FINAL REPORT

submitted to

National Aeronautics and Space Administration
Lyndon B. Johnson Space Center
Space Science Branch
ATTN: Eric L. Christiansen
Houston, TX 77058

for research entitled

DESIGN OF ORBITAL DEBRIS SHIELDS FOR OBLIQUE HYPERVELOCITY IMPACT

Submitted by

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Department of Mechanical Engineering
University of Texas
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ABSTRACT

A new impact debris propagation code has been written to link CTH simulations of space debris shield perforation to the Lagrangian finite element code DYNA3D, for space structure wall impact simulations. This software (DC3D) simulates debris cloud evolution using a nonlinear elastic-plastic deformable particle dynamics model, and renders computationally tractable the supercomputer simulation of oblique impacts on Whipple shield protected structures. Comparison of three dimensional, oblique impact simulations with experimental data shows good agreement over a range of velocities of interest in the design of orbital debris shielding.

Source code developed during this research is provided on the enclosed floppy disk. An abstract based on the work described in this report has been submitted to the 1994 Hypervelocity Impact Symposium.
ACKNOWLEDGMENTS

This work was funded under the NASA Regional Universities Grant Program. The assistance of Eric L. Christiansen (NASA Technical Officer) and Jeanne Lee Crews of the Space Science Branch of Johnson Space Center has been greatly appreciated. Additional support was provided by Cray Research, Inc. under the Cray University Research and Development Grant Program.
SOFTWARE COPYRIGHT NOTICE

Source code developed for NASA under this research project has been copyrighted by the principal investigator.
TABLE OF CONTENTS

Abstract ii
Acknowledgments iii
Software Copyright Notice iv

1. Introduction 1
2. Methodology 2
3. Particle Dynamics Model 3
4. Comparison to Experiments 9
5. Conclusion 12

References 13

Table 1. Example Impact Simulations 15
Table 2. Ballistic Limit Simulations 16

List of Figures 17

Appendix A: Example Input File (CTH simulation) A-1
Appendix B: Example Input File (CTH simulation restart) B-1
Appendix C: Example Input File (DC3D) C-1
Appendix D: Example Input File Header (DYNA3D) D-1
Appendix E: Plotting Routine Source Code (DCMPLT) E-1
Appendix F: Post-processor Source Code (DCPOST) F-1
Appendix G: Analysis Source Code (DC3D) G-1
1. Introduction

The design of the space station Freedom and similar structures for earth orbit must include provisions for the effects of hypervelocity impact, which may arise as a result of space debris or micrometeorite encounters. This problem can be expected to become increasingly important as longer duration space missions are launched, increasing the exposure time of orbiting systems. Such missions provide increased probability of impact damage while placing greater reliability demands on vehicles and structures. Existing light gas gun facilities used in the study of hypervelocity impact effects do not generally allow for tests at velocities above ten kilometers per second, suggesting the use of computer simulation methods for orbital debris shield design at those velocities.

The accomplishment of design goals for the space station and similar structures depends in part upon the development and verification of computationally tractable models capable of describing oblique hypervelocity impact effects at velocities beyond existing experimental capabilities. Experience to date has shown that the extreme CPU time and memory requirements of standard Eulerian hydrocodes (McGlaun et al., 1990) make their use in direct simulation of three dimensional impacts on space debris shields impractical, even given supercomputer resources. In addition, current Eulerian hydrocodes do not in general rigorously account for material history effects on the failure of space structures under impact debris loading. Conventional Lagrangian finite element codes (Goudreau and Hallquist, 1982), on the other hand, are not suitable for use in simulating the shield perforation portion of the impact problem. Mesh distortion effects greatly reduce the size of the time step used in the calculations, and mandate frequent rezoning. As a result of the preceding difficulties, the only general simulation technique demonstrated to date has involved the systematic linking of Eulerian hydrocodes (of shield perforation) to Lagrangian finite element models (of debris cloud evolution and debris impact on the protected structure). This approach has been developed and implemented by the principal investigator (Fahrenthold, 1993).
The development of particle-based debris cloud evolution models [e.g. Fritts et al. (1985), Trease et al. (1990), Monaghan (1988), and Trease (1988)], offers an opportunity to directly simulate complete three-dimensional debris impact problems on existing supercomputers. Particle-based methods address the previously discussed shortcomings of Eulerian and Lagrangian codes in two ways: (1) they effectively eliminate the mesh distortion problems of Lagrangian finite element codes, and (2) they greatly improve on the CPU time efficiency of Eulerian hydrocodes while allowing for accurate tracking of material history dependent effects such as plastic deformation. As an application which has severely taxed the capabilities of conventional Eulerian and Lagrangian computer codes, orbital debris shield design is well suited to capitalize on the strengths of new particle-based modeling techniques. Hence the research presented here has: (1) developed a debris cloud evolution code which links shield perforation and wall impact simulations, (2) conducted three dimensional, supercomputer based simulations of shield impact, debris cloud evolution, and wall impact problems, and (3) evaluated and validated the computer models using data from experiments conducted at NASA Johnson Space Center. This computer simulation methodology allows for the modeling of impacts at velocities beyond ten kilometers per second which are very difficult to duplicate in the laboratory.

2. Methodology

The problem of hypervelocity impact on space structures has been an object of research since the 1950's, as reflected in the summary of Hypervelocity Impact Symposia presented during recent conferences in that series (e.g. Anderson, 1986). However both experimental and analytical research work has accelerated in recent years, with most recent NASA interest focused on debris effects on the space shuttle and planned space station. A significant data base exists for impacts at velocities below ten kilometers per second (Tower et al., 1987), including studies aimed specifically at NASA applications such as space shuttle windows (Schneider and Stilp, 1987) and debris shield
design (Yew and Kendrick, 1986). However, difficulties with conducting experiments at higher velocities, relevant to both the space station and future programs, have limited the ability to evaluate new designs in a laboratory setting.

The preceding facts suggest a combined experimental and analytical approach to micrometeorite and debris shield design, using experimental data at velocities below ten kilometers per second to critique and verify computer models, which then provide a basis for higher velocity design calculations. The simulation work described here was conducted on a Cray Y-MP/864 supercomputer at the University of Texas System Center for High Performance Computing.

The principal investigator has made extensive use of existing supercomputer based Eulerian and Lagrangian hydrocodes to evaluate their use in orbital debris shield design. In general, Eulerian codes are best suited to hypervelocity impact simulations where impact pressures are sufficiently large to render material strength effects generally unimportant. An Eulerian code is best used to predict initial debris cloud mass and distribution as a function of projectile material type and velocity, shield material type and geometry, and other parameters. The protected space structure must be designed to avoid spallation or fracture under the debris cloud impact. Since spallation and fracture processes are very stress and strain history dependent phenomena (Yew and Taylor, 1992, and Grady and Kipp, 1987), and since Lagrangian hydrocodes are best suited to trace stress and strain history in solid materials, a Lagrangian hydrocode model of debris cloud impact on the inner wall is most appropriate. The new modeling approach outlined here links both parts of the impact event using a new analysis methodology, significantly reducing computer resource requirements for oblique impact calculations.

3. Particle Dynamics Model

a. Introduction

This section describes a new modeling approach combining Lagrangian bond graphs (Fahrenthold and Wargo, 1994) with a selected finite element discretization
scheme to allow for direct simulation of the dynamic evolution of debris particles arising from hypervelocity impact.

b. Kinematics

The homogeneous deformation field associated with the finite element discretization employed here allows the position $x$ and velocity $v$ of any mass particle "P" in a particular element to be written in the form (Malvern, 1969)

$$x = F(t) \cdot (r - r_c) + c(t) ; \quad v = \dot{F}(t) \cdot (r - r_c) + \dot{c}(t)$$  \hspace{1cm} (1a,b)

where $c(t)$ and $\dot{c}(t)$ are the position and velocity of the element center of mass "C", $r$ and $r_c$ are the position of P and C in the reference (initial undeformed) configuration of the body, and $F$ is the deformation gradient tensor. Note that since $r$ and $r_c$ in equations (1) are constants, the motion of any particle P in the element is determined by the motion of C and by the time dependent components of the second order tensor $\dot{F}$, related to the rate of deformation ($D$) and velocity gradient ($L$) tensors by

$$D = \frac{1}{2} \{ L + L^T \} ; \quad L = \dot{F}F^{-1}$$  \hspace{1cm} (2a,b)

where the superscripts "-1" and "T" denote the inverse and the transpose. In the special case where $L$ is the skew-symmetric tensor whose axial vector is the angular velocity, equation (1b) represents rigid body motion (Casey, 1983, and Fahrenthold and Wargo, 1991a and b).

c. Kinetic energy

The homogeneous deformation kinematics of equations (1) allows the kinetic co-energy ($T^*$) of a single element of fixed mass "m" and variable volume "V" to be expressed in the form

$$T^* = \frac{1}{2} \int_{V} \rho v \cdot v \, dV$$  \hspace{1cm} (3a)

$$= \frac{1}{2} \left[ \int_{V} \rho \dot{v} \cdot \dot{v} \, dV + \int_{V} \rho \dot{F}(r-r_c) \cdot \dot{F}(r-r_c) \, dV + 2c \cdot \dot{F} \int_{V} \rho (r-r_c) \, dV \right]$$  \hspace{1cm} (3b)

$$= \frac{1}{2} \left[ m \dot{c} \cdot \dot{c} + \text{tr} (\dot{F}^T \dot{F} \cdot J) \right]$$  \hspace{1cm} (3c)

where $\rho$ is the density, "tr" is the trace operator, $J$ is an inertia tensor,
\begin{align*}
J &= \int \rho_0 (r-r_c) \otimes (r-r_c) \, dV_0 \quad (3d) \\
\text{and conservation of mass requires} \\
\frac{dm}{dt} &= \rho \, dV = \rho_0 \, dV_0 \quad (3e)
\end{align*}

with \( \rho_0 \) the density in the reference configuration. Note that the third term in equation (3b) is zero by definition of the center of mass. Since \( J \) is a constant tensor defined in the reference configuration, the element momenta \( p \) and \( H \) are defined by
\begin{align*}
p &= \partial T^*/\partial \dot{c} = m \dot{c} \quad ; \quad H = \partial T^*/\partial \dot{F} = \dot{F} J \\
(4a,b)
\end{align*}

Since the kinetic energy \( (T) \) of the finite element is
\begin{align*}
T &= p \cdot \dot{c} + \text{tr}(HF^T) - T^* \\
(5a)
\end{align*}

it follows that
\begin{align*}
T &= (1/2) \left[ m^{-1} p \cdot p + \text{tr} \left( (HJ^{-1})^T H \right) \right] \\
(5b)
\end{align*}

The preceding results demonstrate that kinetic energy storage in a single finite element may be modeled using the bond graph multiports shown in Figure 1. The kinetic energy function may be represented in the most familiar form by the introduction of a fourth order inertia tensor \( G \), defined by
\begin{align*}
G &= \frac{\partial^2 T^*}{\partial F \partial \dot{F}} \\
(6a)
\end{align*}

so that
\begin{align*}
T^* &= (1/2) \left[ m \dot{c} \cdot \dot{c} + F \dot{c} : G : F \right] \quad ; \quad T = (1/2) \left[ m^{-1} p \cdot p + H : G^{-1} : H \right] \\
(6b,c)
\end{align*}

Now the constitutive relation (4b) takes the form
\begin{align*}
H &= G \dot{F} \\
(6d)
\end{align*}

d. Internal energy

The preceding discussion of inertia effects must be augmented by an RC network description of internal energy storage and energy dissipation in the material. Unlike the inertia multiports, the capacitance and resistance multiports required to model a particular material must be formulated for each material type. To illustrate this procedure, this section considers the large strain deformation of an elastic-viscoplastic material (Haupt,
This case emphasizes the applicability of the bond graph modeling methodology described here to very complex engineering materials (Fahrenthold and Wu, 1988), and hence to system dynamics and impact dynamics problems of a very general nature. Note that the conventional assumptions of infinitesimal strain and linear stress-strain behavior, included in the vast majority of mechanical vibrations models, are not adopted here. Since the large strains and the relatively complex material response considered here often calls for special purpose finite element code development work, the example material selected demonstrates the simplicity of the proposed modeling methodology, as compared to conventional displacement-based finite element analysis.

