01 0.86668730E-01 0.87448001E-01
0002300 0.87710857E-01 0.87448001E-01 0.86668730E-01 0.85403562E-01 0.83666503E-01
EOF
q
```

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.40820204E-02 0.40819757E-02 0.40819384E-02 0.40819347E-02 0.40819459E-02
0000200 0.40819831E-02 0.40820464E-02 0.40821359E-02 0.40822476E-02 0.40823892E-02
0000300 0.40825494E-02 0.40827319E-02 0.40829480E-02 0.40831752E-02 0.40834211E-02
0000400 0.40836744E-02 0.40839501E-02 0.40842257E-02 0.40845126E-02 0.40847920E-02
0000500 0.40850602E-02 0.40853210E-02 0.40855706E-02 0.40857941E-02 0.40860027E-02
0000600 0.40861741E-02 0.40863231E-02 0.40864199E-02 0.40864795E-02 0.40864982E-02
0000700 0.40864646E-02 0.40863752E-02 0.40862449E-02 0.40860511E-02 0.40858164E-02
0000800 0.40855259E-02 0.40851794E-02 0.40847883E-02 0.40843524E-02 0.40838830E-02
0000900 0.40833689E-02 0.40828362E-02 0.40822700E-02 0.40817000E-02 0.40811226E-02
0001000 0.40805526E-02 0.40799864E-02 0.40794425E-02 0.40789396E-02 0.40784739E-02
0001100 0.40780641E-02 0.40777251E-02 0.40774569E-02 0.40772744E-02 0.40771887E-02
0001200 0.40772073E-02 0.40773265E-02 0.40775724E-02 0.40779412E-02 0.40784329E-02
0001300 0.40790588E-02 0.40798038E-02 0.40806830E-02 0.40816814E-02 0.40828027E-02
0001400 0.40840395E-02 0.40853694E-02 0.40867887E-02 0.40882826E-02 0.40898323E-02
0001500 0.40914156E-02 0.40930063E-02 0.40945895E-02 0.40961355E-02 0.40975958E-02
0001600 0.40989853E-02 0.41002147E-02 0.41012876E-02 0.41021556E-02 0.41027851E-02
0001700 0.41031353E-02 0.41031688E-02 0.41028410E-02 0.41021183E-02 0.41009597E-02
0001800 0.40993467E-02 0.40972121E-02 0.40945485E-02 0.40913187E-02 0.40874854E-02
0001900 0.40830411E-02 0.40779449E-02 0.40721931E-02 0.40657818E-02 0.40586889E-02
0002000 0.40509254E-02 0.40424950E-02 0.40334128E-02 0.40236972E-02 0.40133782E-02
0002100 0.40024891E-02 0.39910823E-02 0.39791949E-02 0.39669126E-02 0.39542913E-02
0002200 0.39414167E-02 0.39283745E-02 0.39152727E-02 0.39022132E-02 0.38893127E-02
0002300 0.38766996E-02 0.38645091E-02 0.38528871E-02 0.38419850E-02 0.38319619E-02
0002400 0.38229839E-02 0.38152244E-02 0.38088651E-02 0.38040923E-02 0.38010918E-02
0002500 0.38000732E-02 0.38010918E-02 0.38040923E-02 0.38088651E-02 0.38152244E-02
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.12224829E 00-0.12224728E 00-0.12224668E 00-0.12224633E 00-0.12224567E 00
0000200-0.12224460E 00-0.12224483E 00-0.12224412E 00-0.12224370E 00-0.12224275E 00
0000300-0.12224203E 00-0.12224197E 00-0.12224090E 00-0.12224108E 00-0.12224054E 00
0000400-0.12224072E 00-0.12224084E 00-0.12223977E 00-0.12224066E 00-0.12224072E 00
0000500-0.12224060E 00-0.12224060E 00-0.12224066E 00-0.12224114E 00-0.12224144E 00
0000600-0.12224144E 00-0.12224209E 00-0.12224185E 00-0.12224239E 00-0.12224239E 00
0000700-0.12224287E 00-0.12224257E 00-0.12224263E 00-0.12224269E 00-0.12224209E 00
0000800-0.12224138E 00-0.12224054E 00-0.12223977E 00-0.12223792E 00-0.12223631E 00
0000900-0.12223417E 00-0.12223214E 00-0.12222964E 00-0.12222719E 00-0.12222463E 00
0001000-0.12222141E 00-0.12221754E 00-0.12221462E 00-0.12221098E 00-0.12220746E 00
0001100-0.12220383E 00-0.12220007E 00-0.12219715E 00-0.12219328E 00-0.12219012E 00
0001200-0.12218714E 00-0.12218517E 00-0.12218338E 00-0.12218249E 00-0.12218201E 00
0001300-0.12218237E 00-0.12218362E 00-0.12218606E 00-0.12218899E 00-0.12219357E 00
0001400-0.12219888E 00-0.12220550E 00-0.12221384E 00-0.12222344E 00-0.12223423E 00
0001500-0.12224627E 00-0.12225956E 00-0.12227446E 00-0.12229025E 00-0.12230760E 00
0001600-0.12232506E 00-0.12234354E 00-0.12236238E 00-0.12238193E 00-0.12240142E 00
0001700-0.12242061E 00-0.12243927E 00-0.12245673E 00-0.12247276E 00-0.12248617E 00
0001800-0.12249744E 00-0.12250501E 00-0.12250811E 00-0.12250644E 00-0.12249863E 00
0001900-0.12248361E 00-0.12246060E 00-0.12242854E 00-0.12238580E 00-0.12233144E 00
0002000-0.12226355E 00-0.12218058E 00-0.12208205E 00-0.12196499E 00-0.12182838E 00
0002100-0.12167042E 00-0.12148935E 00-0.12128365E 00-0.12105107E 00-0.12078983E 00
0002200-0.12049830E 00-0.12017512E 00-0.11981839E 00-0.11942667E 00-0.11899865E 00
0002300-0.11853319E 00-0.11802953E 00-0.11748677E 00-0.11690462E 00-0.11628306E 00
0002400-0.11562246E 00-0.11492401E 00-0.11418766E 00-0.11345834E 00-0.11250538E 00
0002500-0.11233377E 00-0.11250538E 00-0.11345834E 00-0.11418766E 00-0.11492401E 00
EOF
```

NA+ LDA a=0.25 DENS.

VEFF

```
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
```

NA+ LDA a=0.5 DENS.

```
        TOP RECORD
0000100 0.40800162E-02 0.40797293E-02 0.40796399E-02 0.40797852E-02 0.40801503E-02
0000200 0.40807463E-02 0.40815622E-02 0.40825494E-02 0.40836558E-02 0.40848404E-02
0000300 0.40860176E-02 0.40870942E-02 0.40880106E-02 0.40886812E-02 0.40890388E-02
0000400 0.40890165E-02 0.40885843E-02 0.40877201E-02 0.40864311E-02 0.40847622E-02
0000500 0.40827654E-02 0.40805601E-02 0.40782429E-02 0.40759817E-02 0.40739253E-02
0000600 0.40722415E-02 0.40711053E-02 0.40706880E-02 0.40711164E-02 0.40724985E-02
0000700 0.40749088E-02 0.40783547E-02 0.40827841E-02 0.40880814E-02 0.40940270E-02
0000800 0.41003786E-02 0.41067488E-02 0.41127317E-02 0.41178241E-02 0.41214786E-02
0000900 0.41231029E-02 0.41220933E-02 0.41178353E-02 0.41097552E-02 0.40973276E-02
0001000 0.40801167E-02 0.40578172E-02 0.40302500E-02 0.39974451E-02 0.39596111E-02
0001100 0.39172173E-02 0.38709661E-02 0.38218212E-02 0.37710264E-02 0.37200816E-02
0001200 0.36707469E-02 0.36250204E-02 0.35851155E-02 0.35534347E-02 0.35325035E-02
0001300 0.35252762E-02 0.35325035E-02 0.35534347E-02 0.35851155E-02 0.36250204E-02
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.12224787E 00-0.12224483E 00-0.12224245E 00-0.12224054E 00-0.12223935E 00
0000200-0.12223881E 00-0.12223887E 00-0.12223911E 00-0.12224019E 00-0.12224340E 00
0000300-0.12224633E 00-0.12225014E 00-0.12225348E 00-0.12225765E 00-0.12226152E 00
0000400-0.12226433E 00-0.12226653E 00-0.12226701E 00-0.12226546E 00-0.12226146E 00
0000500-0.12225527E 00-0.12224680E 00-0.12223643E 00-0.12222415E 00-0.12221086E 00
0000600-0.12219661E 00-0.12218338E 00-0.12217128E 00-0.12216276E 00-0.12215823E 00
0000700-0.12215942E 00-0.12216830E 00-0.12218553E 00-0.12221229E 00-0.12224966E 00
0000800-0.12229741E 00-0.12235522E 00-0.12242299E 00-0.12249774E 00-0.12257701E 00
0000900-0.12265617E 00-0.12272918E 00-0.12278855E 00-0.12282425E 00-0.12282443E 00
0001000-0.12277490E 00-0.12265885E 00-0.12245530E 00-0.12214321E 00-0.12169760E 00
0001100-0.12109196E 00-0.12029779E 00-0.11928809E 00-0.11803430E 00-0.11651212E 00
0001200-0.11470020E 00-0.11258435E 00-0.11015803E 00-0.10757971E 00-0.10400963E 00
0001300-0.10331386E 00-0.10400963E 00-0.10757971E 00-0.11015803E 00-0.11258435E 00
EOF
q
```

```
redit pote6
LOADING POTE6
REKEYED
EDIT
 99
```