Before formulating a stored energy function for an elastic-plastic material, it is appropriate to first define the system kinematics. A very general description of the large strain kinematics of elastic-plastic deformation is provided by a multiplicative decomposition of the deformation gradient tensor $F$ in the form (Haupt, 1985)

$$F = F^e F^P ; \dot{F} = \dot{F}^e F^P + F^e \dot{F}^P$$

(7a,b)

where $F^e$ describes the elastic deformation of the solid material from the unloaded plastically deformed configuration and $F^P$ relates the unloaded plastically deformed configuration of the material to the original undeformed reference configuration. Hence the rate of change of $F$ may be decomposed as in equation (7b) into a first term governing the rate of elastic energy storage and a second term governing the rate of plastic energy dissipation. In this case, the presence of both complex kinematics and energy dissipation effects highlights the value of bond graphs in nonlinear system modeling.

Since most elastic-plastic modeling work begins with a Helmholtz free energy function and then derives the internal energy, that procedure is followed here. The elastic-plastic kinematics just described are associated with a Helmholtz free energy density function of the form (Dashner, 1986)
\[ \psi = \psi(F^c, F^p, \theta) \quad (7c) \]

Here \( \psi \) is assumed to take the conventional functional form (Bowen, 1989)

\[ \psi = \frac{1}{(\rho \alpha)} \left\{ \frac{(\lambda/2)}{\mu} \text{tr}(E^c) + \mu \text{tr}(E^c^2) - \beta(\theta - \theta_o) \text{tr}(E^c) - \frac{[(c p_o)/(2 \theta_o)](\theta - \theta_o)^2}{1} \right\} \quad (7d) \]

where \( \lambda \) and \( \mu \) are Lame constants for an isotropic solid, \( c \) is the specific heat, \( \theta_o \) is a reference temperature, \( \rho \alpha \) is the density in the unloaded plastically deformed configuration, and

\[ E^c = \frac{1}{(2)} \left[ F^e F^e ^t \right] ; \quad \beta = k \left( 3 \lambda + 2 \mu \right) ; \quad \rho_o/\rho \alpha = \text{det}(F^p) \quad (7e,f,g) \]

with "k" the thermal expansion coefficient and "det" the determinant operator. For an element of mass "m", this corresponds to a (conserved) internal energy function

\[ U = m \psi + \theta S \quad (8a) \]

where \( S \) is the total entropy, defined by the thermodynamic identity

\[ S = - \frac{\partial(m \psi)}{\partial \theta} = (m/\rho \alpha) \left\{ c p_o \left( \frac{(\theta - \theta_o)}{1} \right) + \beta \text{tr}(E^c) \right\} \quad (8b) \]

Equations (7) and (8) may be combined to yield

\[ U = \frac{(m/\rho_o)}{\text{det}(F^p)} \left\{ \mu \text{tr}(E^c^2) + \frac{(\lambda/2)}{\mu} \text{tr}(E^c) + \beta \theta_o \text{tr}(E^c) \right\} + \]

\[ \frac{((c m \theta_o)/2)}{(1 + S/(m c) - (\beta/(c p_o))) \text{det}(F^p) \text{tr}(E^c)} - 1 \quad (8c) \]

The functional form for the internal energy

\[ U = U(F^e, F^p, S) \quad (9a) \]

leads to the multiport capacitor shown in Figure 2, where in this case

\[ K^e = \frac{\partial U}{\partial F^e} |_{F^p, S} = (m/\rho \alpha) \left[ \lambda \left( \beta^2 \frac{\theta_o}{(c p_o)} \right) \text{tr}(E^c) \right] F^e + \]

\[ 2 \mu E^e - \left( \beta \theta_o S \right)/(m c) \right\} I \right \} \quad (9b) \]

\[ K^p = \frac{\partial U}{\partial F^p} |_{F^e, S} = (m/\rho \alpha) \left\{ \left( \frac{(\lambda/2)}{\mu} + \left( \beta^2 \frac{\theta_o}{(c p_o)} \right) \right) \text{tr}(E^c) + \frac{\mu \text{tr}(E^c^2)}{\left( \beta \theta_o S \right)/(m c)} \text{tr}(E^c) \right\} F^p \quad (9c) \]

\[ \theta = \frac{\partial U}{\partial S} |_{F^e, F^p} = \theta_o \left( 1 + S/(m c) - \right) \beta/(c p_o) \text{tr}(E^c) \right\} \quad (9d) \]
e. Plastic deformation

The material description is completed by defining the plastic constitutive relations. For simplicity, the rate form

\[ \dot{K}^d = \eta (m/\rho \alpha) L^p; \quad L^p = F^p F^{-1} \]  

is adopted here, with \( \eta \) a viscosity coefficient. The second order tensor \( K^d \) (dimensionally an extensive chemical potential) is the effort power conjugate to \( L^p \).

A model for the elastic-viscoplastic material just defined is shown in Figure 2. Note that a transformer with fourth order tensor modulus \( M \), defined by components

\[ M_{ijrs} = \delta_{ir} F_{sp} F_{jq} \]  

is introduced in order to conform to the fundamental kinematic relation (10b).

f. Bond graph model

The bond graph structure of Figure 2 may be directly augmented with inertia multiports representing the kinetic energy contributions associated with \( p \) and \( H \). Finally, if the appropriate RC network model representing elastic-viscoplastic materials is introduced, the result is the complete element-level bond graph shown in Figure 3, representing the "ith" element of the system. Assuming adiabatic deformation, thermal energy is stored, as indicated by the thermomechanical coupling shown in Figure 3. Note that in Figure 3 transformers with moduli

\[ M_{ijkl}^e = \delta_{jl} F_{ip}^{-1}; \quad M_{ijkl}^p = \delta_{ik} F_{pq}^{-1} \]  

are introduced in accordance with the kinematics of equations (7a and b).

g. State equation derivation

The causally augmented bond graph of Figure 3 and the constitutive relations previously defined yield (Rosenberg and Karnopp, 1983) state equations for the "ith" element of the form:

\[ \dot{p}^{(i)} = 0 \]  

\[ \dot{H}^{(i)} = \dot{M} p^{(i)} T K e^{(i)} (F e^{(i)}, F p^{(i)}, S^{(i)}) \]
\[ \dot{\mathbf{e}}(i) = \mathbf{M}^{(i)} \mathbf{G}^{(i)-1} \mathbf{H}^{(i)} - \left[ \mathbf{\rho}^{(i)}/(\eta \mathbf{m}^{(i)}) \right] \mathbf{M}^{(i)} \mathbf{M}^{(i)-1} \mathbf{M}^{(i)-1} \mathbf{K}^{d(i)} \]  

(13c)

\[ \dot{\mathbf{F}}^{p(i)} = \left[ \mathbf{\rho}^{(i)}/(\eta \mathbf{m}^{(i)}) \right] \mathbf{M}^{(i)-1} \mathbf{K}^{d(i)} \]  

(13d)

\[ \dot{\mathbf{s}}^{(i)} = \left[ 1/\vartheta^{(i)}(\mathbf{F}^{e(i)}, \mathbf{F}^{p(i)}, \mathbf{S}^{(i)}) \right] \left[ \mathbf{\rho}^{(i)}/(\eta \mathbf{m}^{(i)}) \right] \mathbf{\tau} \left[ \mathbf{K}^{d(i)} \mathbf{T} \mathbf{K}^{d(i)} \right] \]  

(13e)

where

\[ \mathbf{K}^{d(i)} = \mathbf{M}^{(i)-T} \left[ \mathbf{M}^{(i)-T} \mathbf{M}^{(i)} \mathbf{T} \mathbf{K}^{e(i)} \mathbf{F}^{e(i)}, \mathbf{F}^{p(i)}, \mathbf{S}^{(i)} \right] \]  

(13f)

and the functions \( \mathbf{K}^{e(i)} \), \( \mathbf{K}^{p(i)} \), and \( \vartheta^{(i)} \) are defined by equations (9). Note that

\[ M^{(i)-1}_{ijkl} = \delta_{ij} F^{e(i)}_{kl}; \quad M^{(i)-1}_{ijkl} = \delta_{ik} F^{p(i)}_{lj}; \quad M^{(i)-1}_{ijkl} = \delta_{ik} F^{p(i)}_{lj} \]  

(14a,b,c)

Equations (13) are nonlinear equations in the state variables: \( \mathbf{F}^{(i)}, \mathbf{H}^{(i)}, \mathbf{F}^{e(i)}, \mathbf{F}^{p(i)}, \) and \( \mathbf{S}^{(i)} \).

h. Conclusion

The outlined modeling methodology may be implemented numerically, for a variety of internal energy functions and plasticity models, for use in engineering analysis and design. The source code listing at Appendix G represents an isothermal, variable compressibility implementation using the plasticity theory of Green and Naghdi (1971).

4. Comparison to Experiments

a. Introduction

Three dimensional simulation of hypervelocity impacts on space structures places extreme demands on even supercomputer resources. To reduce the computer time and memory requirements of oblique impact simulations, a three-dimensional, deformable particle dynamics model of the type just described has been coded and linked to an Eulerian hydrocode and a Lagrangian structural code, and applied in the simulation of oblique hypervelocity impacts on Whipple shield protected structures. Comparison of the results to experimental data shows good agreement at a computer time and memory cost much less than that associated with conventional hydrocode calculations.
This section describes evaluation of the preceding modeling approach using data from Whipple shield impact experiments conducted at NASA Johnson Space Center, including CPU time requirements for the simulation of representative oblique impact problems.

b. Methodology

The deformable particle dynamics model of debris cloud evolution is referred to here by the title DC3D. This numerical model is used in combination with the Eulerian hydrocode CTH (McGlaun et al., 1990) and the structural finite element code DYNA3D (Goudreau and Hallquist, 1982) as follows. An Eulerian simulation is first employed to model impact on the shield. Then post-processing of the velocity, mass density, and void space distribution data from the Eulerian simulation is used to establish the initial state of the elastic-plastic model of the debris cloud. Numerical integration of the particle dynamics model DC3D, using established system dynamics modeling techniques (Rosenberg and Karnopp, 1983) provides a thermodynamically rigorous yet computationally efficient basis for predictions of debris cloud evolution over the relatively large spaces which normally separate shields from the space structure which they protect. Output from the debris cloud evolution model then provides a basis for the simulation of impact on the wall plate, using DYNA3D. Input data for the wall impact simulation is generated automatically by DC3D, based on the final state of the debris cloud propagation model. By using a momentum deposition representation of the debris cloud loading on the wall plate (calculated from the DC3D results), meshing of each debris particle in DYNA3D can be avoided, yielding additional reductions in computer time and memory requirements.

c. Oblique impact example

The analysis procedure just discussed may be illustrated by considering an oblique impact simulation for a Whipple shield configuration. Specifically, consider the oblique (23 degree) impact of a 15/64 inch diameter aluminum (2017-T4) sphere, at 7.1 kilometers per second, on a 0.063 inch thick aluminum (7075-T6) shield, protecting a
0.125 inch thick aluminum (7075-T6) wall plate. The shield to wall plate spacing is 4.0 inches. Figure 4 shows the CTH simulation results for impact on the shield, at four microseconds after impact. (Note that due to symmetry, all of the figures discussed here depict only one-half of the physical system modeled.) The code DC3D was then employed to: (1) post-processes the CTH results to formulate a debris cloud model, (2) propagate the debris to the wall plate, and (3) generate a DYNA3D input file for use in modeling impact of the debris cloud on the wall plate. DC3D uses a variable step method for numerical integration of the first order state equations describing the elastic-plastic debris cloud dynamics, and commercial plotting routines for graphical representation of the simulation results. Figure 5 shows the predicted impact momentum distribution on the wall plate. Finally a DYNA3D simulation of the wall plate impact was conducted, using a momentum deposition approach to represent the effects of the debris. Figures 6 and 7 show front and rear views of the wall plate impact simulation, including extensive spallation observed in the experiment.

By making appropriate use of Eulerian and Lagrangian codes for those parts of the simulation where they are both accurate and computationally tractable, this approach does not suffer from the limiting assumptions of many previous attempts to model shield impact problems (e.g. Swift et al., 1983). In addition, that portion of the total impact simulation described by the debris cloud model incorporates arbitrarily nonuniform, three-dimensional velocity, density, and void space distributions not admitted by many simplified debris models published to date (Grady and Passman, 1990). In summary, the approach used here makes use of the known strengths of available codes while providing an essential improvement in computational efficiency for oblique impact simulation. Such an improvement is essential before computer codes can provide a practical analytical design tool.

The preceding example demonstrates the feasibility of the modeling approach. Its computational efficiency is such that computer resource requirements are relatively
modest, considering the three dimensional nature of the simulations. Typical CPU time requirements are listed in Table 1.

d. Ballistic limit calculations

Finally it is worthwhile to compare some hypervelocity impact simulation results with ballistic limit calculations based on published experimental research. Figure 8 depicts a typical Ballistic limit curve, and indicates the velocities and impact particle diameters used in the simulations. Figures 9 through 20 show results of the simulation of oblique Whipple shield impacts at 7 and 10 kilometers per second, using the debris propagation code and the general modeling methodology developed under this project. The cases represented are listed in Table 2.

Note that the simulations were conducted for particle diameters above and below the expected ballistic limits for the two velocities. The simulations are consistent with the ballistic limit curve data at 7 km/sec. At 10 km/sec, the simulations suggest slightly less wall damage than might be expected from the ballistic limit curve. Computer time requirements are very modest, considering the complexity of the problems.

5. Conclusion

The outlined research has addressed fundamental problems relevant to the development of space vehicles and structures for a variety of missions. It makes use of state of the art supercomputer resources while applying the newest numerical modeling techniques, designed to make oblique impact simulations computationally tractable. It included numerical implementation of a nonlinear, elastic-plastic debris cloud dynamics model important to accurate shield impact calculations. The resulting simulation capability can provide an important adjunct to experimental work on space shield design for a variety of future missions. The outlined work has been coordinated directly with NASA JSC experimental research efforts, and the final source code has been provided to NASA. It is therefore suggested that the proposed research has addressed important objectives of the NASA Regional Universities Grant Program.
REFERENCES


Table 1. Example Oblique Impact Simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>shield to wall spacing</td>
<td>4.0-8.0 inches</td>
</tr>
<tr>
<td>shield thickness:</td>
<td>0.063-0.071 inches</td>
</tr>
<tr>
<td>wall thickness:</td>
<td>0.125-0.160 inches</td>
</tr>
<tr>
<td>impact velocity:</td>
<td>7.1-7.6 km/sec</td>
</tr>
<tr>
<td>impact obliquity:</td>
<td>23.0-58.4 degrees</td>
</tr>
<tr>
<td>impact mass:</td>
<td>0.202-0.376 grams</td>
</tr>
<tr>
<td>material:</td>
<td>aluminum</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Simulation type</th>
<th>Computer system</th>
<th>Code</th>
<th>Memory</th>
<th>CPU time</th>
</tr>
</thead>
<tbody>
<tr>
<td>shield impact</td>
<td>Cray Y-MP/864</td>
<td>CTH</td>
<td>&lt; 64 MB</td>
<td>2.0-6.0 hrs</td>
</tr>
<tr>
<td>debris evolution</td>
<td>IBM RS/6000*</td>
<td>DC3D</td>
<td>&lt; 16 MB</td>
<td>0.5-3.0 days</td>
</tr>
<tr>
<td>wall impact</td>
<td>Cray Y-MP/864</td>
<td>DYNA3D</td>
<td>&lt; 64 MB</td>
<td>0.5-1.0 hrs</td>
</tr>
</tbody>
</table>

*The CPU time range given is for a Model 320, a very low performance system.*
Table 2. Ballistic Limit Simulations

bumper thickness = 0.127 cm
wall thickness = 0.3175 cm
impact obliquity = 25 degrees
material = Al 6061-T6

(Also see the ballistic limit plot in Figure 8)

<table>
<thead>
<tr>
<th>Simulation #</th>
<th>Impact velocity</th>
<th>Particle diameter</th>
<th>Figures</th>
</tr>
</thead>
<tbody>
<tr>
<td>7a</td>
<td>7 km/sec</td>
<td>0.575 cm</td>
<td>9 through 11</td>
</tr>
<tr>
<td>7b</td>
<td>7 km/sec</td>
<td>0.475 cm</td>
<td>12 through 14</td>
</tr>
<tr>
<td>10a</td>
<td>10 km/sec</td>
<td>0.530 cm</td>
<td>15 through 17</td>
</tr>
<tr>
<td>10b</td>
<td>10 km/sec</td>
<td>0.430 cm</td>
<td>18 through 20</td>
</tr>
</tbody>
</table>

**CPU time requirements**

- Bumper impact simulations (CTH): 1.80-2.11 CPU hrs, Cray YMP
- Debris transport calculations (DC3D): 3.34-5.67 CPU hrs, IBM RS/6000
- Wall impact calculations (DYNA3D): 0.27-0.28 CPU hrs, Cray YMP
List of Figures

Figure 1. Inertia multiports: deformable particle dynamics model.
Figure 2. RC multiports: deformable particle dynamics model.
Figure 3. Bond graph: deformable particle dynamics model.
Figure 4. CTH simulation of oblique impact on a Whipple shield (t = 4 μsec).
Figure 5. DC3D simulation results for impact momentum distribution on the wall plate.
Figure 6. DYNA3D simulation results: front surface of the wall plate.
Figure 7. DYNA3D simulation results: rear surface of the wall plate.
Figure 8. Ballistic limit plot.
Figure 9. CTH simulation 7a results: the shield and the debris cloud at four microseconds after impact.
Figure 10. DC3D simulation 7a results: areal density of the debris cloud momentum deposited on the wall plate.
Figure 11. DYNA3D simulation 7a results: front surface of the wall plate.
Figure 12. CTH simulation 7b results: the shield and the debris cloud at four microseconds after impact.
Figure 13. DC3D simulation 7b results: areal density of the debris cloud momentum deposited on the wall plate.
Figure 14. DYNA3D simulation 7b results: front surface of the wall plate.
Figure 15. CTH simulation 10a results: the shield and the debris cloud at three microseconds after impact.
Figure 16. DC3D simulation 10a results: areal density of the debris cloud momentum deposited on the wall plate.
Figure 17. DYNA3D simulation 10a results: front surface of the wall plate.
Figure 18. CTH simulation 10b results: the shield and the debris cloud at three microseconds after impact.
Figure 19. DC3D simulation 10b results: areal density of the debris cloud momentum deposited on the wall plate.
Figure 20. DYNA3D simulation 10b results: front surface of the wall plate.
Figure 4

Time = 4.0160E-06
Materials 1 2
StudyV 07/21/93 10:02:33
Block 1

Oblique whipple shield impact (B324)
Impact Momentum Areal Density

g/cm·msec
+0.00
+43.68
+87.37
+131.05
+174.73
+218.41
+262.10
+305.78

Figure 5
Debris Cloud Wall Impact Model

time = 0.49974E+02

B324: front surface

disp. scale factor = 0.100E+01 (default)
Debris Cloud Wall Impact Model

time = 0.49974E+02

B324: rear surface

disp. scale factor = 0.100E+01 (default)
Whipple shield ballistic limit

- Bumper thickness = 0.127 cm
- Wall thickness = 0.3175 cm
- Wall to bumper spacing = 10.16 cm
- Impact obliquity = 25 degrees
- Yield stress = 40 ksi
- Projectile density = 2.7 g/cc
- Bumper density = 2.7 g/cc
Fig. 9

Oblique whipple shield impact (7a)

Time = 4.0090E-06

Materials

K1SECN

1 11/28/93

20:33:27

Block 1
Figure 10

Impact Momentum Areal Density

$g/cm\cdot msec$

$+0.00$
$+117.28$
$+234.57$
$+351.85$
$+469.14$
$+586.42$
$+703.71$
$+820.99$

$x(cm)$

$z(cm)$
Debris Cloud Wall Impact Model

time = 0.99799E+01

disp. scale factor = 0.100E+01 (default)
Oblique whipple shield impact (7b)
Figure 13

Impact Momentum Areal Density

<table>
<thead>
<tr>
<th>g/cm-msec</th>
</tr>
</thead>
<tbody>
<tr>
<td>+0.00</td>
</tr>
<tr>
<td>+41.27</td>
</tr>
<tr>
<td>+82.54</td>
</tr>
<tr>
<td>+123.81</td>
</tr>
<tr>
<td>+165.09</td>
</tr>
<tr>
<td>+206.36</td>
</tr>
<tr>
<td>+247.63</td>
</tr>
<tr>
<td>+288.90</td>
</tr>
</tbody>
</table>

z(cm)

x(cm)
Figure 15

Oblique whipple shield impact (10a)
Figure 16

Impact Momentum Areal Density

$g/cm-msec$

- +0.00
- +64.88
- +129.77
- +194.65
- +259.53
- +324.41
- +389.30
- +454.18
Debris Cloud Wall Impact Model

time = 0.99761E+01

disp. scale factor = 0.100E+01 (default)
APPENDIX A

Example Input File (CTH simulation)
* Title record
* Oblique whipple shield impact (7a)
* control records