NA+ LDA a=0.75 DENS.

```
        TOP RECORD
0000100 0.40778182E-02 0.40775388E-02 0.40773377E-02 0.40772036E-02 0.40771551E-02
0000200 0.40771775E-02 0.40772930E-02 0.40774941E-02 0.40777810E-02 0.40781647E-02
0000300 0.40786229E-02 0.40791705E-02 0.40798001E-02 0.40805042E-02 0.40812567E-02
0000400 0.40820800E-02 0.40829256E-02 0.40838271E-02 0.40847398E-02 0.40856525E-02
0000500 0.40865503E-02 0.40874407E-02 0.40882789E-02 0.40890686E-02 0.40897839E-02
0000600 0.40904135E-02 0.40909536E-02 0.40913671E-02 0.40916651E-02 0.40918253E-02
0000700 0.40918291E-02 0.40916875E-02 0.40913895E-02 0.40909164E-02 0.40902868E-02
0000800 0.40894970E-02 0.40885396E-02 0.40874369E-02 0.40861890E-02 0.40848032E-02
0000900 0.40833093E-02 0.40817149E-02 0.40800571E-02 0.40783472E-02 0.40765926E-02
0001000 0.40748417E-02 0.40731207E-02 0.40714554E-02 0.40698834E-02 0.40684305E-02
0001100 0.40671341E-02 0.40660389E-02 0.40651485E-02 0.40645041E-02 0.40641576E-02
0001200 0.40641092E-02 0.40643960E-02 0.40650293E-02 0.40660389E-02 0.40674172E-02
0001300 0.40691942E-02 0.40713698E-02 0.40739328E-02 0.40768720E-02 0.40801838E-02
0001400 0.40838346E-02 0.40877983E-02 0.40920414E-02 0.40965192E-02 0.41011833E-02
0001500 0.41059703E-02 0.41108131E-02 0.41156448E-02 0.41203797E-02 0.41249357E-02
0001600 0.41292161E-02 0.41331276E-02 0.41365698E-02 0.41394383E-02 0.41416136E-02
0001700 0.41429885E-02 0.41434541E-02 0.41428842E-02 0.41411817E-02 0.41382313E-02
0001800 0.41339062E-02 0.41281357E-02 0.41208044E-02 0.41118115E-02 0.41011088E-02
0001900 0.40886030E-02 0.40742420E-02 0.40579811E-02 0.40397979E-02 0.40196702E-02
0002000 0.39976165E-02 0.39736442E-02 0.39478093E-02 0.39201640E-02 0.38908080E-02
0002100 0.38598385E-02 0.38273879E-02 0.37936163E-02 0.37586954E-02 0.37228295E-02
0002200 0.36862413E-02 0.36491763E-02 0.36119025E-02 0.35747099E-02 0.35379075E-02
0002300 0.35018208E-02 0.34667973E-02 0.34332012E-02 0.34014070E-02 0.33718115E-02
0002400 0.33448213E-02 0.33208549E-02 0.33003469E-02 0.32837456E-02 0.32715057E-02
0002500 0.32640013E-02 0.32614840E-02 0.32640013E-02 0.32715057E-02 0.32837456E-02
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.12224829E 00-0.12224627E 00-0.12224454E 00-0.12224299E 00-0.12224126E 00
0000200-0.12224102E 00-0.12223923E 00-0.12223816E 00-0.12223762E 00-0.12223691E 00
0000300-0.12223679E 00-0.12223625E 00-0.12223685E 00-0.12223679E 00-0.12223768E 00
0000400-0.12223893E 00-0.12224013E 00-0.12224221E 00-0.12224412E 00-0.12224603E 00
0000500-0.12224817E 00-0.12225085E 00-0.12225443E 00-0.12225699E 00-0.12225991E 00
0000600-0.12226355E 00-0.12226659E 00-0.12226993E 00-0.12227267E 00-0.12227595E 00
0000700-0.12227821E 00-0.12228048E 00-0.12228262E 00-0.12228340E 00-0.12228429E 00
0000800-0.12228364E 00-0.12228328E 00-0.12228084E 00-0.12227863E 00-0.12227499E 00
0000900-0.12227088E 00-0.12226534E 00-0.12225944E 00-0.12225264E 00-0.12224495E 00
0001000-0.12223607E 00-0.12222719E 00-0.12221742E 00-0.12220711E 00-0.12219685E 00
0001100-0.12218601E 00-0.12217575E 00-0.12216562E 00-0.12215608E 00-0.12214661E 00
0001200-0.12213880E 00-0.12213200E 00-0.12212670E 00-0.12212336E 00-0.12212116E 00
0001300-0.12212211E 00-0.12212557E 00-0.12213147E 00-0.12214065E 00-0.12215281E 00
0001400-0.12216860E 00-0.12218827E 00-0.12221175E 00-0.12223923E 00-0.12227023E 00
0001500-0.12230533E 00-0.12234432E 00-0.12238711E 00-0.12243408E 00-0.12248379E 00
0001600-0.12253672E 00-0.12259215E 00-0.12264961E 00-0.12270874E 00-0.12276852E 00
0001700-0.12282866E 00-0.12288654E 00-0.12294233E 00-0.12299424E 00-0.12304080E 00
0001800-0.12308002E 00-0.12310988E 00-0.12312841E 00-0.12313300E 00-0.12312084E 00
0001900-0.12308979E 00-0.12303609E 00-0.12295634E 00-0.12284714E 00-0.12270433E 00
0002000-0.12252378E 00-0.12230182E 00-0.12203282E 00-0.12171274E 00-0.12133694E 00
0002100-0.12089944E 00-0.12039566E 00-0.11982006E 00-0.11916786E 00-0.11843359E 00
0002200-0.11761248E 00-0.11669862E 00-0.11568886E 00-0.11457729E 00-0.11336176E 00
0002300-0.11203802E 00-0.11060292E 00-0.10905522E 00-0.10739368E 00-0.10561782E 00
0002400-0.10372812E 00-0.10172725E 00-0.99617124E-01-0.97402811E-01-0.95543742E-01
0002500-0.94281554E-01-0.94105184E-01-0.94281554E-01-0.95543742E-01-0.97402811E-01
EOF
```

```
q
redit pote8
LOADING POTE8
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.40771998E-02 0.40763244E-02 0.40758289E-02 0.40757693E-02 0.40761791E-02
0000200 0.40770993E-02 0.40784888E-02 0.40802881E-02 0.40824264E-02 0.40847845E-02
0000300 0.40872321E-02 0.40896088E-02 0.40917471E-02 0.40934756E-02 0.40946491E-02
0000400 0.40951222E-02 0.40947907E-02 0.40935911E-02 0.40915161E-02 0.40885992E-02
0000500 0.40849335E-02 0.40806942E-02 0.40760897E-02 0.40713884E-02 0.40669143E-02
0000600 0.40629841E-02 0.40599704E-02 0.40581934E-02 0.40579736E-02 0.40595718E-02
0000700 0.40631704E-02 0.40688552E-02 0.40766038E-02 0.40862635E-02 0.40975064E-02
0000800 0.41098893E-02 0.41227825E-02 0.41354336E-02 0.41469224E-02 0.41562207E-02
0000900 0.41622072E-02 0.41636974E-02 0.41595064E-02 0.41484646E-02 0.41295104E-02
0001000 0.41017160E-02 0.40643848E-02 0.40170774E-02 0.39597042E-02 0.38925498E-02
0001100 0.38163152E-02 0.37321663E-02 0.36417299E-02 0.35470866E-02 0.34507483E-02
0001200 0.33556237E-02 0.32649632E-02 0.31823097E-02 0.31114563E-02 0.30564039E-02
0001300 0.30212260E-02 0.30092793E-02 0.30212260E-02 0.30564039E-02 0.31114563E-02
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.12224823E 00-0.12224078E 00-0.12223393E 00-0.12222832E 00-0.12222332E 00
0000200-0.12222010E 00-0.12221865E 00-0.12221974E 00-0.12222201E 00-0.12222755E 00
0000300-0.12223369E 00-0.12224174E 00-0.12225103E 00-0.12226069E 00-0.12227041E 00
0000400-0.12227863E 00-0.12228549E 00-0.12228906E 00-0.12228984E 00-0.12228554E 00
0000500-0.12227714E 00-0.12226355E 00-0.12224549E 00-0.12222242E 00-0.12219650E 00
0000600-0.12216872E 00-0.12214047E 00-0.12211376E 00-0.12209189E 00-0.12207681E 00
0000700-0.12207144E 00-0.12207896E 00-0.12210226E 00-0.12214321E 00-0.12220496E 00
0000800-0.12228692E 00-0.12239105E 00-0.12251520E 00-0.12265724E 00-0.12281203E 00
0000900-0.12297338E 00-0.12313133E 00-0.12327355E 00-0.12338245E 00-0.12343845E 00
0001000-0.12341523E 00-0.12328345E 00-0.12300706E 00-0.12254602E 00-0.12185478E 00
0001100-0.12086400E 00-0.11956039E 00-0.11788994E 00-0.11575842E 00-0.11313438E 00
0001200-0.10997391E 00-0.10624152E 00-0.10191709E 00-0.96996129E-01-0.91627777E-01
0001300-0.86821139E-01-0.86115003E-01-0.86821139E-01-0.91627777E-01-0.96996129E-01
EOF
q
redit
```

NA+ LDA a=1.0 DENS.

VEFF

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.40733740E-02 0.40707961E-02 0.40688366E-02 0.40676631E-02 0.40673912E-02
0000200 0.40681250E-02 0.40698797E-02 0.40726103E-02 0.40762275E-02 0.40805377E-02
0000300 0.40853284E-02 0.40903091E-02 0.40951632E-02 0.40995590E-02 0.41031539E-02
0000400 0.41056350E-02 0.41067116E-02 0.41061863E-02 0.41039288E-02 0.40998943E-02
0000500 0.40941760E-02 0.40869787E-02 0.40786192E-02 0.40695220E-02 0.40602386E-02
0000600 0.40513612E-02 0.40435791E-02 0.40375665E-02 0.40339939E-02 0.40334761E-02
0000700 0.40364936E-02 0.40434375E-02 0.40544420E-02 0.40694736E-02 0.40881820E-02
0000800 0.41099899E-02 0.41339919E-02 0.41589960E-02 0.41835196E-02 0.42058378E-02
0000900 0.42239651E-02 0.42357817E-02 0.42391047E-02 0.42316839E-02 0.42114407E-02
0001000 0.41764490E-02 0.41251369E-02 0.40564090E-02 0.39697029E-02 0.38651151E-02
0001100 0.37434825E-02 0.36064358E-02 0.34563751E-02 0.32964442E-02 0.31304443E-02
0001200 0.29627115E-02 0.27979708E-02 0.26411796E-02 0.24973785E-02 0.23715994E-02
0001300 0.22687486E-02 0.21928241E-02 0.21463367E-02 0.21307629E-02 0.21463367E-02
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.12224829E 00-0.12222791E 00-0.12220985E 00-0.12219393E 00-0.12218028E 00
0000200-0.12217027E 00-0.12216347E 00-0.12216145E 00-0.12216359E 00-0.12217116E 00
0000300-0.12218142E 00-0.12219733E 00-0.12221509E 00-0.12223631E 00-0.12225848E 00
0000400-0.12227958E 00-0.12229961E 00-0.12231463E 00-0.12232471E 00-0.12232727E 00
0000500-0.12232143E 00-0.12230647E 00-0.12228155E 00-0.12224668E 00-0.12220377E 00
0000600-0.12215340E 00-0.12209964E 00-0.12204432E 00-0.12199295E 00-0.12194949E 00
0000700-0.12191951E 00-0.12190837E 00-0.12192118E 00-0.12196422E 00-0.12204170E 00
0000800-0.12215686E 00-0.12231219E 00-0.12250859E 00-0.12274396E 00-0.12301379E 00
0000900-0.12351057E 00-0.12362126E 00-0.12392914E 00-0.12421018E 00-0.12443417E 00
0001000-0.12456340E 00-0.12455010E 00-0.12433603E 00-0.12386167E 00-0.12304538E 00
0001100-0.12180459E 00-0.12064721E 00-0.11767501E 00-0.11458814E 00-0.11068630E 00
0001200-0.10587746E 00-0.10068049E 00-0.93233168E-01-0.85299075E-01-0.76273263E-01
0001300-0.67657325E-01-0.61915837E-01-0.57957642E-01-0.57262003E-01-0.57957642E-01
EOF
q
```

NA+ LDA a=2.0 DENS.

VEFF

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p 99
        TOP RECORD
0000100 0.40731728E-02 0.40736571E-02 0.40748157E-02 0.40760336E-02 0.40790327E-02
0000200 0.40819012E-02 0.40850788E-02 0.40884092E-02 0.40916689E-02 0.4094671 5E-02
0000300 0.40972084E-02 0.40990934E-02 0.41001886E-02 0.41003376E-02 0.40995032E-02
0000400 0.40976703E-02 0.40948838E-02 0.40912591E-02 0.40869638E-02 0.40822178E-02
0000500 0.40772930E-02 0.40724725E-02 0.40680654E-02 0.40643737E-02 0.40616654E-02
0000600 0.40601678E-02 0.40600523E-02 0.40614232E-02 0.40642768E-02 0.40685385E-02
0000700 0.40740222E-02 0.40804520E-02 0.40874779E-02 0.40946752E-02 0.41015819E-02
0000800 0.41076951E-02 0.41125603E-02 0.41157119E-02 0.41167773E-02 0.41154847E-02
0000900 0.41116811E-02 0.41053068E-02 0.40967017E-02 0.40860139E-02 0.40738098E-02
0001000 0.40607378E-02 0.40475967E-02 0.40352754E-02 0.40247291E-02 0.40169321E-02
0001100 0.40128119E-02 0.40131807E-02 0.40187016E-02 0.40297955E-02 0.40466189E-02
0001200 0.40689781E-02 0.40963143E-02 0.41276887E-02 0.41617304E-02 0.41966567E-02
0001300 0.42303279E-02 0.42602494E-02 0.42836592E-02 0.42976104E-02 0.42991154E-02
0001400 0.42852014E-02 0.42531788E-02 0.42006709E-02 0.41258559E-02 0.40276274E-02
0001500 0.39057059E-02 0.37607497E-02 0.35944623E-02 0.34095633E-02 0.3209746 2E-02
0001600 0.29995556E-02 0.27841998E-02 0.25693076E-02 0.23606729E-02 0.21639946E-02
0001700 0.19846577E-02 0.182 75296E-02 0.16962695E-02 0.15930224E-02 0.15188723E-02
0001800 0.14742685E-02 0.14594207E-02 0.14742685E-02 0.15188723E-02 0.15930224E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p 99
        TOP RECORD
0000100-0.12224787E 00-0.12225175E 00-0.12225592E 00-0.12225974E 00-0.12226427E 00
0000200-0.12226826E 00-0.12227243E 00-0.12227690E 00-0.12228185E 00-0.12228686E 00
0000300-0.12229192E 00-0.12229615E 00-0.12229931E 00-0.12230116E 00-0.1223021 7E 00
0000400-0.12229967E 00-0.12229520E 00-0.1222881 7E 00-0.1222 7839E 00-0.122265 70E 00
0000500-0.12225074E 00-0.1222332 7E 00-0.12221503E 00-0.12219548E 00-0.12217695E 00
0000600-0.12215984E 00-0.12214571E 00-0.12213463E 00-0.12212771E 00-0.12212551E 00
0000700-0.12212992E 00-0.12213868E 00-0.12215388E 00-0.12217319E 00-0.12219673E 00
0000800-0.12222248E 00-0.12224960E 00-0.1222 7625E 00-0.12229884E 00-0.122316 72E 00
0000900-0.12232590E 00-0.12232631E 00-0.12231529E 00-0.122291 74E 00-0.12225503E 00
0001000-0.12220585E 00-0.12214470E 00-0.1220 7651E 00-0.12200189E 00-0.12192893E 00
0001100-0.12186182E 00-0.12180781E 00-0.12177455E 00-0.12176991E 00-0.12180179E 00
0001200-0.12187654E 00-0.12199938E 00-0.12217522E 00-0.12240565E 00-0.12268978E 00
0001300-0.12302470E 00-0.12340260E 00-0.12381071E 00-0.12423146E 00-0.12464088E 00
0001400-0.12500614E 00-0.12528557E 00-0.12542653E 00-0.12536538E 00-0.12502426E 00
0001500-0.12431312E 00-0.12312675E 00-0.12134904E 00-0.11885059E 00-0.11549425E 00
0001600-0.11113715E 00-0.10563916E 00-0.98867536E-01-0.90708256E-01-0.81073046E-01
0001700-0.69922388E-01-0.58983687E-01-0.49983475E-01-0.42943832E-01-0.37950959E-01
0001800-0.34685798E-01-0.34021251E-01-0.34685798E-01-0.37950959E-01-0.42943832E-01
EOF
q
```

NA+ LDA a=3.0 DENS.

VEFF

```
redit pote14
LOADING POTE14
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.40671155E-02 0.40678084E-02 0.40695481E-02 0.40722825E-02 0.40759146E-02
0000200 0.40802583E-02 0.40850788E-02 0.40901229E-02 0.40950887E-02 0.40996708E-02
0000300 0.41035600E-02 0.41064806E-02 0.41082092E-02 0.41085556E-02 0.41074343E-02
0000400 0.41048229E-02 0.41007921E-02 0.40955134E-02 0.40892363E-02 0.40822960E-02
0000500 0.40750764E-02 0.40680058E-02 0.40615350E-02 0.40560924E-02 0.40520914E-02
0000600 0.40498450E-02 0.40496103E-02 0.40515214E-02 0.40555820E-02 0.40616766E-02
0000700 0.40695257E-02 0.40787272E-02 0.40887855E-02 0.40990822E-02 0.41089356E-02
0000800 0.41176714E-02 0.41245818E-02 0.41290708E-02 0.41305684E-02 0.41287318E-02
0000900 0.41233525E-02 0.41144378E-02 0.41022524E-02 0.40872470E-02 0.40701739E-02
0001000 0.40519536E-02 0.40337034E-02 0.40166713E-02 0.40021986E-02 0.39916001E-02
0001100 0.39861426E-02 0.39869249E-02 0.39948113E-02 0.40103495E-02 0.40336610E-02
0001200 0.40644854E-02 0.41019766E-02 0.41447915E-02 0.41910075E-02 0.42382218E-02
0001300 0.42834841E-02 0.43234378E-02 0.43544210E-02 0.43725334E-02 0.43738820E-02
0001400 0.43546744E-02 0.43114908E-02 0.42415000E-02 0.41426346E-02 0.40178550E-02
0001500 0.38552752E-02 0.36683120E-02 0.34557362E-02 0.32216010E-02 0.29711188E-02
0001600 0.27104022E-02 0.24461274E-02 0.21851428E-02 0.19340529E-02 0.16988304E-02
0001700 0.14844632E-02 0.12942369E-02 0.11295399E-02 0.99039217E-03 0.87595941E-03
0001800 0.78496756E-03 0.71601872E-03 0.66781696E-03 0.63933106E-03 0.62991655E-03
EOF
q
redit pote15
LOADING POTE15
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.12224633E 00-0.12225312E 00-0.12225956E 00-0.12226633E 00-0.12227356E 00
0000200-0.12228101E 00-0.12228924E 00-0.12229794E 00-0.12230712E 00-0.12231654E 00
0000300-0.12232590E 00-0.12233442E 00-0.12234080E 00-0.12234682E 00-0.12234861E 00
0000400-0.12234843E 00-0.12234479E 00-0.12233692E 00-0.12232530E 00-0.12230915E 00
0000500-0.12228930E 00-0.12226695E 00-0.12224215E 00-0.12221640E 00-0.12219077E 00
0000600-0.12216693E 00-0.12214619E 00-0.12212926E 00-0.12211794E 00-0.12211442E 00
0000700-0.12211651E 00-0.12212658E 00-0.12214351E 00-0.12216729E 00-0.12219602E 00
0000800-0.12222761E 00-0.12226093E 00-0.12229186E 00-0.12231952E 00-0.12233865E 00
0000900-0.12234896E 00-0.12234646E 00-0.12232953E 00-0.12229711E 00-0.12224871E 00
0001000-0.12218523E 00-0.12210965E 00-0.12202412E 00-0.12193501E 00-0.12184829E 00
0001100-0.12177145E 00-0.12171352E 00-0.12168300E 00-0.12168950E 00-0.12174141E 00
0001200-0.12184620E 00-0.12201166E 00-0.12224138E 00-0.12253845E 00-0.12290221E 00
0001300-0.12332928E 00-0.12381053E 00-0.12433255E 00-0.12487274E 00-0.12540197E 00
0001400-0.12587827E 00-0.12624848E 00-0.12644410E 00-0.12638086E 00-0.12595707E 00
0001500-0.12505269E 00-0.12352926E 00-0.12123060E 00-0.11798543E 00-0.11361146E 00
0001600-0.10791987E 00-0.10072333E 00-0.91845512E-01-0.81130564E-01-0.68453610E-01
0001700-0.55483896E-01-0.43912817E-01-0.33692449E-01-0.24789155E-01-0.17170500E-01
0001800-0.10871768E-01-0.59146918E-02-0.23559078E-02-0.91230564E-04 0.48506330E-03
0001900
EOF
q
```

NA+ LDA a=5.0 DENS.