control

control

control

endc

edit records

edit

edit

mesh records

mesh

mesh

material insertion records
insertion of material
*
block 1
*
package projectile
material 1
numsub 49
velocities xvel 0.0 yvel 6.3441545e5 zvel 2.9583278e5
insert sphere
    center 0.0 -10.5745 0.0
    r 0.2875
endi
endp
*
package shield
material 1
numsub 49
velocities xvel 0. yvel 0. zvel 0.
insert box
    x1 0.0 y1 -10.287 z1 -1.00 x2 1.5875 y2 -10.16 z2 2.96875
endi
endp
*
endb
*
end
*
*******************************************************************************
*
* eos records
*
*
* eos num 2
eos
mat1 mgrun eos=6061-t6_al
* mat1 mgrun eos=2024-t4_al
* mat2 mgrun eos=7075-t6_al
* aneos1 -1 'Aluminum library' lib=6 type=4 rhug=-1. thug=-1.
* ende
*
*******************************************************************************
*
* material strength records
*
epdata
* matep 1 jfrac=7
* matep 2 jfrac=8
* matep 1 st=6061-t6_aluminum
* matep 1 st=2024-t4_aluminum
* matep 2 st=7075-t6_aluminum
* matep 1 st=user r0=1.0
* matep 2 st=user r0=1.0
mix = 5
ende
*
*******************************************************************************
*
endinput
*
* end of cthgen input
*
*******************************************************************************
*
*eor* cthin
*
*******************************************************************************
*
* cth input
*
*******************************************************************************
*
* Title record
*
Oblique whipple shield impact (7a)
*
*******************************************************************************
*
* control records
*
restart
   nu = 1
endr
*
control
   tst = 1.0e-6
   nsc = 5000
   cpshift = 60.
* mmp
endc
*
convect
   convection = 1
endc
*
*******************************************************************************
*
* time step records
*
mtndt
   time = 0.  dt = 1.e-12
endn
*
maxdt
   time=0.   dt=0.5e-10
   time=3.e-10  dt=1.
endx
*
*******************************************************************************
*
* tracer records
*
tracer
   add 0.0 -10.528 0.0
   add 0.0 -10.368 0.0
   add 0.0 -10.287 0.0
* add 0.0 -9.368
* add 0.0 -0.127
* add 0.0 -9.368 to 1.0 -9.368 n 3
* add 0.0 -0.127 to 1.0 -0.127 n 9
end
*
* edit records
*
edit
  shortt
    time=0.  d=5.e-6
    time=1.e-5  d=1.e-5
    time=1.e-4  d=1.e-4
  ends
  longt
    time=0.  d=5.e-6
    time=1.e-5  d=1.e-5
    time=1.e-4  d=1.e-4
  endl
plott
  time=0.  d=0.5e-6
  time=15.0e-6  d=1.0e-6
  time=30.0e-6  d=2.0e-6
endp
histt
  time = 0.  d=1.e-8
  htracer1
  htracer2
  htracer3
  bxyz 1 0.0 -8.01 0.0
  bxyz 1 0.2 -8.01 0.0
  bxyz 1 0.4 -8.01 0.0
  bxyz 1 0.6 -8.01 0.0
  bxyz 1 0.8 -8.01 0.0
  bxyz 1 1.0 -8.01 0.0
endh
ende
*
*
* boundary condition records
*
boundary
  bhydro
    block 1
      bxb=0  bxt=1  byb=1  byt=1  bzb=1  bzt=1
  endb
endh
endb
*
* end of cth input
*
*--------------------------------------------------------------------------*
* eor* hisinp
*--------------------------------------------------------------------------
* hisplt input
  * bottom=off
  plot time cpu v2=dt v3=etot
  *plot time pressure.1 v2=pressure.2 v3=pressure.3
  *plot time yvelocity.1 v2=yvelocity.2 v3=yvelocity.3
  *plot time zvelocity.1 v2=zvelocity.2 v3=zvelocity.3
  *plot time pressure.4 v2=pressure.5 v3=pressure.6
  *plot time pressure.7 v2=pressure.8 v3=pressure.9
  * end of hisplt input
  *
  *eor* pltinp
  *
  * cthplt input
  *
  units cgsk
  bottom=off
  *
  *color table = 6
  *color material = 16 112
  *color nmaterial = 31 127
  *3dplot
  *tcolor = 6
  *
  *3dline, mat=0
  3dortho, mat=0
  *
  *2dfix x=0.0
  *2dplot if tracer dots=density=3.0
  * end of cthplt input
  *
  ************************************************************
APPENDIX B

Example Input File (CTH simulation restart)
**Oblique whipple shield impact (7a)**

*control records*

```plaintext
*control
ep
mmp
dnc
```

*edit records*

```plaintext
*edit
block 1
  expanded
endb
ende
```

*mesh records*

```plaintext
*mesh
block 1 geom=3dr type=e
  x0  0.0
  x1  n=50  w=1.5875  rat=1.0
endx
  y0  -11.5
  y1  n=125  w=3.96875  rat=1.0
endy
  z0  -1.000
  z1  n=125  w=3.96875  rat=1.0
endz
  xact  =  0.0  1.00
  yact  = -11.5  -10.40
  zact  =  -0.50  1.00
endb
endm
```

*material insertion records*
insertion of material

block 1

package projectile
material 1
numsub 49
velocities xvel 0.0  yvel 6.3441545e5  zvel 2.9583278e5
insert sphere
   center  0.0  -10.5745  0.0
   r       0.2875
endi
endp

package shield
material 1
numsub 49
velocities xvel 0.  yvel 0.  zvel 0.
insert box
   x1  0.0  y1 -10.287  z1 -1.00  x2  1.5875  y2 -10.16  z2 2.96875
endi
endp

endb
endi

* eos records

* eos  num 2
eos
   mat1  mgrun eos=6061-t6_al
   mat1  mgrun eos=2024-t4_al
   mat2  mgrun eos=7075-t6_al
   * aneos1 -1 'Aluminum library' lib=6 type=4  rhug=-1.  thug=-1.
ende

* material strength records

epdata
   * matep 1  jfrac=7
   * matep 2  jfrac=8
   matep 1  st=6061-t6_aluminum
   matep 1  st=2024-t4_aluminum
   matep 2  st=7075-t6_aluminum
   matep 1  st=user  r0=1.0
   matep 2  st=user  r0=1.0
     mix  = 5
ende

*
endinput

* end of cthgen input
*

************************************************************************************
*
* eor* cthin
*
************************************************************************************
*
* cth input
*
************************************************************************************
*
* Title record
*
Oblique whipple shield impact (7a)
*
************************************************************************************
*
* control records
*
restart
  newfile
  nu = 3
endr
*
control
  tst = 4.0e-6
  nsc = 5000
  cpshift = 60.
* mmp
endc
*
convect
  convection = 1
endc
*
************************************************************************************
*
* time step records
*
mindt
  time = 0.  dt = 1.e-12
endn
*
maxdt
  time=0.  dt=0.5e-10
  time=3.e-10  dt=1.
endx
*
************************************************************************************
*
* tracer records
*
tracer
  * add 0.0  -10.528  0.0
  * add 0.0  -10.368  0.0
* add 0.0 -10.287 0.0
* add 0.0 -9.368
* add 0.0 -0.127
* add 0.0 -9.368 to 1.0 -9.368 n 3
* add 0.0 -0.127 to 1.0 -0.127 n 9
endt

* edit records
* edit
  shortt
    time=0.  dtf=5.e-6
    time=1.e-5 dtf=1.e-5
    time=1.e-4 dtf=1.e-4
  ends
longt
    time=0.  dtf=5.e-6
    time=1.e-5 dtf=1.e-5
    time=1.e-4 dtf=1.e-4
  endl
plott
    time=0.  dtf=1.5e-6
    time=15.0e-6 dtf=1.0e-6
    time=30.0e-6 dtf=2.0e-6
endp
histt
  time = 0.  dtf = 1.e-8
*  htracer1
*  htracer2
*  htracer3
  * bxyz 1 0.0 -8.01 0.0
  * bxyz 1 0.2 -8.01 0.0
  * bxyz 1 0.4 -8.01 0.0
  * bxyz 1 0.6 -8.01 0.0
  * bxyz 1 0.8 -8.01 0.0
  * bxyz 1 1.0 -8.01 0.0
endh
.ende

* boundary condition records
* boundary
  bydro
    block 1
      bxb=0 bxt=1 byb=1 byt=1 bzb=1 bzt=1
  endb
endh
endb

* end of cth input
* 
**********************************************************************
* *eor* hisinp
*
hisplt input

plot time cpu v2=dt v3=etot
*plot time pressure.1 v2=pressure.2 v3=pressure.3
*plot time yvelocity.1 v2=yvelocity.2 v3=yvelocity.3
*plot time zvelocity.1 v2=zvelocity.2 v3=zvelocity.3
*plot time pressure.4 v2=pressure.5 v3=pressure.6
*plot time pressure.7 v2=pressure.8 v3=pressure.9
*
* end of hisplt input

pltinp

cthplt input

units cgsk
bottom=off
*color table = 6
*color material = 16 112
*color nmaterial = 31 127
*3dplot
*tcolor = 6
*
*3dline, mat=0
3dortho, mat=0
*
*2dfix x=0.0
*2dplot if tracer dots=density=3.0
*
* end of cthplt input
APPENDIX C

Example Input File (DC3D)
* dc3d input file

* itype  jtype
  2   1
* i1  i2
  2   33
* j1  j2
  64  112
* k1  k2
  17  80

* xlow  delta x
  0.0  0.031750
* ylow  delta y
-11.5000  0.031750
* zlow  delta z
-1.0000  0.031750
* tcut  tmin  dencut
  25.0  0.0  0.01
* idmax  jdm max  kdm ax  idmaxn  jdm axn  kdm axn
  51   5   101      51   5   101
* xdm in  xdm ax  xdm in n  xdm ax n
  0.0  8.00   0.0  4.00
* ydm in  ydm ax  ydm in n  ydm ax n
  0.0  0.3175  0.0  0.3175
* zd min  zdm ax  zd min n  zdm ax n
-4.00  12.00   2.0  10.0
* vmu  vlamb  denref  eta
  0.259  0.503  2.703  1.0e-3
* zeta  eps  ymxref
  1.0e-9  1.0e-6  1.0e-6
* mdfactor
  1.0
APPENDIX D

Example Input File Header (DYNA3D)
Debris Cloud Wall Impact Model

<p>| | | |</p>
<table>
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</tr>
</thead>
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<tr>
<td>2</td>
<td>25763</td>
<td>20001</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>100.0e-01</td>
<td>-2.0e+4</td>
<td>50.0e-01</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>13</td>
<td>2.703</td>
</tr>
<tr>
<td>e-p w/failure</td>
<td>0.276</td>
<td>2.900e-03</td>
</tr>
<tr>
<td>7.20e-1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>elastic</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>0.3</td>
</tr>
</tbody>
</table>
APPENDIX E

Plotting Routine Source Code (DCMPLT)
program dcmplt

dimension x(500),y(500),z(500),
1 zz(500,500),cval(10)

external grcrt,efsplt
external grcrt,egsgl,efsplt

open(1, file='dcpost.plt')
open(2, file='dc3din')
open(9, file='dcmplt.out')

do 11 i=1,500
  x(i)=0.0
  y(i)=0.0
  z(i)=0.0
  continue

scale=1.0e+6
scale=1.0e+3

jmax=1
kmax=1
zmax=0.0

do 10 i=1,500000
  read(1,101,end=98) j,k,xx,yy,pmag
101  format(2i6,3e15.3)
  x(j)=xx
  y(k)=yy
  zz(j,k)=pmag*scale
  if(zz(j,k).gt.zmax) zmax=zz(j,k)
  if(j.gt.jmax) jmax=j
  if(k.gt.kmax) kmax=k
  continue

98  dummy=1.0

iunit=0
ldzz=500
iopt=1+2+4
iopt=2+8
ncv=8

x= (1.0e-33)
cval(2)=zmax

call grcrt(jmax,kmax,x,y,zz,ldzz,iopt,ncv,cval)
call egsgl('!contour.plot useS', 'dcmplt.dl$')
call egsgl('!useS', 'dcmplt.d2$')
call egsgl('!viewport$', 0.1,0.9,0.1,0.9)
call efsplt(iunit, '')

stop
end
APPENDIX F

Post-processor Source Code (DCPOST)
program dcpost

!**** program dcpost

dimension iflg(100000), px(100000), py(100000), pz(100000),
1 jenew(100000)
dimension xcen(500), zcen(500), emom(500, 500)

character*8 ch0, ch1, ch2, ch3, ch4, ch5, ch6, ch7, ch8, ch9

open(1, file = 'dc3din')
open(12, file = 'dc3d.dyn')
open(61, file = 'dc3d.mom')
open(13, file = 'dcbase')

open(21, file = 'dcpost.out')
open(22, file = 'dcpost.plt')

time = 1.0

time = 0.0

factor = 0.75
factor = 1.0

read(1, 110) itype, jtype
110 format(///2iii)
read(1, 111) li, i2, j1, j2, k1, k2
111 format(/2i8)
read(1, 112) xlow, deltx, ylow, delty, zlow, deltz
112 format(/2e15.6)
read(1, 113) tcut
113 format(/e15.3)
read(1, 114) idmax, jdmax, kdmax, idmaxn, jdmaxn, kdmaxn
114 format(/6i10)
read(1, 115) xdmin, xdmax, xdminn, xdmaxn,
1 ydmin, ydmax, ydminn, ydmaxn,
2 zdmin, zdmax, zdminn, zdmaxn
115 format(/4e15.3)
read(1, 116) factor
116 format(////e15.3)

ncnt = idmax*jdmax*kdmax + (idmax-1)*(jdmax-1)*(kdmax-1) +
1 8+1+5

if(itype.ne.1) go to 777
if(itype.eq.0) go to 777

do 14 i = 1, ncnt
14 read(12, 202) ch0, ch1, ch2, ch3, ch4, ch5, ch6, ch7, ch8, ch9
202 format(10a8)

if(itype.eq.3) go to 14

write(21, 203) ch0, ch1, ch2, ch3, ch4, ch5, ch6, ch7, ch8, ch9
203 format(10a8)
14 continue

777 dummy = 1.0
do 10 j=1,1000000  
    iflg(j)=0  
    px(j)=0.0  
    py(j)=0.0  
    pz(j)=0.0  
 10 continue  

do 11 i=1,500000  
  read(12,102,end=75) j,dpx,dpy,dpz  
  read(61,102,end=75) j,dpx,dpy,dpz  
 102 format(i8,3e10.3)  
    iflg(j)=1  
    px(j)=px(j)+dpx*factor  
    py(j)=py(j)+dpy*factor  
    pz(j)=pz(j)+dpz*factor  
 11 continue  

dummy=1.0  
  ridmax=idmax  
  rkdmax=kdmax  
  deldx=(xdmax-xdmin)/(ridmax-1.0)  
  deldz=(zdmax-zdmin)/(rkdmax-1.0)  
  ridmxn=ridmaxn  
  rkdmxn=kdmmaxn  
  deldxn=(xdmaxn-xdminn)/(ridmxn-1.0)  
  deldzn=(zdmaxn-zdminn)/(rkdmxn-1.0)  

do 710 k=1,kdmax-1  
  do 711 i=1,idmax-1  
    rk=k  
    ri=i  
    zcen(k)=zdmin+deldz/2.0+(rk-1.0)*deldz  
    xcen(i)=xdmin+deldx/2.0+(ri-1.0)*deldx  
    emom(i,k)=0.0  
 711 continue  
 710 continue  

do 12 j=1,1000000  
    jout=j  
    if(jtype.eq.3) jout=jenew(j)  
    if(jout.eq.0) go to 12  
    if(iflg(j).eq.0) go to 12  
  write(21,201) jout,px(j),py(j),pz(j),time
201 format(i8,4e10.3)
  c  if(jtype.eq.3) go to 12
  c  iel=mod(j,idmax-1)
  c  kel=j/(idmax-1)+1
  c  pmag=(px(j)**2+py(j)**2+pz(j)**2)**0.5
  c  emom(iel,kel)=pmag/(deldx*deldz)
  c  emom(iel,kel)=pmag
  c  riel=iel
  c  rkel=kel
  c  xi=xdmin+deldx+(riel-1.0)*deldx
  c  zi=zdmin+deldz+(rkel-1.0)*deldz
  c  write(22,212) iel,kel,xi,zi,pmag,time
  c  212 format(2i6,4e15.3)
  c  12 continue
  c  if(jtype.eq.3) go to 99
  c  do 721 k=1,kdmax-1
  c  do 722 i=1,idmax-1
  c    write(22,213) i,k,xcen(i),zcen(k),emom(i,k)
  c  213 format(2i6,3e15.5)
  c  722 continue
  c  721 continue
  c  99 dummy=2.0
  c  stop
  end
APPENDIX G

Analysis Source Code (DC3D)
program dc3d

**** program dc3d

common/attype/itype, jtype
common/mesh/i1, i2, j1, j2, k1, k2, deltx, delty, deltz,
 1 xlow, ylow, zlow
common/waldat/ywall, tcut, tmin, dencut,
 1 idmax, jdmax, kdmax, xdmn, xdmx, ydmn, ydxm, zdmn, zdxm
common/walnew/idmaxn, jdmaxn, kdmaxn,
 1 xdmnn, xdmxn, ydmnn, ydxmn, zdmnn, zdxmn
common/props/den, denref, rmass, vmu, vlamb, eta, zeta, phi, rj(3, 3)
common/intpar/epsint, ymxref

open (1, file='dc3din')

open(7, file='pltdat/dc3d.pltl')
open(8, file='pltdat/dc3d.plt2')
open(4, file='dc3d.cth')
open(9, file='dc3d.dyn')

open(61, file='dc3d.mom')
open(10, file='dc3d.dbg')

read(1,110) itype, jtype
 110 format (///2i10)
read(1,111) i1, i2, j1, j2, k1, k2
 111 format (///2i10)
read(1,112) xlow, deltx, ylow, delty, zlow, deltz
 112 format (///2e15.6)
read(1,113) tcut, tmin, dencut
 113 format (///3e15.3)
read(1,114) idmax, jdmax, kdmax, idmaxn, jdmaxn, kdmaxn
 114 format (///6i10)
read(1,115) xdmn, xdmx, xdmnn, xdmxn,
 1 ydmn, ydxm, ydmnn, ydxmn,
 2 zdmn, zdmx, zdmnn, zdxmn
 115 format (///4e15.3)
read(1,116) vmu, vlamb, denref, eta
 116 format (///4e15.3)
read(1,117) zeta, epsint, ymxref
 117 format (///3e15.3)

ywall=ydmn

call rdavs

c if(itype.eq.2) call dyngen
  if(itype.eq.2 .and. jtype.eq.1) call dyngen
  if(itype.eq.2 .and. jtype.eq.2) call dyngen
  if(itype.eq.2 .and. jtype.eq.3) call dyngen
  if(jtype.eq.2) go to 99
  if(jtype.eq.3) go to 99

c call rdavs

c ifst=2
jfst = 2
kfst = 2

ilast = 2
jlast = 2
klast = 2

ilast = i2 - il
jlast = j2 - j1
klast = k2 - kl

lfst = 1
llast = 5

do 10 i = ifst, ilast
do 11 j = jfst, jlast
do 12 k = kfst, klast
do 13 l = ifst, llast

call dcelem(i, j, k, l)

13 continue
12 continue
11 continue
10 continue

99 dummy = 1.0

stop
end

subroutine dyngen

** subroutine dyngen

common/atypetype, jtype
common/walnew/idmaxn, jdmaxn, kdmaxn,
1 xdmnin, xdmnax, ydmnin, ydmnax, zdnmin, zdmaxn
common/waldat/ywall, tcut, tmin, dencut,
1 idmax, jdmax, kdmax, xdmnin, xdmnax, ydmnin, ydmnax, zdmin, zdmaxn
dimension x(8), y(8), z(8), xn(501), yn(501), zn(501)

if (jtype .ne. 3) go to 88

idmax = idmaxn
jdmax = jdmaxn
kdmax = kdmaxn
xdmin = xdmnin
ydmin = ydmnin
zdmin = zdmin
xdmax = xdmnax
ydmax = ydmnax
zdmax = zdmaxn

88 dummy = 1.0

ridmax = idmax
delx = (xdmax - xdmnin) / (ridmax - 1.0)

rjmax = jdmax
dely = (ydmax - ydmnin) / (rjmax - 1.0)

rkmax = kdmax
\[ \text{delz} = \frac{(z_{\text{max}} - z_{\text{min}})}{(r_{k_{\text{max}}} - 1.0)} \]

\[ \text{do } 10 \text{ i=1,idmax} \]
\[ \text{ri}=i \]
\[ \text{xn}(i) = (ri - 1.0) \times \text{delx} \]
\[ 10 \text{ continue} \]

\[ \text{do } 11 \text{ j=1,jdmax} \]
\[ \text{rj}=j \]
\[ \text{yn}(j) = (rj - 1.0) \times \text{dely} \]
\[ 11 \text{ continue} \]

\[ \text{do } 12 \text{ k=i,kdmax} \]
\[ \text{rk}=k \]
\[ \text{zn}(k) = (rk - 1.0) \times \text{delz} \]
\[ 12 \text{ continue} \]

\[ \text{define the nodes} \]

\[ \text{nconst}=0 \]

\[ \text{do } 20 \text{ j=1,jdmax} \]
\[ \text{do } 21 \text{ k=1,kdmax} \]
\[ \text{do } 22 \text{ i=1,idmax} \]

\[ \text{nconst}=0 \]
\[ \text{if (i.eq.1)} \quad \text{nconst}=1 \]

\[ \text{go to 761} \]

\[ \text{if (i.eq.idmax)} \quad \text{nconst}=4 \]
\[ \text{if (k.eq.1)} \quad \text{nconst}=5 \]
\[ \text{if (k.eq.kdmax)} \quad \text{nconst}=5 \]
\[ \text{if (i.eq.1.and.k.eq.1)} \quad \text{nconst}=7 \]
\[ \text{if (i.eq.1.and.k.eq.kdmax)} \quad \text{nconst}=7 \]
\[ \text{if (i.eq.idmax.and.k.eq.1)} \quad \text{nconst}=7 \]
\[ \text{if (i.eq.idmax.and.k.eq.kdmax)} \quad \text{nconst}=7 \]

\[ 761 \text{ dummy}=1.0 \]

\[ \text{nnode}=i+idmax*(k-1)+idmax*kdmax*(j-1) \]
\[ \text{write}(9,101) \text{ nnnode,nconst,xn(i),yn(j),zn(k)} \]

\[ 101 \text{ format}(i5,i5,3e20.8) \]

\[ 101 \text{ format}(i8,i5,3e20.8) \]

\[ 20 \text{ continue} \]

\[ \text{nconst}=0 \]

\[ x(1)=x_{\text{min}} \]
\[ y(1)=y_{\text{min}}-1.0 \]
\[ z(1)=z_{\text{min}} \]
\[ x(2)=x_{\text{min}}+1.0 \]
\[ y(2)=y_{\text{min}}-1.0 \]
\[ z(2)=z_{\text{min}} \]
\[ x(3)=x_{\text{min}}+1.0 \]
\[ y(3)=y_{\text{min}}-1.0 \]
G-5