VEFF

```
redit pote16
LOADING POTE16
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.40637217E-02 0.40624589E-02 0.40624999E-02 0.40639192E-02 0.40666871E-02
0000200 0.40707141E-02 0.40758401E-02 0.40817633E-02 0.40881895E-02 0.40947273E-02
0000300 0.41009896E-02 0.41065551E-02 0.41110553E-02 0.41141324E-02 0.41155294E-02
0000400 0.41150488E-02 0.41126162E-02 0.41082650E-02 0.41021518E-02 0.40945411E-02
0000500 0.40858388E-02 0.40765032E-02 0.40670633E-02 0.40581152E-02 0.40502399E-02
0000600 0.40439889E-02 0.40398575E-02 0.40382333E-02 0.40393621E-02 0.40433668E-02
0000700 0.40501840E-02 0.40595420E-02 0.40710457E-02 0.40840842E-02 0.40979460E-02
0000800 0.41117966E-02 0.41247383E-02 0.41358620E-02 0.41442886E-02 0.41492395E-02
0000900 0.41501001E-02 0.41464493E-02 0.41381009E-02 0.41251704E-02 0.41080713E-02
0001000 0.40875077E-02 0.40644817E-02 0.40402673E-02 0.40163323E-02 0.39942972E-02
0001100 0.39758570E-02 0.39626546E-02 0.39562285E-02 0.39578751E-02 0.39685704E-02
0001200 0.39888695E-02 0.40187798E-02 0.40578172E-02 0.41047931E-02 0.41578822E-02
0001300 0.42146184E-02 0.42719245E-02 0.43261126E-02 0.43730699E-02 0.44083297E-02
0001400 0.44272393E-02 0.44252612E-02 0.43980666E-02 0.43419339E-02 0.42539388E-02
0001500 0.41322522E-02 0.39763898E-02 0.37873478E-02 0.35677094E-02 0.33216355E-02
0001600 0.30546754E-02 0.27735063E-02 0.24855265E-02 0.21983832E-02 0.19194575E-02
0001700 0.16553891E-02 0.14116275E-02 0.11917148E-02 0.99711493E-03 0.82770642E-03
0001800 0.68229227E-03 0.55899913E-03 0.45559183E-03 0.36970852E-03 0.29901322E-03
0001900 0.24130799E-03 0.19459019E-03 0.15708648E-03 0.12726152E-03 0.10381313E-03
0002000 0.85660664E-04 0.71928211E-04 0.61927247E-04 0.55140816E-04 0.51209747E-04
0002100 0.49922673E-04 0.51209747E-04 0.55140816E-04 0.61927247E-04 0.71928211E-04
EOF
q
redit pote17
LOADING POTE17
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.12224811E 00-0.12224740E 00-0.12224710E 00-0.12224633E 00-0.12224776E 00
0000200-0.12224984E 00-0.12225342E 00-0.12225968E 00-0.12226802E 00-0.12227815E 00
0000300-0.12228972E 00-0.12230235E 00-0.12231511E 00-0.12232655E 00-0.12233728E 00
0000400-0.12234432E 00-0.12234777E 00-0.12234652E 00-0.12233943E 00-0.12232703E 00
0000500-0.12230825E 00-0.12228411E 00-0.12225503E 00-0.12222195E 00-0.12218732E 00
0000600-0.12215251E 00-0.12211967E 00-0.12209058E 00-0.12206757E 00-0.12205237E 00
0000700-0.12204760E 00-0.12205261E 00-0.12206906E 00-0.12209618E 00-0.12213480E 00
0000800-0.12218261E 00-0.12223732E 00-0.12229693E 00-0.12235665E 00-0.12241423E 00
0000900-0.12246293E 00-0.12250042E 00-0.12252116E 00-0.12252039E 00-0.12249494E 00
0001000-0.12244266E 00-0.12236243E 00-0.12225568E 00-0.12212515E 00-0.12197739E 00
0001100-0.12181932E 00-0.12166178E 00-0.12151575E 00-0.12139434E 00-0.12131160E 00
0001200-0.12128079E 00-0.12131464E 00-0.12142462E 00-0.12162054E 00-0.12190902E 00
0001300-0.12229389E 00-0.12277550E 00-0.12334704E 00-0.12399691E 00-0.12470382E 00
0001400-0.12543577E 00-0.12614906E 00-0.12678438E 00-0.12726724E 00-0.12750429E 00
0001500-0.12738431E 00-0.12677693E 00-0.12553561E 00-0.12349671E 00-0.12048560E 00
0001600-0.11631906E 00-0.11081231E 00-0.10378301E 00-0.95059574E-01-0.84486485E-01
0001700-0.71931660E-01-0.58889586E-01-0.46864450E-01-0.35768762E-01-0.25517676E-01
0001800-0.16033281E-01-0.72459951E-02 0.90476684E-03 0.84703900E-02 0.15492946E-01
0001900 0.22004411E-01 0.28026864E-01 0.33571079E-01 0.38635444E-01 0.43203782E-01
0002000 0.47243547E-01 0.50704498E-01 0.53519782E-01 0.55609781E-01 0.56911375E-01
0002100 0.57336688E-01 0.56911375E-01 0.55609781E-01 0.53519782E-01 0.50704498E-01
EOF
q
```

NA+ LDA a=10.0 DENS.

VEFF

```
redit pote18
LOADING POTE18
REKEYED
EDIT
p 99
        TOP RECORD
0000100 0.40614419E-02 0.40601976E-02 0.40603094E-02 0.40618442E-02 0.40647872E-02
0000200 0.40690228E-02 0.40743761E-02 0.40805787E-02 0.40872917E-02 0.40941313E-02
0000300 0.41006953E-02 0.41065551E-02 0.41113198E-02 0.41146390E-02 0.41162111E-02
0000400 0.41158609E-02 0.41135028E-02 0.41091666E-02 0.41029938E-02 0.40952675E-02
0000500 0.40863864E-02 0.40768273E-02 0.40671341E-02 0.40579177E-02 0.40497631E-02
0000600 0.40432550E-02 0.40388927E-02 0.40370636E-02 0.40380768E-02 0.40420368E-02
0000700 0.40488765E-02 0.40583536E-02 0.40700547E-02 0.40833876E-02 0.40976144E-02
0000800 0.41118972E-02 0.41253045E-02 0.41369237E-02 0.41458495E-02 0.41512810E-02
0000900 0.41525476E-02 0.41492321E-02 0.41411221E-02 0.41282997E-02 0.41111670E-02
0001000 0.40904172E-02 0.40670596E-02 0.40423572E-02 0.40177926E-02 0.39950162E-02
0001100 0.39757341E-02 0.39616413E-02 0.39543062E-02 0.39550699E-02 0.39649531E-02
0001200 0.39845444E-02 0.40139146E-02 0.40525794E-02 0.40994138E-02 0.41526295E-02
0001300 0.42097457E-02 0.42676702E-02 0.43227635E-02 0.43708533E-02 0.44074580E-02
0001400 0.44278912E-02 0.44275187E-02 0.44019967E-02 0.43474995E-02 0.42610466E-02
0001500 0.41407272E-02 0.39860010E-02 0.37978052E-02 0.35786903E-02 0.33327949E-02
0001600 0.30656713E-02 0.27840126E-02 0.24952460E-02 0.22070555E-02 0.19268729E-02
0001700 0.16613849E-02 0.14160918E-02 0.11945905E-02 0.99838804E-03 0.82741166E-03
0001800 0.68049831E-03 0.55579492E-03 0.45107608E-03 0.36397344E-03 0.29213680E-03
0001900 0.23334283E-03 0.18555333E-03 0.14695176E-03 0.11594915E-03 0.91179172E-04
0002000 0.71483475E-04 0.55891724E-04 0.43599619E-04 0.33946446E-04 0.26393900E-04
0002100 0.20506923E-04 0.15936181E-04 0.12403199E-04 0.96875556E-05 0.76162169E-05
0002200 0.60546390E-05 0.48997153E-05 0.40740651E-05 0.35217035E-05 0.32048147E-05
0002300 0.31015652E-05 0.32048147E-05 0.35217035E-05 0.40740651E-05 0.48997153E-05
EOF
q
redit pote19
LOADING POTE19
REKEYED
EDIT
p 99
        TOP RECORD
0000100-0.12224823E 00-0.12225002E 00-0.12225169E 00-0.12225384E 00-0.12225801E 00
0000200-0.12226152E 00-0.12226731E 00-0.12227595E 00-0.12228638E 00-0.12229943E 00
0000300-0.12231362E 00-0.12232918E 00-0.12234467E 00-0.12235898E 00-0.12237233E 00
0000400-0.12238157E 00-0.12238753E 00-0.12238801E 00-0.12238264E 00-0.12237054E 00
0000500-0.12235260E 00-0.12232792E 00-0.12229776E 00-0.12226349E 00-0.12222713E 00
0000600-0.12219000E 00-0.12215447E 00-0.12212288E 00-0.12209725E 00-0.12208021E 00
0000700-0.12207353E 00-0.12207711E 00-0.12209386E 00-0.12212175E 00-0.12216157E 00
0000800-0.12221241E 00-0.12227160E 00-0.12233657E 00-0.12240273E 00-0.12246758E 00
0000900-0.12252504E 00-0.12257081E 00-0.12260008E 00-0.12260723E 00-0.12258822E 00
0001000-0.12254059E 00-0.12246245E 00-0.12235546E 00-0.12222099E 00-0.12206548E 00
0001100-0.12189585E 00-0.12172335E 00-0.12155980E 00-0.12141943E 00-0.12131578E 00
0001200-0.12126434E 00-0.12127811E 00-0.12137032E 00-0.12155110E 00-0.12182832E 00
0001300-0.12220639E 00-0.12268543E 00-0.12326002E 00-0.12391740E 00-0.12463659E 00
0001400-0.12538546E 00-0.12611926E 00-0.12677842E 00-0.12728703E 00-0.12755144E 00
0001500-0.12745929E 00-0.12687963E 00-0.12566513E 00-0.12365294E 00-0.12066966E 00
0001600-0.11653435E 00-0.11106443E 00-0.10408175E 00-0.95417619E-01-0.84920406E-01
0001700-0.72459459E-01-0.59506170E-01-0.47541015E-01-0.36476344E-01-0.26227191E-01
0001800-0.16714826E-01-0.78678280E-02 0.37739705E-03 0.80770589E-02 0.15280213E-01
0001900 0.22029329E-01 0.28361313E-01 0.34307651E-01 0.39895676E-01 0.45148864E-01
0002000 0.50087489E-01 0.54728951E-01 0.59088297E-01 0.63176990E-01 0.67007184E-01
0002100 0.70586979E-01 0.73920012E-01 0.77008843E-01 0.79849601E-01 0.82431197E-01
0002200 0.84734440E-01 0.86728096E-01 0.88368297E-01 0.89601338E-01 0.90372205E-01
0002300 0.90633214E-01 0.90372205E-01 0.89601338E-01 0.88368297E-01 0.86728096E-01
EOF
q
```

NA+ LDA a=15.0 DENS.