z(3) = z_{\text{min}} + 1.0
x(4) = x_{\text{min}}
y(4) = y_{\text{min}} - 1.0
z(4) = z_{\text{min}} + 1.0
x(5) = x_{\text{min}}
y(5) = y_{\text{min}} - 2.0
z(5) = z_{\text{min}}
x(6) = x_{\text{min}} + 1.0
y(6) = y_{\text{min}} - 2.0
z(6) = z_{\text{min}}
x(7) = x_{\text{min}}
y(7) = y_{\text{min}} - 2.0
z(7) = z_{\text{min}} + 1.0
x(8) = x_{\text{min}}
y(8) = y_{\text{min}} - 2.0
z(8) = z_{\text{min}} + 1.0

do 40 i=1,8
nnode = \text{id}_{\text{max}} + \text{id}_{\text{max}}* (\text{kd}_{\text{max}} - 1) + \text{id}_{\text{max}}\text{kd}_{\text{max}}* (\text{jd}_{\text{max}} - 1) + i
write (9,103) nnode, nconst, x(1), y(1), z(1)
format(i5,i5,3e20.8)
format (i8, i5,3e20.8)
continue

define the elements

nmat = 1
ngen = 0

do 30 j=1, \text{jd}_{\text{max}} - 1
do 31 k=1, \text{kd}_{\text{max}} - 1
do 32 i=1, \text{id}_{\text{max}} - 1
nelem = i + (\text{id}_{\text{max}} - 1)*(k-1) + (\text{id}_{\text{max}} - 1)* (\text{kd}_{\text{max}} - 1)*(j-1)
n1 = i + \text{id}_{\text{max}}*(k-1) + \text{id}_{\text{max}}\text{kd}_{\text{max}}*(j-1)
n2 = n1 + 1
n3 = n2 + \text{id}_{\text{max}}
n4 = n3 + 1
n5 = n1 + \text{id}_{\text{max}}\text{kd}_{\text{max}}
n6 = n5 + 1
n7 = n6 + \text{id}_{\text{max}}
n8 = n7 - 1
write(9,102) nelem, nmat, ngen, n5, n6, n7, n8, n1, n2, n3, n4
format(i11i5)
write(9,102) nelem, nmat, ngen, n5, n6, n7, n8, n1, n2, n3, n4
format (i8, i5,8i8)
continue

nmat = 2

nelem = \text{id}_{\text{max}} - 1 + (\text{id}_{\text{max}} - 1)*(\text{kd}_{\text{max}} - 1-1) +
1 (\text{id}_{\text{max}} - 1)* (\text{kd}_{\text{max}} - 1-1) + 1
n1 = \text{id}_{\text{max}}\text{id}_{\text{max}} (\text{kd}_{\text{max}} - 1) + \text{id}_{\text{max}}\text{kd}_{\text{max}} (\text{jd}_{\text{max}} - 1) + 1
n2 = n1 + 1
n3 = n1 + 2
n4 = n1 + 3
n5 = n1 + 4
n6=n1+5
n7=n1+6
n8=n1+7

write(9,104) nelem,nmat,ngen,n1,n2,n3,n4,n5,n6,n7,n8
104 format (i11)
write(9,104) nelem,nmat,n2,n3,n4,n5,n6,n7,n8
104 format (i8,i5,8i8)

write(9,110)

format(' 1 1 11',/,' 1 0',/,' 1')
idmpl=idmax+1
idmp2=idmax+2
write(9,111) idmp2,idmpl,n4,n3,n2,n1
111 format(' 1 0 1 2',2i5,
1 /,' 1 0',4i5)

write (9,110)

format(' 1 1 11',/,' 1 0',/,' 1')
idmpl=idmax+1
idmp2=idmax+2
write(9,111) idmp2,idmpl,n4,n3,n2,n1
111 format(' 1 1 2',2i8,
1 /,' 1',4i8)

return
end

subroutine rdavs

subroutine rdavs

common/mesh/il,i2,j1,j2,k1,k2,deltx,delty,deltz,
1 xlow,ylow,zlow

common/cthdat/ velx(75,75,75),vely(75,75,75),
1 velz(75,75,75),pres(75,75,75),temp(75,75,75),
2 gama(75,75,75),spen(75,75,75),vmas(75,75,75),
3 vphi(75,75,75),cspd(75,75,75)

common/cthxyz/xcth(100),ycth(100),zcth(100)

common/vellng/vfx(75,75,75),vfy(75,75,75),vfz(75,75,75)

character*1 chdum

open(2,file='avsout')
open(3,file='avschk')

calculate the nodal coordinates

do 20 i=il,i2
vi=i
xcth(i-il+1)=xlow+(vi-1.0)*deltx-deltx
continue

do 21 j=j1,j2
vj=j
ycth(j-j1+1)=ylow+(vj-1.0)*delty-delty
21 continue

c  do 22 k=k1,k2
   vk=k
   zcth(k-k1+1)=zlow+(vk-1.0)*deltz-deltz
22 continue

c  read in the mesh data

c  do 400 idum=1,27
   read(2,901) chdum
901 format(a)
400 continue

c  do 10 k1,k2-k1+1
   do 11 j=j1-j1+1
   do 12 i=i1-i1+1
   read(2,902) velx(i,j,k),velx(i,j,k),velz(i,j,k),
   1 pres(i,j,k),temp(i,j,k),gama(i,j,k),spen(i,j,k)
   read(2,902) vmas(i,j,k),vphi(i,j,k),
   1 cspd(i,j,k)
   unit conversion factors

   velx(i,j,k)=velx(i,j,k)/1.0e+6
   vely(i,j,k)=vely(i,j,k)/1.0e+6
   velz(i,j,k)=velz(i,j,k)/1.0e+6
   pres(i,j,k)=pres(i,j,k)/1.0e+12
902 format(7ell.3)
12 continue
11 continue
10 continue

c  do 30 k=k1,k2-k1+1
   do 31 j=j2-j1+1
   do 32 i=i2-i1+1
   write(3,903) velx(i,j,k),velx(i,j,k),velx(i,j,k),
   1 pres(i,j,k),temp(i,j,k),gama(i,j,k),
   write(3,903) vmas(i,j,k),vphi(i,j,k),
   1 xcth(i),ycth(j),zcth(k)
903 format(7ell.3)
32 continue
31 continue
30 continue

c  calculate the nodal velocities

c  do 40 k=2,k2-k1+1
   do 41 j=2,j2-j1+1
   do 42 i=2,i2-i1+1
   wta=vmas(i,j,k-1)
   wtb=vmas(i,j-1,k-1)
   wtc=vmas(i,j-1,k)
   wtd=vmas(i,j,k)
   va=velx(i,j,k-1)
   vb=velx(i,j-1,k-1)
   vc=velx(i,j-1,k)
vd=velx(i,j,k)
if(wta+wtb+wtc+wtd.gt.0.0) then
  vfx(i,j,k)=(wta*va+wtb*vb+wtc*vc+wtd*vd)/(wta+wtb+wtc+wtd)
else
  vfx(i,j,k)=0.0
endif

write(10,910) wta,wtb,wtc,wtd,va,vb,vc,vd
format(8e10.2)

wta=vmas(i-1,j,k-1)
wtb=vmas(i,j-1,k)
wtc=vmas(i-1,j,k-1)
wtd=vmas(i-1,j,k)
va=vely(i-1,j,k-1)
vb=vely(i,j,k-1)
vc=vely(i,j,k)
v=vely(i-1,j,k)
if(wta+wtb+wtc+wtd.gt.0.0) then
  vfy(i,j,k)=(wta*va+wtb*vb+wtc*vc+wtd*vd)/(wta+wtb+wtc+wtd)
else
  vfy(i,j,k)=0.0
endif

write(10,911) wta,wtb,wtc,wtd,va,vb,vc,vd
format(8e10.2)

wta=vmas(i,j,k)
wtb=vmas(i,j-1,k)
wtc=vmas(i-1,j,k)
wtd=vmas(i-1,j,k-1)
va=velz(i,j,k)
vb=velz(i,j-1,k)
vc=velz(i-1,j,k)
v=velz(i-1,j,k)
if(wta+wtb+wtc+wtd.gt.0.0) then
  vfz(i,j,k)=(wta*va+wtb*vb+wtc*vc+wtd*vd)/(wta+wtb+wtc+wtd)
else
  vfz(i,j,k)=0.0
endif

write(10,912) wta,wtb,wtc,wtd,va,vb,vc,vd
format(8e10.2)

42 continue
41 continue
40 continue

return
end

subroutine dcelem(ii,jj,kk,ll)

**** subroutine dcelem
common/atypetype, jtype,
common/waldat/ywall,tcut,tmin,dencut,
idmax,jdmax,kdmax,xdmin,xdmax,ydmin,ydmax,zdmin,zdmax
common/props/den,denref,rmass,vmu,vlamb,eta,zeta,phi,rj(3,3)
common/ndata/xl(3),x2(3),x3(3),x4(3),
v1(3),v2(3),v3(3),v4(3),xc(3)
dimension h(3,3),f(3,3),e(3,3),ep(3,3),p(3),
y(33),yt(33,101)
dimension param(50),time(101)

eexternal fcn
call eldata(ii,jj,kk,ll)
c
rden=den/denref
if(rden.gt.1000.0) go to 99
if(rden.lt.0.01) go to 99
if(phi.gt.0.999) go to 99
denblk=(1.-phi)*den/denref
if(denblk.lt.0.01) go to 99
if(denblk.lt.dencut) go to 99
call nddata(ii,jj,kk,ll)
call jcalc(den,xl,x2,x3,x4,xc,rj)
call jcalc(xl,x2,x3,x4,xc,rj)
call initlz(h,f,ep,p)
c
write(10,558) rmass
558 format(/,'inertia tensor ( mass = ',ell.3, ' ) ','/)
do 555 io=1,3
do 556 jo=1,3
write(10,557) rj(io,jo)
557 format(e20.8)
556 continue
555 continue

c set the state vector
do 10 i=1,3
do 11 j=1,3
y(3*(i-1)+j) = h(i,j)
y(3*(i-1)+j+9) = f(i,j)
y(3*(i-1)+j+18) = ep(i,j)
c
write(10,1000) h(i,j),f(i,j),ep(i,j)
c1000 format(3e15.4)
11 continue
10 continue

do 12 i=1,3
y(i+27)= p(i)
y(i+30)=xc(i)
c
write(10,1001) p(i),xc(i)
c1001 format(2e15.4)
12 continue