VEFF

```
redit pote2
LOADING POTE2
REKEYED
EDIT
p99
```

NA^+ NL a=0.25 DENS.

```
        TOP RECORD
0000100 0.40813684E-02 0.40813871E-02 0.40814206E-02 0.40814802E-02 0.40815547E-02
0000200 0.40816292E-02 0.40817410E-02 0.40818639E-02 0.40820055E-02 0.40821619E-02
0000300 0.40823482E-02 0.40825419E-02 0.40827543E-02 0.40829740E-02 0.40832125E-02
0000400 0.40834546E-02 0.40837005E-02 0.40839538E-02 0.40842108E-02 0.40844604E-02
0000500 0.40847100E-02 0.40849447E-02 0.40851682E-02 0.40853731E-02 0.40855594E-02
0000600 0.40857196E-02 0.40858574E-02 0.40859617E-02 0.40860362E-02 0.40860772E-02
0000700 0.40860735E-02 0.40860400E-02 0.40859617E-02 0.40858462E-02 0.40856935E-02
0000800 0.40854998E-02 0.40852763E-02 0.40850118E-02 0.40847100E-02 0.40843859E-02
0000900 0.40840358E-02 0.40836632E-02 0.40832832E-02 0.40828884E-02 0.40824898E-02
0001000 0.40821023E-02 0.40817261E-02 0.40813722E-02 0.40810443E-02 0.40807500E-02
0001100 0.40805079E-02 0.40803142E-02 0.40801838E-02 0.40801242E-02 0.40801391E-02
0001200 0.40802248E-02 0.40804073E-02 0.40806755E-02 0.40810443E-02 0.40815063E-02
0001300 0.40820651E-02 0.40827282E-02 0.40834844E-02 0.40843189E-02 0.40852427E-02
0001400 0.40862486E-02 0.40873103E-02 0.40884279E-02 0.40895902E-02 0.40907748E-02
0001500 0.40919669E-02 0.40931404E-02 0.40942729E-02 0.40953569E-02 0.40963478E-02
0001600 0.40972196E-02 0.40979534E-02 0.40985048E-02 0.40988475E-02 0.40989555E-02
0001700 0.40988028E-02 0.40983297E-02 0.40975250E-02 0.40963441E-02 0.40947571E-02
0001800 0.40927343E-02 0.40902458E-02 0.40872619E-02 0.40837601E-02 0.40797181E-02
0001900 0.40751137E-02 0.40699244E-02 0.40641539E-02 0.40577874E-02 0.40508173E-02
0002000 0.40432438E-02 0.40351041E-02 0.40263832E-02 0.40171109E-02 0.40073171E-02
0002100 0.39970390E-02 0.39863214E-02 0.39752088E-02 0.39637685E-02 0.39520524E-02
0002200 0.39401464E-02 0.39281361E-02 0.39161034E-02 0.39041466E-02 0.38923707E-02
0002300 0.38808896E-02 0.38698250E-02 0.38593025E-02 0.38494547E-02 0.38404220E-02
0002400 0.38323486E-02 0.38253840E-02 0.38196892E-02 0.38154209E-02 0.38127413E-02
0002500 0.38118341E-02 0.38127413E-02 0.38154209E-02 0.38196892E-02 0.38253840E-02
EOF
q
redit pote3
LOADING POTE3
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.12225020E 00-0.12226659E 00-0.12226886E 00-0.12226772E 00-0.12226909E 00
0000200-0.12227136E 00-0.12227100E 00-0.12227070E 00-0.12227356E 00-0.12227130E 00
0000300-0.12227142E 00-0.12227273E 00-0.12227231E 00-0.12227130E 00-0.12227052E 00
0000400-0.12227136E 00-0.12227011E 00-0.12226945E 00-0.12226927E 00-0.12226778E 00
0000500-0.12226731E 00-0.12226695E 00-0.12226582E 00-0.12226439E 00-0.12226466E 00
0000600-0.12226522E 00-0.12226349E 00-0.12226254E 00-0.12226361E 00-0.12226409E 00
0000700-0.12226301E 00-0.12226295E 00-0.12226528E 00-0.12226492E 00-0.12226462E 00
0000800-0.12226492E 00-0.12226623E 00-0.12226725E 00-0.12226683E 00-0.12226820E 00
0000900-0.12226921E 00-0.12226874E 00-0.12227041E 00-0.12227148E 00-0.12227166E 00
0001000-0.12227237E 00-0.12227237E 00-0.12227201E 00-0.12227219E 00-0.12227345E 00
0001100-0.12227362E 00-0.12227219E 00-0.12227315E 00-0.12227339E 00-0.12227267E 00
0001200-0.12227184E 00-0.12227136E 00-0.12227255E 00-0.12227219E 00-0.12227315E 00
0001300-0.12227345E 00-0.12227327E 00-0.12227601E 00-0.12227827E 00-0.12227976E 00
0001400-0.12228239E 00-0.12228656E 00-0.12229162E 00-0.12229550E 00-0.12230116E 00
0001500-0.12230915E 00-0.12231451E 00-0.12232220E 00-0.12233096E 00-0.12234080E 00
0001600-0.12235010E 00-0.12235892E 00-0.12236959E 00-0.12237924E 00-0.12238753E 00
0001700-0.12239581E 00-0.12240392E 00-0.12241167E 00-0.12241477E 00-0.12241566E 00
0001800-0.12241530E 00-0.12241071E 00-0.12240118E 00-0.12238771E 00-0.12236708E 00
0001900-0.12233824E 00-0.12230366E 00-0.12226015E 00-0.12220496E 00-0.12214071E 00
0002000-0.12206352E 00-0.12196928E 00-0.12186283E 00-0.12174308E 00-0.12160289E 00
0002100-0.12144220E 00-0.12126344E 00-0.12106287E 00-0.12083912E 00-0.12059200E 00
0002200-0.12031901E 00-0.12001932E 00-0.11969203E 00-0.11933541E 00-0.11895013E 00
0002300-0.11853474E 00-0.11808795E 00-0.11760992E 00-0.11710006E 00-0.11655831E 00
0002400-0.11598456E 00-0.11538088E 00-0.11474478E 00-0.11412376E 00-0.11329126E 00
0002500-0.11315954E 00-0.11329126E 00-0.11412376E 00-0.11474478E 00-0.11538088E 00
EOF
```

```
q
redit pote4
LOADING POTE4
REKEYED
EDIT
p99
```

NA NL a=0.5 DENS.

```
       TOP RECORD
0000100 0.37555236E-02 0.37556163E-02 0.37558787E-02 0.37563127E-02 0.37569085E-02
0000200 0.37576479E-02 0.37584982E-02 0.37594219E-02 0.37603744E-02 0.37613038E-02
0000300 0.37621555E-02 0.37628757E-02 0.37634135E-02 0.37637271E-02 0.37637793E-02
0000400 0.37635486E-02 0.37630303E-02 0.37622359E-02 0.37611930E-02 0.37599513E-02
0000500 0.37585760E-02 0.37571553E-02 0.37557830E-02 0.37545713E-02 0.37536311E-02
0000600 0.37530758E-02 0.37530074E-02 0.37535201E-02 0.37546789E-02 0.37565236E-02
0000700 0.37590521E-02 0.37622259E-02 0.37659539E-02 0.37700930E-02 0.37744436E-02
0000800 0.37787561E-02 0.37827224E-02 0.37859885E-02 0.37881574E-02 0.37888028E-02
0000900 0.37874805E-02 0.37837410E-02 0.37771512E-02 0.37673141E-02 0.37538840E-02
0001000 0.37365986E-02 0.37152919E-02 0.36899259E-02 0.36606016E-02 0.36275811E-02
0001100 0.35912991E-02 0.35523786E-02 0.35116263E-02 0.34700392E-02 0.34287975E-02
0001200 0.33892498E-02 0.33529119E-02 0.33214439E-02 0.32966307E-02 0.32803123E-02
0001300 0.32747008E-02 0.32803123E-02 0.32966307E-02 0.33214439E-02 0.33529119E-02
EOF
q
redit pote5
LOADING POTE5
REKEYED
EDIT
p99
```

VEFF

```
       TOP RECORD
0000100-0.11567718E 00-0.11568040E 00-0.11568141E 00-0.11568248E 00-0.11568362E 00
0000200-0.11568487E 00-0.11568558E 00-0.11568618E 00-0.11568743E 00-0.11568958E 00
0000300-0.11569095E 00-0.11569351E 00-0.11569542E 00-0.11569870E 00-0.11570227E 00
0000400-0.11570561E 00-0.11571044E 00-0.11571401E 00-0.11571813E 00-0.11572105E 00
0000500-0.11572409E 00-0.11572605E 00-0.11572725E 00-0.11572778E 00-0.11572719E 00
0000600-0.11572623E 00-0.11572546E 00-0.11572474E 00-0.11572504E 00-0.11572766E 00
0000700-0.11573249E 00-0.11574078E 00-0.11575335E 00-0.11577141E 00-0.11579555E 00
0000800-0.11582506E 00-0.11585999E 00-0.11589962E 00-0.11594105E 00-0.11598182E 00
0000900-0.11601752E 00-0.11604244E 00-0.11604953E 00-0.11602944E 00-0.11597186E 00
0001000-0.11586440E 00-0.11569273E 00-0.11544102E 00-0.11509287E 00-0.11463052E 00
0001100-0.11403555E 00-0.11328965E 00-0.11237562E 00-0.11127645E 00-0.10997790E 00
0001200-0.10846800E 00-0.10673952E 00-0.10478133E 00-0.10276127E 00-0.99881649E-01
0001300-0.99389076E-01-0.99881649E-01-0.10276127E 00-0.10478133E 00-0.10673952E 00
EOF
q
```

```
redit pote6
LOADING POTE6
REKEYED
EDIT
p99
```

NA^+ NL a=0.75 DENS.

```
        TOP RECORD
0000100+0.407871606-02+0.407846066-02+0.407826766-02+0.407814986-02+0.407807166-02
0000200+0.407807166-02+0.407813126-02+0.407826166-02+0.407845906-02+0.407872356-02
0000300+0.407905886-02+0.407944996-02+0.407991196-02+0.408042596-02+0.408098476-02
0000400+0.408158456-02+0.408222536-02+0.408289586-02+0.408357356-02+0.408425936-02
0000500+0.408494476-02+0.408560416-02+0.408624496-02+0.408684096-02+0.408736856-02
0000600+0.408786916-02+0.408827516-02+0.408859926-02+0.408883776-02+0.408897166-02
0000700+0.408900166-02+0.408891596-02+0.408870736-02+0.408839066-02+0.408794736-02
0000800+0.408738856-02+0.408671056-02+0.408593196-02+0.408506396-02+0.408408796-02
0000900+0.408304466-02+0.408193476-02+0.408077516-02+0.407959156-02+0.407839576-02
0001000+0.407721856-02+0.407607486-02+0.407498706-02+0.407398066-02+0.407310206-02
0001100+0.407234586-02+0.407174676-02+0.407133026-02+0.407113136-02+0.407114256-02
0001200+0.407141456-02+0.407194726-02+0.407276306-02+0.407386206-02+0.407525906-02
0001300+0.407695776-02+0.407896566-02+0.408125366-02+0.408383466-02+0.408668956-02
0001400+0.408975416-02+0.409304726-02+0.409652296-02+0.410014766-02+0.410384666-02
0001500+0.410759456-02+0.411131226-02+0.411494066-02+0.411842396-02+0.412169756-02
0001600+0.412457446-02+0.412709646-02+0.412911556-02+0.413054606-02+0.413129116-02
0001700+0.413126136-02+0.413034116-02+0.412844126-02+0.412546476-02+0.412131166-02
0001800+0.411590566-02+0.410914056-02+0.410093746-02+0.409123306-02+0.407996036-02
0001900+0.406705226-02+0.405246256-02+0.403620666-02+0.401820996-02+0.399844626-02
0002000+0.397706406-02+0.395395616-02+0.392921276-02+0.390290736-02+0.387511666-02
0002100+0.384594766-02+0.381552876-02+0.378400326-02+0.375153226-02+0.371830516-02
0002200+0.368452586-02+0.365041366-02+0.361621056-02+0.358217616-02+0.354855666-02
0002300+0.351573296-02+0.348391856-02+0.345346406-02+0.342470066-02+0.339797446-02
0002400+0.337363906-02+0.335206516-02+0.333363036-02+0.331872316-02+0.330774306-02
0002500+0.330101446-02+0.329875656-02+0.330101446-02+0.330774306-02+0.331872316-02
EOF
q
redit pote7
LOADING POTE7
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.122249606-00-0.122252176-00-0.122252526-00-0.122253186-00-0.122253786-00
0000200-0.122252946-00-0.122251516-00-0.122253246-00-0.122250806-00-0.122249016-00
0000300-0.122249316-00-0.122246926-00-0.122244366-00-0.122241686-00-0.122240136-00
0000400-0.122239356-00-0.122235366-00-0.122232976-00-0.122232026-00-0.122228686-00
0000500-0.122226546-00-0.122225946-00-0.122223446-00-0.122221596-00-0.122221416-00
0000600-0.122220756-00-0.122219386-00-0.122219566-00-0.122220996-00-0.122220466-00
0000700-0.122221536-00-0.122224516-00-0.122225466-00-0.122227436-00-0.122229406-00
0000800-0.122231486-00-0.122234646-00-0.122237156-00-0.122239116-00-0.122242276-00
0000900-0.122245616-00-0.122247826-00-0.122251636-00-0.122253956-00-0.122255036-00
0001000-0.122256936-00-0.122261176-00-0.122263076-00-0.122263376-00-0.122265226-00
0001100-0.122266176-00-0.122268626-00-0.122270646-00-0.122268926-00-0.122269396-00
0001200-0.122272736-00-0.122273506-00-0.122274766-00-0.122279056-00-0.122281556-00
0001300-0.122283766-00-0.122288586-00-0.122295626-00-0.122303966-00-0.122311956-00
0001400-0.122321316-00-0.122335316-00-0.122350696-00-0.122367566-00-0.122386996-00
0001500-0.122407736-00-0.122431816-00-0.122457626-00-0.122486776-00-0.122516336-00
0001600-0.122549186-00-0.122582386-00-0.122614206-00-0.122649136-00-0.122683946-00
0001700-0.122715066-00-0.122744086-00-0.122770736-00-0.122791536-00-0.122806496-00
0001800-0.122812516-00-0.122808646-00-0.122792786-00-0.122762566-00-0.122716376-00
0001900-0.122648066-00-0.122558836-00-0.122444276-00-0.122300926-00-0.122127416-00
0002000-0.121914806-00-0.121666136-00-0.121374916-00-0.121033916-00-0.120644876-00
0002100-0.120202306-00-0.119700676-00-0.119137646-00-0.118508226-00-0.117809536-00
0002200-0.117038196-00-0.116190256-00-0.115263466-00-0.114253886-00-0.113159956-00
0002300-0.111978896-00-0.110708366-00-0.109347406-00-0.107895796-00-0.106351856-00
0002400-0.104715946-00-0.102989086-00-0.101175436-00-0.992676626-00-0.976771716-01
0002500-0.965823536-01-0.964505676-01-0.965823536-01-0.976771716-01-0.992676626-01
EOF
```

```
q
redit pote6
LOADING POTE6
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.40780045E-02 0.40772557E-02 0.40768161E-02 0.40767156E-02 0.40769838E-02
0000200 0.40776357E-02 0.40786453E-02 0.40799752E-02 0.40815733E-02 0.40833242E-02
0000300 0.40851496E-02 0.40869378E-02 0.40885359E-02 0.40898398E-02 0.40907376E-02
0000400 0.40911138E-02 0.40909089E-02 0.40900819E-02 0.40886141E-02 0.40865503E-02
0000500 0.40839724E-02 0.40810183E-02 0.40778555E-02 0.40746927E-02 0.40717633E-02
0000600 0.40693767E-02 0.40677562E-02 0.40671527E-02 0.40678196E-02 0.40699281E-02
0000700 0.40735938E-02 0.40788651E-02 0.40856786E-02 0.40938407E-02 0.41030683E-02
0000800 0.41129291E-02 0.41228570E-02 0.41321479E-02 0.41400008E-02 0.41455105E-02
0000900 0.41476786E-02 0.41454919E-02 0.41379035E-02 0.41239150E-02 0.41026548E-02
0001000 0.40733367E-02 0.40354095E-02 0.39885752E-02 0.39328374E-02 0.38665317E-02
0001100 0.37963747E-02 0.37174902E-02 0.36333932E-02 0.35459921E-02 0.34575565E-02
0001200 0.33706774E-02 0.32882402E-02 0.32133623E-02 0.31493697E-02 0.30997626E-02
0001300 0.30681074E-02 0.30573762E-02 0.30681074E-02 0.30997626E-02 0.31493697E-02
EOF
q
redit pote9
LOADING POTE9
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.12224883E 00-0.12225312E 00-0.12225366E 00-0.12225181E 00-0.12224901E 00
0000200-0.12224549E 00-0.12224013E 00-0.12223417E 00-0.12222767E 00-0.12222177E 00
0000300-0.12221497E 00-0.12220955E 00-0.12220514E 00-0.12220299E 00-0.12220281E 00
0000400-0.12220395E 00-0.12220728E 00-0.12221193E 00-0.12221891E 00-0.12222570E 00
0000500-0.12223351E 00-0.12224162E 00-0.12224871E 00-0.12225485E 00-0.12226081E 00
0000600-0.12226450E 00-0.12226844E 00-0.12227082E 00-0.12227440E 00-0.12227929E 00
0000700-0.12228692E 00-0.12229937E 00-0.12231904E 00-0.12234658E 00-0.12238508E 00
0000800-0.12243563E 00-0.12249857E 00-0.12257373E 00-0.12265879E 00-0.12274998E 00
0000900-0.12284094E 00-0.12292302E 00-0.12298375E 00-0.12300682E 00-0.12297273E 00
0001000-0.12285630E 00-0.12263143E 00-0.12226576E 00-0.12172413E 00-0.12096810E 00
0001100-0.11995924E 00-0.11865705E 00-0.11702144E 00-0.11501461E 00-0.11260263E 00
0001200-0.10975659E 00-0.10645366E 00-0.10267925E 00-0.98430276E-01-0.93830407E-01
0001300-0.89649796E-01-0.89134276E-01-0.89649796E-01-0.93830407E-01-0.98430276E-01
EOF
q
```

NA+ NL a=1.0 DENS.

VEFF

```
redit pote10
LOADING POTE10
REKEYED
EDIT
p99
        TOP RECORD
0000100 0.40751398E-02 0.40731318E-02 0.40716045E-02 0.40706806E-02 0.40704645E-02
0000200 0.40710010E-02 0.40723011E-02 0.40743314E-02 0.40770322E-02 0.40802434E-02
0000300 0.40838011E-02 0.40874965E-02 0.40910989E-02 0.40943511E-02 0.40970035E-02
0000400 0.40988252E-02 0.40996149E-02 0.40992387E-02 0.40975846E-02 0.40946640E-02
0000500 0.40905513E-02 0.40854067E-02 0.40794984E-02 0.40731840E-02 0.40668622E-02
0000600 0.40610284E-02 0.40561967E-02 0.40528849E-02 0.40516071E-02 0.40528066E-02
0000700 0.40568374E-02 0.40639341E-02 0.40741563E-02 0.40873699E-02 0.41032284E-02
0000800 0.41211508E-02 0.41402951E-02 0.41595548E-02 0.41776113E-02 0.41929185E-02
0000900 0.42037442E-02 0.42082183E-02 0.42044334E-02 0.41904822E-02 0.41645728E-02
0001000 0.41251145E-02 0.40708408E-02 0.40009096E-02 0.39149895E-02 0.38133252E-02
0001100 0.36968307E-02 0.35671042E-02 0.34264089E-02 0.32776359E-02 0.31242147E-02
0001200 0.29700128E-02 0.28192042E-02 0.26761396E-02 0.25452389E-02 0.24309163E-02
0001300 0.23375058E-02 0.22685677E-02 0.22263508E-02 0.22122145E-02 0.22263508E-02
EOF
q
redit pote11
LOADING POTE11
REKEYED
EDIT
p99
        TOP RECORD
0000100-0.12224889E 00-0.12225777E 00-0.12226254E 00-0.12226295E 00-0.12226057E 00
0000200-0.12225574E 00-0.12224704E 00-0.12223703E 00-0.12222475E 00-0.12221158E 00
0000300-0.12219805E 00-0.12218589E 00-0.12217504E 00-0.12216693E 00-0.12216240E 00
0000400-0.12216157E 00-0.12216461E 00-0.12217075E 00-0.12218106E 00-0.12219334E 00
0000500-0.12220776E 00-0.12222403E 00-0.12224001E 00-0.12225443E 00-0.12226802E 00
0000600-0.12227929E 00-0.12228853E 00-0.12229431E 00-0.12230009E 00-0.12230539E 00
0000700-0.12231266E 00-0.12232548E 00-0.12234706E 00-0.12238014E 00-0.12242985E 00
0000800-0.12249970E 00-0.12259281E 00-0.12271053E 00-0.12285310E 00-0.12301797E 00
0000900-0.12319720E 00-0.12338066E 00-0.12355119E 00-0.12368459E 00-0.12375158E 00
0001000-0.12371439E 00-0.12352693E 00-0.12313616E 00-0.12248218E 00-0.12149912E 00
0001100-0.12011629E 00-0.11826026E 00-0.11585718E 00-0.11283690E 00-0.10913360E 00
0001200-0.10469103E 00-0.99462271E-01-0.93413889E-01-0.86533844E-01-0.78787029E-01
0001300-0.71641743E-01-0.66669703E-01-0.63305736E-01-0.62807858E-01-0.63305736E-01
EOF
q
```

NA+ NL a=2.0 DENS.