C set up and call the integration routine

ido=1
neq=33
tol=1.0e-6

do 20 i=1,50
param(i)=0.0
20 continue

C
param(1)=1.0e-6
param(3)=1.0e-3
param(4)=100000
param(9)=1.0e-1
param(10)=3
param(12)=2

do 32 i=1,neq
yt(i,1)=y(i)
32 continue

C iend=2
iend=1
riend=iend

tarr=1.0e+33
vceny=p(2)/rmass
avceny=abs(vceny)
if(avceny.gt.0.0)
1 tarr=abs((ywall-y(32))/vceny)
if(itype.eq.2.and.tarr.gt.tcut) go to 99
if(itype.eq.2.and.tarr.lt.tmin) go to 99
if(tarr.gt.tcut) go to 99
if(tarr.ge.tcut) go to 99
if(tarr.lt.tmin) go to 99
if(ii.ne.3) go to
99
if(jj.ne.38) go to 99
if(kk.ne.44) go to 99

delt=tarr/riend
if(itype.eq.2) delt=tarr/riend
if(itype.eq.1) delt=0.2

t=0.0
time(1)=0.0

do 30 i=1,iend
ri=i
C t=(ri-1.0)*delt
tend=t+delt
C call ivprk(ido, neq, fcn, t, tend, tol, param, y)
call ivpbs(ido, neq, fcn, t, tend, tol, param, y)
call ivpag(ido, neq, fcn, fcnj, aaa, t, tend, tol, param, y)
call ifdcrk(ido, neq, t, tend, tol, param, y)
call ivdcrk(ido, neq, t, tend, tol, param, y)
write(10,101) tarr,t,tend,y(32)
101 format(5e15.3)
do 31 j=1,neq
   yt(j,i+1)=y(j)
31 continue
t=tend
time(i+1)=tend
continue
write cth input data
if (itype.eq.1)
   1 call cthout(ii, jj, kk, ll, y)
if (itype.eq.2)
   1 call dynout(ii, jj, kk, ll, y, tarr)
ido=3
call ivprk(ido, neq, fcn, t, tend, tol, param, y)
call ivpbs(ido, neq, fcn, t, tend, tol, param, y)
call ivpag(ido, neq, fcn, fcnj, aaa, t, tend, tol, param, y)
call prtout(iend, time, yt)
go to 99
write(7,501) ii, jj, kk, ll, yt(31,1), yt(32,1), yt(33,1)
write(8,501) ii, jj, kk, ll,
   1 yt(31,iend+1), yt(32,iend+1), yt(33,iend+1)
501 format(4i6, 3e15.4)
99 return
end
subroutine dynout(ip, jp, kp, lp, y, tarr)
subroutine dynout
common/props/den, denref, rmass, vmu, vlamb, eta, zeta, phi, rj(3,3)
common/ndata/x1(3), x2(3), x3(3), x4(3),
   1 v1(3), v2(3), v3(3), v4(3), xc(3)
common/waldat/ywall, tcut, tmin, dencut,
   1 idmax, jdmax, kmax, xmin, xmax, ydmin, ydmax, zdmin, zdmax
dimension y(33), f(3,3), xt1(3), xt2(3), xt3(3), xt4(3), xt5(3),
   1 ptc(3), id(5), jd(5), kd(5)
c1=(denref/den)**(-1./3.)
do 10 i=1,3
do 11 j=1,3
   f(i,j)=y(3*(i-1)+j+9)
11 continue
10 continue
write(4,101) i,j,f(i,j)
101 format(i5,i5,el5.6)
11 continue
10 continue

call detcal(f, detf)
denout = denref/detf

momentum enhancement

ridmax = idmax
rjmax = jmax
rkmax = kmax

tmass = denref * ((xtdmax - xtdmin) / (ridmax - 1.0)) * 
1 * ((ytdmax - ytdmin) / (rjmax - 1.0)) * ((ztdmax - ztdmin) / (rkmax - 1.0))
enhmom = ((tmass + rmass) / rmass) ** 0.5

do 12 i = 1, 3
  ptc(i) = enhmom * y (27+i) / 5.0
12 continue

do 20 i = 1, 3
  xt1(i) = 0.0
  xt2(i) = 0.0
  xt3(i) = 0.0
  xt4(i) = 0.0
  xt5(i) = 0.0
20 continue

do 23 i = 1, 3
  do 21 j = 1, 3
    xt1(i) = xt1(i) + cl * f(i,j) * (xl(j) - xc(j))
    xt2(i) = xt2(i) + cl * f(i,j) * (x2(j) - xc(j))
    xt3(i) = xt3(i) + cl * f(i,j) * (x3(j) - xc(j))
    xt4(i) = xt4(i) + cl * f(i,j) * (x4(j) - xc(j))
 21 continue
23 continue

do 22 i = 1, 3
  xt1(i) = xt1(i) + y (30+i)
  xt2(i) = xt2(i) + y (30+i)
  xt3(i) = xt3(i) + y (30+i)
  xt4(i) = xt4(i) + y (30+i)
  xt5(i) = y (30+i)
22 continue

calculate the element numbers

c nelmax = (idmax-1) * (jmax-1) * (kmax-1)
c

ridmax = idmax
delx = (xtdmax - xtdmin) / (ridmax - 1.0)
rjmax = jmax
dely = (ytdmax - ytdmin) / (rjmax - 1.0)
rkmax = kmax
delz = (ztdmax - ztdmin) / (rkmax - 1.0)
id(1)=int((xt1(1)-xmin)/delx)+1
kd(1)=int((xt1(3)-zmin)/delz)+1
id(2)=int((xt2(1)-xmin)/delx)+1
kd(2)=int((xt2(3)-zmin)/delz)+1
id(3)=int((xt3(1)-xmin)/delx)+1
kd(3)=int((xt3(3)-zmin)/delz)+1
id(4)=int((xt4(1)-xmin)/delx)+1
kd(4)=int((xt4(3)-zmin)/delz)+1
id(5)=int((xt5(1)-xmin)/delx)+1
kd(5)=int((xt5(3)-zmin)/delz)+1

write(9,501) ip, jp, kp, lp
format(4i5)

do 303 ic=1,5
ia=id(ic)
if(ia.gt.idmax-l) go to 303
if(ia.lt.1) go to 303
ka=kd(ic)
if(ka.gt.kdmax-l) go to 303
if(ka.lt.1) go to 303
nelem=ia+(idmax-l)*ka
write(9,503) nelem, ptc(1),ptc(2),ptc(3),tarr
write(61,503) nelem, ptc(1),ptc(2),ptc(3),tarr
format(i5, 4e20.8)
format(i8, 4e20.8)
continue

go to 301
write(9,506) xtl(1),xtl(2),xtl(3)
format(3e20.8)
write(9,507) xt2(1),xt2(2),xt2(3)
format(3e20.8)
write(9,508) xt3(1),xt3(2),xt3(3)
format(3e20.8)
write(9,598) xt4(1),xt4(2),xt4(3)
format(3e20.8)
write(9,597) xt5(1),xt5(2),xt5(3)
format(3e20.8)

dummy=1.0
return
end

subroutine cthout(ip, jp, kp, lp, y)
nummat=1
numsub=49
c

c1=(denref/den)**(1./3.)
c2=(1.-phi)**(1./3.)
c3=c2/c1

do 10 i=1,3
    do 11 j=1,3
       f(i,j)=y(3*(i-1)+j+9)
    write(4,101) i,j,f(i,j)
10 continue

101 format (i5,i5,e15.6)

continue

c
    call detcal(f,detf)
    denout=denref/detf

do 12 i=1,3
    vtc(i)=1.0e+6*y(27+i)/rmass
12 continue

do 20 i=1,3
    xt1(i)=0.0
    xt2(i)=0.0
    xt3(i)=0.0
    xt4(i)=0.0
write(4,102) x1(i),x2(i),x4(i),x4(i),xc(i)
102 format (5e15.6)

continue

do 23 i=1,3
    do 21 j=1,3
       xt1(i)=xt1(i)+c3*f(i,j)*(x1(j)-xc(j))
       xt2(i)=xt2(i)+c3*f(i,j)*(x2(j)-xc(j))
       xt3(i)=xt3(i)+c3*f(i,j)*(x3(j)-xc(j))
       xt4(i)=xt4(i)+c3*f(i,j)*(x4(j)-xc(j))
21 continue
23 continue

go to 301

do 22 i=1,3
    xt1(i)=xt1(i)+y(30+i)
    xt2(i)=xt2(i)+y(30+i)
    xt3(i)=xt3(i)+y(30+i)
    xt4(i)=xt4(i)+y(30+i)
22 continue

c
301 dummy=1.0

write(4,501) ip,jp,kp,lp
501 format (5x,'package ',i3,',',i3,',',i3,',',i3,',',i3)
write(4,502) nummat,numsub
502 format (7x,'material ',i3,/'numsub ',i3)
write(4,532) denout
532 format (7x,'density = ',e20.8)
write(4,503) vtc(1)
503 format (7x,'xvel1 = ',e20.8)
write(4,504) vtc(2)
504 format(7x,'yvel = ',e20.8)  
write(4,594) vtc(3)  
594 format(7x,'zvel = ',e20.8)  
write(4,505)  
505 format(7x,'insert pyramid')  
write(4,506) xtl(1),xt1(2),xt1(3)  
506 format(9x,'point = ',e15.6,',',e15.6,',',e15.6)  
write(4,507) xtl(2),xt2(2),xt2(3)  
507 format(9x,'point = ',e15.6,',',e15.6,',',e15.6)  
write(4,508) xtl(3),xt3(2),xt3(3)  
508 format(9x,'point = ',e15.6,',',e15.6,',',e15.6)  
write(4,509) xtl(4),xt4(2),xt4(3)  
509 format(9x,'vertex = ',e15.6,',',e15.6,',',e15.6)  
write(4,509)  
591 format(5x,'endpackage')  
write(4,591)  
return  
end  
subroutine prtout (iend, time, yt)  
c**** subroutine prtout  
c  
dimension yt(33,101)  
dimension time(101), out(18,101), f(3,3), e(3,3), ep(3,3), 
c  
c  
print output  
open(9, file='pltdat/dc3d.out')  
open(11, file='pltdat/h11.plt')  
open(12, file='pltdat/h12.plt')  
open(13, file='pltdat/h13.plt')  
open(14, file='pltdat/h21.plt')  
open(15, file='pltdat/h22.plt')  
open(16, file='pltdat/h23.plt')  
open(17, file='pltdat/h31.plt')  
open(18, file='pltdat/h32.plt')  
open(19, file='pltdat/h33.plt')  
open(20, file='pltdat/f11.plt')  
open(21, file='pltdat/f12.plt')  
open(22, file='pltdat/f13.plt')  
open(23, file='pltdat/f21.plt')  
open(24, file='pltdat/f22.plt')  
open(25, file='pltdat/f23.plt')  
open(26, file='pltdat/f31.plt')  
open(27, file='pltdat/f32.plt')  
open(28, file='pltdat/f33.plt')  
open(29, file='pltdat/epl1.plt')  
open(30, file='pltdat/epl2.plt')  
open(31, file='pltdat/epl3.plt')  
open(32, file='pltdat/epl21.plt')
open(33, file='pltdat/ep22.plt')
open(34, file='pltdat/ep23.plt')
open(35, file='pltdat/ep31.plt')
open(36, file='pltdat/ep32.plt')
open(37, file='pltdat/ep33.plt')
c
open(38, file='pltdat/pl.plt')
open(39, file='pltdat/p2.plt')
open(40, file='pltdat/p3.plt')
c
open(41, file='pltdat/xcl.plt')
open(42, file='pltdat/xc2.plt')
open(43, file='pltdat/xc3.plt')
c
open(44, file='pltdat/detf.plt')
open(45, file='pltdat/ile.plt')
open(46, file='pltdat/j2e.plt')
open(47, file='pltdat/ilep.plt')
open(48, file='pltdat/j2ep.plt')
open(49, file='pltdat/detc.plt')
open(50, file='pltdat/out7.plt')
open(51, file='pltdat/out8.plt')
open(52, file='pltdat/out9.plt')
c
c print out the states
do 80 i=1,iend+1
   write(9,111) (yt(j,i), j=1, 33)
c 111 format(1le15.6)
c 80 continue
c
c calculate output variables
do 61 j=1,iend+1
   out(i,j)=0.0
61 continue
c 60 continue
c
do 611 j=1,3
do 612 k=1,3
   f(j,k) =yt(3*(j-1)+k+9,i)
   ep(j,k)=yt(3*(j-1)+k+18,i)
612 continue
611 continue
c
call detcal(f,detval)
call ecalc(f,e)
c
do 614 j=1,3
do 615 k=1,3
   if(j.eq.k) then
      deljk=1.0
   else
      deljk=0.0
   endif
\[ c(j, k) = \delta_{jk} + 2.0e(j, k) \]