VEFF

```
redit pote12
LOADING POTE12
REKEYED
EDIT
p 99
        TOP RECORD
0000100 0.40740520E-02 0.40741935E-02 0.40749051E-02 0.40761493E-02 0.40778965E-02
0000200 0.40800534E-02 0.40824972E-02 0.40851049E-02 0.40877201E-02 0.40901825E-02
0000300 0.40923432E-02 0.40940419E-02 0.40951557E-02 0.40955916E-02 0.40952824E-02
0000400 0.40942132E-02 0.40924139E-02 0.40899515E-02 0.40869489E-02 0.40835775E-02
0000500 0.40800236E-02 0.40765032E-02 0.40732510E-02 0.40704906E-02 0.40684193E-02
0000600 0.40672272E-02 0.40670373E-02 0.40679462E-02 0.40699355E-02 0.40729530E-02
0000700 0.40768981E-02 0.40815435E-02 0.40866211E-02 0.40918440E-02 0.40968470E-02
0000800 0.41012764E-02 0.41047819E-02 0.41070282E-02 0.41077361E-02 0.41067265E-02
0000900 0.41038878E-02 0.40992461E-02 0.40929317E-02 0.40852316E-02 0.40765367E-02
0001000 0.40673651E-02 0.40583573E-02 0.40501989E-02 0.40436424E-02 0.40394217E-02
0001100 0.40382445E-02 0.40407069E-02 0.40472671E-02 0.40581934E-02 0.40734969E-02
0001200 0.40929429E-02 0.41159429E-02 0.41415691E-02 0.41685738E-02 0.41953400E-02
0001300 0.42199381E-02 0.42401403E-02 0.42535327E-02 0.42575411E-02 0.42495281E-02
0001400 0.42269751E-02 0.41875727E-02 0.41293651E-02 0.40509142E-02 0.39514340E-02
0001500 0.38308911E-02 0.36901226E-02 0.35308718E-02 0.33557657E-02 0.31682586E-02
0001600 0.29724955E-02 0.27731471E-02 0.25751870E-02 0.23836815E-02 0.22035772E-02
0001700 0.20395436E-02 0.18958345E-02 0.17757036E-02 0.16811071E-02 0.16130933E-02
0001800 0.15721449E-02 0.15585115E-02 0.15721449E-02 0.16130933E-02 0.16811071E-02
EOF
q
redit pote13
LOADING POTE13
REKEYED
EDIT
p 99
        TOP RECORD
0000100-0.12224901E 00-0.12225366E 00-0.12225282E 00-0.12224841E 00-0.12224376E 00
0000200-0.12223750E 00-0.12222964E 00-0.12222195E 00-0.12221450E 00-0.12220860E 00
0000300-0.12220442E 00-0.12220287E 00-0.12220323E 00-0.12220562E 00-0.12221241E 00
0000400-0.12222177E 00-0.12223172E 00-0.12224436E 00-0.12225688E 00-0.12226981E 00
0000500-0.12228233E 00-0.12229270E 00-0.12230009E 00-0.12230432E 00-0.12230396E 00
0000600-0.12229991E 00-0.12229145E 00-0.12227863E 00-0.12226212E 00-0.12224239E 00
0000700-0.12222081E 00-0.12219781E 00-0.12217546E 00-0.12215513E 00-0.12213814E 00
0000800-0.12212533E 00-0.12211704E 00-0.12211543E 00-0.12211913E 00-0.12212884E 00
0000900-0.12214303E 00-0.12216103E 00-0.12218291E 00-0.12220550E 00-0.12222743E 00
0001000-0.12224960E 00-0.12226820E 00-0.12228453E 00-0.12229621E 00-0.12230682E 00
0001100-0.12231457E 00-0.12232214E 00-0.12233353E 00-0.12235266E 00-0.12238270E 00
0001200-0.12243074E 00-0.12250274E 00-0.12260336E 00-0.12273669E 00-0.12290716E 00
0001300-0.12311238E 00-0.12334812E 00-0.12360495E 00-0.12386543E 00-0.12410396E 00
0001400-0.12428761E 00-0.12437195E 00-0.12430215E 00-0.12401426E 00-0.12343115E 00
0001500-0.12246799E 00-0.12103289E 00-0.11902684E 00-0.11634845E 00-0.11289835E 00
0001600-0.10858196E 00-0.10331535E 00-0.97028315E-01-0.89668393E-01-0.81210554E-01
0001700-0.71613550E-01-0.62349252E-01-0.54864656E-01-0.49093138E-01-0.45081858E-01
0001800-0.42427793E-01-0.41981082E-01-0.42427793E-01-0.45081858E-01-0.49093138E-01
EOF
q
```

NA+ NL a=3.0 DENS.

VFFF

```
redit pote14
LOADING POTE14   NA+ NL a=5.0
REKEYED
EDIT             DENS.
p99
        TOP RECORD
0000100 0.40682591E-02 0.40684119E-02 0.40694438E-02 0.40713176E-02 0.40739477E-02
0000200 0.40772222E-02 0.40809661E-02 0.40849671E-02 0.40890016E-02 0.40928237E-02
0000300 0.40961877E-02 0.40988661E-02 0.41006841E-02 0.41014552E-02 0.41011162E-02
0000400 0.40996149E-02 0.40970147E-02 0.40933937E-02 0.40889643E-02 0.40839501E-02
0000500 0.40786453E-02 0.40733777E-02 0.40684789E-02 0.40642917E-02 0.40611364E-02
0000600 0.40592588E-02 0.40588714E-02 0.40600933E-02 0.40629469E-02 0.40673316E-02
0000700 0.40730760E-02 0.40798783E-02 0.40873587E-02 0.40950626E-02 0.41024685E-02
0000800 0.41090660E-02 0.41143075E-02 0.41177571E-02 0.41189864E-02 0.41177087E-02
0000900 0.41137971E-02 0.41072629E-02 0.40983148E-02 0.40873364E-02 0.40749162E-02
0001000 0.40617883E-02 0.40488541E-02 0.40370971E-02 0.40275864E-02 0.40213540E-02
0001100 0.40193833E-02 0.40225238E-02 0.40314011E-02 0.40463805E-02 0.40674694E-02
0001200 0.40942915E-02 0.41260459E-02 0.41614361E-02 0.41987300E-02 0.42356700E-02
0001300 0.42696297E-02 0.42975880E-02 0.43162517E-02 0.43221787E-02 0.43119118E-02
0001400 0.42821579E-02 0.42299815E-02 0.41529909E-02 0.40495843E-02 0.39190613E-02
0001500 0.37618242E-02 0.35794459E-02 0.33746990E-02 0.31514666E-02 0.29145975E-02
0001600 0.26696578E-02 0.24226170E-02 0.21795095E-02 0.19460823E-02 0.17274937E-02
0001700 0.15280466E-02 0.13506159E-02 0.11964696E-02 0.10657175E-02 0.95774257E-03
0001800 0.87153399E-03 0.80596749E-03 0.75998995E-03 0.73275901E-03 0.72374986E-03
EOF
q
redit pote15
LOADING POTE15
REKEYED
EDIT             VEFF
p99
        TOP RECORD
0000100-0.12224871E 00-0.12225527E 00-0.12225759E 00-0.12225604E 00-0.12225097E 00
0000200-0.12224311E 00-0.12223417E 00-0.12222290E 00-0.12221354E 00-0.12220591E 00
0000300-0.12219971E 00-0.12219745E 00-0.12219864E 00-0.12220353E 00-0.12221301E 00
0000400-0.12222600E 00-0.12224251E 00-0.12226146E 00-0.12228197E 00-0.12230200E 00
0000500-0.12232125E 00-0.12233800E 00-0.12235081E 00-0.12235832E 00-0.12236047E 00
0000600-0.12235612E 00-0.12234479E 00-0.12232685E 00-0.12230313E 00-0.12227446E 00
0000700-0.12224233E 00-0.12220889E 00-0.12217522E 00-0.12214482E 00-0.12211937E 00
0000800-0.12209874E 00-0.12208581E 00-0.12208122E 00-0.12208515E 00-0.12209678E 00
0000900-0.12211639E 00-0.12214184E 00-0.12217158E 00-0.12220353E 00-0.12223697E 00
0001000-0.12226796E 00-0.12229753E 00-0.12232184E 00-0.12234282E 00-0.12235880E 00
0001100-0.12237120E 00-0.12238342E 00-0.12239844E 00-0.12242067E 00-0.12245804E 00
0001200-0.12251765E 00-0.12260723E 00-0.12273520E 00-0.12290961E 00-0.12313348E 00
0001300-0.12340814E 00-0.12372839E 00-0.12408078E 00-0.12444347E 00-0.12478334E 00
0001400-0.12505496E 00-0.12520111E 00-0.12514734E 00-0.12480599E 00-0.12407655E 00
0001500-0.12284344E 00-0.12098259E 00-0.11835963E 00-0.11483830E 00-0.11028337E 00
0001600-0.10456640E 00-0.97572029E-01-0.89204192E-01-0.79398930E-01-0.68084240E-01
0001700-0.56714833E-01-0.46727058E-01-0.38057815E-01-0.30694354E-01-0.24603575E-01
0001800-0.19746728E-01-0.16069520E-01-0.13542585E-01-0.11937432E-01-0.11606116E-01
EOF
q
```

```
redit pote16
LOADING POTE16
REKEYED
EDIT
p99
```

NA+ NL a.=100

DENS.

```
        TOP RECORD
0000100 0.40654689E-02 0.40636472E-02 0.40629283E-02 0.40633939E-02 0.40650517E-02
0000200 0.40678568E-02 0.40716827E-02 0.40763244E-02 0.40815473E-02 0.40870421E-02
0000300 0.40924922E-02 0.40975586E-02 0.41019209E-02 0.41052625E-02 0.41073412E-02
0000400 0.41079707E-02 0.41070506E-02 0.41045584E-02 0.41005798E-02 0.40952973E-02
0000500 0.40889718E-02 0.40819570E-02 0.40746741E-02 0.40675551E-02 0.40610768E-02
0000600 0.40556826E-02 0.40517896E-02 0.40497296E-02 0.40497482E-02 0.40519685E-02
0000700 0.40563866E-02 0.40628463E-02 0.40710680E-02 0.40806159E-02 0.40909685E-02
0000800 0.41014813E-02 0.41114874E-02 0.41202679E-02 0.41271448E-02 0.41315183E-02
0000900 0.41328780E-02 0.41308850E-02 0.41253939E-02 0.41164681E-02 0.41044317E-02
0001000 0.40898100E-02 0.40734112E-02 0.40562153E-02 0.40393993E-02 0.40242374E-02
0001100 0.40120743E-02 0.40042214E-02 0.40018706E-02 0.40060505E-02 0.40174872E-02
0001200 0.40365495E-02 0.40631667E-02 0.40967911E-02 0.41363165E-02 0.41800737E-02
0001300 0.42258091E-02 0.42707361E-02 0.43116026E-02 0.43447241E-02 0.43661669E-02
0001400 0.43718442E-02 0.43577254E-02 0.43201223E-02 0.42557865E-02 0.41622594E-02
0001500 0.40380768E-02 0.38829625E-02 0.36979583E-02 0.34855276E-02 0.32494955E-02
0001600 0.29949055E-02 0.27277707E-02 0.24547218E-02 0.21825891E-02 0.19179704E-02
0001700 0.16668106E-02 0.14340340E-02 0.12226906E-02 0.10347853E-02 0.86972257E-03
0001800 0.72674081E-03 0.60426351E-03 0.50037564E-03 0.41302526E-03 0.34016604E-03
0001900 0.27985475E-03 0.23030570E-03 0.18992336E-03 0.15731504E-03 0.13128993E-03
0002000 0.11085084E-03 0.95182942E-04 0.83640829E-04 0.75736330E-04 0.71127972E-04
0002100 0.69614238E-04 0.71127972E-04 0.75736330E-04 0.83640829E-04 0.95182942E-04
EOF
q
redit pote17
LOADING POTE17
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.12224907E 00-0.12226188E 00-0.12226897E 00-0.12226957E 00-0.12226552E 00
0000200-0.12225646E 00-0.12224334E 00-0.12222731E 00-0.12220937E 00-0.12219203E 00
0000300-0.12217623E 00-0.12216246E 00-0.12215364E 00-0.12214977E 00-0.12215078E 00
0000400-0.12215883E 00-0.12217176E 00-0.12219048E 00-0.12221402E 00-0.12224090E 00
0000500-0.12226880E 00-0.12229764E 00-0.12232465E 00-0.12234724E 00-0.12236434E 00
0000600-0.12237525E 00-0.12237740E 00-0.12237126E 00-0.12235612E 00-0.12233102E 00
0000700-0.12229848E 00-0.12226033E 00-0.12221813E 00-0.12217420E 00-0.12213099E 00
0000800-0.12209284E 00-0.12206167E 00-0.12203938E 00-0.12202644E 00-0.12202549E 00
0000900-0.12203640E 00-0.12205809E 00-0.12208945E 00-0.12212849E 00-0.12217271E 00
0001000-0.12222081E 00-0.12226784E 00-0.12231332E 00-0.12235302E 00-0.12238729E 00
0001100-0.12241328E 00-0.12243176E 00-0.12244356E 00-0.12245178E 00-0.12245929E 00
0001200-0.12247467E 00-0.12250596E 00-0.12256229E 00-0.12265342E 00-0.12279344E 00
0001300-0.12299025E 00-0.12324953E 00-0.12357223E 00-0.12395287E 00-0.12437487E 00
0001400-0.12481111E 00-0.12522173E 00-0.12555140E 00-0.12572908E 00-0.12566757E 00
0001500-0.12526035E 00-0.12438679E 00-0.12291276E 00-0.12069029E 00-0.11756361E 00
0001600-0.11337501E 00-0.10796916E 00-0.10119802E 00-0.92929125E-01-0.83055973E-01
0001700-0.71462095E-01-0.59544444E-01-0.48675366E-01-0.38735561E-01-0.29658854E-01
0001800-0.21369189E-01-0.13793349E-01-0.68649389E-02-0.52191387E-03 0.52960888E-02
0001900 0.10647297E-01 0.15588414E-01 0.20174772E-01 0.24461694E-01 0.28494000E-01
0002000 0.32289207E-01 0.35812672E-01 0.38947422E-01 0.41481234E-01 0.43166488E-01
0002100 0.43740261E-01 0.43166488E-01 0.41481234E-01 0.38947422E-01 0.35812672E-01
EOF
q
```

```
redit pote13
LOADING POTE13
REKEYED
EDIT
p99
```

NA+ NL a=15.0 DENS.

```
        TOP RECORD
0000100 0.40633306E-02 0.40615574E-02 0.40609241E-02 0.40615313E-02 0.40633865E-02
0000200 0.40664412E-02 0.40705353E-02 0.40754750E-02 0.40810071E-02 0.40866260E-02
0000300 0.40925890E-02 0.40979497E-02 0.41025653E-02 0.41061193E-02 0.41083656E-02
0000400 0.41090958E-02 0.41082054E-02 0.41056797E-02 0.41015968E-02 0.40961392E-02
0000500 0.40896013E-02 0.40823296E-02 0.40747523E-02 0.40673278E-02 0.40605478E-02
0000600 0.40548854E-02 0.40507577E-02 0.40485151E-02 0.40484332E-02 0.40506423E-02
0000700 0.40551201E-02 0.40617324E-02 0.40701926E-02 0.40800683E-02 0.40907897E-02
0000800 0.41017495E-02 0.41122101E-02 0.41214526E-02 0.41287802E-02 0.41335411E-02
0000900 0.41352399E-02 0.41334778E-02 0.41281097E-02 0.41191801E-02 0.41069873E-02
0001000 0.40920973E-02 0.40752776E-02 0.40575469E-02 0.40400885E-02 0.40242113E-02
0001100 0.40112808E-02 0.40026382E-02 0.39995462E-02 0.40030479E-02 0.40139072E-02
0001200 0.40325485E-02 0.40589310E-02 0.40925369E-02 0.41322783E-02 0.41765012E-02
0001300 0.42229965E-02 0.42689480E-02 0.43111034E-02 0.43457374E-02 0.43689013E-02
0001400 0.43764450E-02 0.43643005E-02 0.43286942E-02 0.42663217E-02 0.41746236E-02
0001500 0.40520579E-02 0.38982772E-02 0.37142320E-02 0.35023326E-02 0.32663611E-02
0001600 0.30113435E-02 0.27432991E-02 0.24686938E-02 0.21950172E-02 0.19283441E-02
0001700 0.16749077E-02 0.14397227E-02 0.12261206E-02 0.10355737E-02 0.86813699E-03
0001800 0.72288164E-03 0.59825159E-03 0.49233669E-03 0.40307618E-03 0.32840390E-03
0001900 0.26634568E-03 0.21507464E-03 0.17294353E-03 0.13849654E-03 0.11046608E-03
0002000 0.87762441E-04 0.69458736E-04 0.54772740E-04 0.43048640E-04 0.33739227E-04
0002100 0.26389593E-04 0.20622945E-04 0.16128717E-04 0.12652715E-04 0.99893041E-05
0002200 0.79746042E-05 0.64809365E-05 0.54110551E-05 0.46942951E-05 0.42827069E-05
0002300 0.41485382E-05 0.42827069E-05 0.46942951E-05 0.54110551E-05 0.64809365E-05
EOF
q
redit pote19
LOADING POTE19
REKEYED
EDIT
p99
```

VEFF

```
        TOP RECORD
0000100-0.12224871E 00-0.12226868E 00-0.12228000E 00-0.12228417E 00-0.12228352E 00
0000200-0.12227571E 00-0.12226373E 00-0.12224811E 00-0.12223011E 00-0.12221253E 00
0000300-0.12219602E 00-0.12218213E 00-0.12217271E 00-0.12216794E 00-0.12216955E 00
0000400-0.12217790E 00-0.12219137E 00-0.12221193E 00-0.12223619E 00-0.12226456E 00
0000500-0.12229466E 00-0.12232548E 00-0.12235391E 00-0.12237906E 00-0.12239856E 00
0000600-0.12241042E 00-0.12241477E 00-0.12241018E 00-0.12239528E 00-0.12237042E 00
0000700-0.12233925E 00-0.12230027E 00-0.12225705E 00-0.12221247E 00-0.12216896E 00
0000800-0.12213010E 00-0.12209779E 00-0.12207472E 00-0.12206215E 00-0.12206119E 00
0000900-0.12207162E 00-0.12209457E 00-0.12212807E 00-0.12216830E 00-0.12221420E 00
0001000-0.12226421E 00-0.12231266E 00-0.12235975E 00-0.12240088E 00-0.12243617E 00
0001100-0.12246251E 00-0.12247974E 00-0.12248975E 00-0.12249571E 00-0.12249905E 00
0001200-0.12250865E 00-0.12253356E 00-0.12258130E 00-0.12266433E 00-0.12279564E 00
0001300-0.12298352E 00-0.12323439E 00-0.12355095E 00-0.12392789E 00-0.12434816E 00
0001400-0.12478709E 00-0.12520546E 00-0.12554824E 00-0.12574512E 00-0.12570900E 00
0001500-0.12533551E 00-0.12450331E 00-0.12307733E 00-0.12091053E 00-0.11784649E 00
0001600-0.11372662E 00-0.10839361E 00-0.10169899E 00-0.93507707E-01-0.83711386E-01
0001700-0.72190523E-01-0.60339283E-01-0.49525071E-01-0.39625395E-01-0.30570894E-01
0001800-0.22280000E-01-0.14676131E-01-0.76854974E-02-0.12376555E-02 0.47366060E-02
0001900 0.10308988E-01 0.15553381E-01 0.20549547E-01 0.25386829E-01 0.30162655E-01
0002000 0.34980040E-01 0.39938617E-01 0.45115888E-01 0.50541110E-01 0.56162708E-01
0002100 0.61830591E-01 0.67310154E-01 0.72338939E-01 0.76709926E-01 0.80336928E-01
0002200 0.83256245E-01 0.85567653E-01 0.87358236E-01 0.88661075E-01 0.89463651E-01
0002300 0.89734375E-01 0.89463651E-01 0.88661075E-01 0.87358236E-01 0.85567653E-01
EOF
q
```