615 continue
614 continue

\[
\begin{align*}
\text{call detcal}(c, \text{detc})
\end{align*}
\]

out(1, i) = detval
out(2, i) = (1.0/3.0) * (e(1, 1) + e(2, 2) + e(3, 3))
out(4, i) = (1.0/3.0) * (ep(1, 1) + ep(2, 2) + ep(3, 3))
out(6, i) = detc

610 continue

\[
\begin{align*}
do 52 & \quad j = 1, 9 \\
& \quad j1 = j \\
& \quad j2 = j + 9 \\
& \quad j3 = j + 18 \\
& \quad k1 = j + 10 \\
& \quad k2 = j + 19 \\
& \quad k3 = j + 28 \\
do 51 & \quad i = 1, \text{iend} + 1 \\
& \quad \text{write}(k1, 112) \text{ time}(i), yt(j1, i) \\
& \quad \text{write}(k2, 112) \text{ time}(i), yt(j2, i) \\
& \quad \text{write}(k3, 112) \text{ time}(i), yt(j3, i) \\
112 & \quad \text{format}(2e20.8) \\
& \quad 51 \quad \text{continue} \\
& \quad 52 \quad \text{continue} \\
\end{align*}
\]

\[
\begin{align*}
do 53 & \quad j = 1, 3 \\
& \quad j1 = j + 27 \\
& \quad j2 = j + 30 \\
& \quad k1 = j + 37 \\
& \quad k2 = j + 40 \\
do 54 & \quad i = 1, \text{iend} + 1 \\
& \quad \text{write}(k1, 102) \text{ time}(i), yt(j1, i) \\
& \quad \text{write}(k2, 102) \text{ time}(i), yt(j2, i) \\
102 & \quad \text{format}(2e20.8) \\
& \quad 54 \quad \text{continue} \\
& \quad 53 \quad \text{continue} \\
\end{align*}
\]

\[
\begin{align*}
do 55 & \quad j = 1, 9 \\
& \quad jj = j + 43 \\
do 56 & \quad i = 1, \text{iend} + 1 \\
& \quad \text{write}(jj, 113) \text{ time}(i), \text{out}(j, i) \\
113 & \quad \text{format}(2e20.8) \\
& \quad 56 \quad \text{continue} \\
& \quad 55 \quad \text{continue} \\
\end{align*}
\]

\[
\begin{align*}
do 50 & \quad i = 1, \text{iend} + 1 \\
& \quad \text{out1}(i) = yt(19, i) + yt(23, i) + yt(27, i) \\
& \quad \text{out2}(i) = \text{abs}(yt(19, i) - yt(23, i)) \\
& \quad \text{out3}(i) = \text{abs}(yt(23, i) - yt(27, i)) \\
& \quad \text{out4}(i) = \text{abs}(yt(19, i) - yt(27, i)) \\
& \quad \text{write}(11, 101) \text{ time}(i), \text{out1}(i), \text{out2}(i), \text{out3}(i), \text{out4}(i) \\
101 & \quad \text{format}(5e15.6) \\
& \quad 50 \quad \text{continue} \\
\end{align*}
\]

\[
\begin{align*}
\text{return}
\end{align*}
\]
subroutine detcal(a,deta)

**** subroutine detcal

dimension a(3,3)

deta = a(1,1)*(a(2,2)*a(3,3)-a(3,2)*a(2,3)) -
1 a(1,2)*(a(2,1)*a(3,3)-a(2,3)*a(3,1)) +
2 a(1,3)*(a(2,1)*a(3,2)-a(3,1)*a(2,2))

return
end

subroutine eldata(ii, jj, kk, ll)

**** subroutine eldata

common/props/den, denref, rmass, vmu, vlamb, eta, zeta, phi, rj(3,3)

common/mesh/il, i2, jl, j2, kl, k2, deltx, delty, deltz, 1 xlow, ylow, zlow

common/cthdat/ velx(75,75,75), vely(75,75,75),
1 velz(75,75,75), pres(75,75,75), temp(75,75,75),
2 gama(75,75,75), spen(75,75,75), vmas(75,75,75),
3 vphi(75,75,75), cspd(75,75,75)

rmass = vmas(ii, jj, kk)

den = gama(ii, jj, kk)

phi = vphi(ii, jj, kk)

denref = 2.7

dmge = 0.0

vmu = (1. - dmge) * 1.0

vlamb = (1. - dmge) * 1.0

eta = 1.0

write(10,100) velx(ii, jj, kk), vely(ii, jj, kk), velz(ii, jj, kk),
1 pres(ii, jj, kk), temp(ii, jj, kk), gama(ii, jj, kk), spen(ii, jj, kk),
2 vmas(ii, jj, kk), vphi(ii, jj, kk), cspd(ii, jj, kk)

100 format (/7e11.3,/3e11.3,/)  

return
end

subroutine nddata(ii, jj, kk, ll)

**** subroutine nddata

common/ndata/x1(3), x2(3), x3(3), x4(3),
1 v1(3), v2(3), v3(3), v4(3), xc(3)

common/mesh/il, i2, j1, j2, k1, k2, deltx, delty, deltz, 1 xlow, ylow, zlow
common/cthdat/ velx(75,75,75), vely(75,75,75),
velz(75,75,75), pres(75,75,75), temp(75,75,75),
gama(75,75,75), spen(75,75,75), vmas(75,75,75),
vphi(75,75,75), cspd(75,75,75)

common/cthxyz/xcth(100), ycth(100), zcth(100)

common/vellng/vfx(75,75,75), vfy(75,75,75), vfz(75,75,75)

set cell coordinates

xn1=xcth(ii)
yn1=ycth(jj)
zn1=zcth(kk)

xn2=xcth(ii+1)
yn2=ycth(jj)
zn2=zcth(kk)

xn3=xcth(ii+1)
yn3=ycth(jj+1)
zn3=zcth(kk)

xn4=xcth(ii)
yn4=ycth(jj+1)
zn4=zcth(kk+1)

xn5=xcth(ii)
yn5=ycth(jj)
zn5=zcth(kk+1)

xn6=xcth(ii+1)
yn6=ycth(jj)
zn6=zcth(kk+1)

xn7=xcth(ii+1)
yn7=ycth(jj+1)
zn7=zcth(kk+1)

xn8=xcth(ii)
yn8=ycth(jj+1)
zn8=zcth(kk+1)

set element coordinates

go to (301,302,303,304,305) 11

301 x1(1)=xn1
x1(2)=yn1
x1(3)=zn1
x2(1)=xn2
x2(2)=yn2
x2(3)=zn2
x3(1)=xn4
x3(2)=yn4
x3(3)=zn4
x4(1)=xn5
x4(2)=yn5
x4(3)=zn5

go to 306

302 x1(1)=xn3
x1(2)=yn3
x1(3) = zn3
x2(1) = xn4
x2(2) = yn4
x2(3) = zn4
x3(1) = xn2
x3(2) = yn2
x3(3) = zn2
x4(1) = xn7
x4(2) = yn7
x4(3) = zn7
go to 306

303 x1(1) = xn4
x1(2) = yn4
x1(3) = zn4
x2(1) = xn2
x2(2) = yn2
x2(3) = zn2
x3(1) = xn7
x3(2) = yn7
x3(3) = zn7
x4(1) = xn5
x4(2) = yn5
x4(3) = zn5
go to 306

304 x1(1) = xn8
x1(2) = yn8
x1(3) = zn8
x2(1) = xn5
x2(2) = yn5
x2(3) = zn5
x3(1) = xn7
x3(2) = yn7
x3(3) = zn7
x4(1) = xn4
x4(2) = yn4
x4(3) = zn4
go to 306

305 x1(1) = xn6
x1(2) = yn6
x1(3) = zn6
x2(1) = xn7
x2(2) = yn7
x2(3) = zn7
x3(1) = xn5
x3(2) = yn5
x3(3) = zn5
x4(1) = xn2
x4(2) = yn2
x4(3) = zn2
go to 306

306 dummy = 1.0
c
set cell velocities
vxn1 = vfx(ii, jj, kk)
vxn2 = vfx(ii+1, jj, kk)
vxn3 = vfx(ii+1, jj+1, kk)
vxn4 = vfx(ii, jj+1, kk)
vxn5 = vfx(ii, jj, kk+1)
vxn6 = vfx(ii+1, jj, kk+1)
vxn7 = vfx(ii, jj+1, kk+1)
vxn8 = vfx(ii+1, jj+1, kk+1)

vyn1 = vfy(ii, jj, kk)
vyn2 = vfy(ii+1, jj, kk)
vyn3 = vfy(ii+1, jj+1, kk)
vyn4 = vfy(ii, jj+1, kk)
vyn5 = vfy(ii, jj, kk+1)
vyn6 = vfy(ii+1, jj, kk+1)
vyn7 = vfy(ii, jj+1, kk+1)
vyn8 = vfy(ii+1, jj+1, kk+1)

vzn1 = vfx(ii, jj, kk)
vzn2 = vfx(ii+1, jj, kk)
vzn3 = vfx(ii+1, jj+1, kk)
vzn4 = vfx(ii, jj+1, kk)
vzn5 = vfx(ii, jj, kk+1)
vzn6 = vfx(ii+1, jj, kk+1)
vzn7 = vfx(ii, jj+1, kk+1)
vzn8 = vfx(ii+1, jj+1, kk+1)

set nodal velocities

go to (331, 332, 333, 334, 335) 11

331 v1(1) = vxn1
v1(2) = vyn1
v1(3) = vzn1
v2(1) = vxn2
v2(2) = vyn2
v2(3) = vzn2
v3(1) = vxn4
v3(2) = vyn4
v3(3) = vzn4
v4(1) = vxn5
v4(2) = vyn5
v4(3) = vzn5
go to 336

332 v1(1) = vxn3
v1(2) = vyn3
v1(3) = vzn3
v2(1) = vxn4
v2(2) = vyn4
v2(3) = vzn4
v3(1) = vxn2
v3(2) = vyn2
v3(3) = vzn2
v4(1) = vxn7
v4(2) = vyn7
v4(3) = vzn7
go to 336
c

333 v1(1)=vxn4
v1(2)=vyn4
v1(3)=vzn4
v2(1)=vxn2
v2(2)=vyn2
v2(3)=vzn2
v3(1)=vxn7
v3(2)=vyn7
v3(3)=vzn7
v4(1)=vxn5
v4(2)=vyn5
v4(3)=vzn5
go to 336

c

334 v1(1)=vxn8
v1(2)=vyn8
v1(3)=vzn8
v2(1)=vxn5
v2(2)=vyn5
v2(3)=vzn5
v3(1)=vxn7
v3(2)=vyn7
v3(3)=vzn7
v4(1)=vxn4
v4(2)=vyn4
v4(3)=vzn4
go to 336

c

335 v1(1)=vxn6
v1(2)=vyn6
v1(3)=vzn6
v2(1)=vxn7
v2(2)=vyn7
v2(3)=vzn7
v3(1)=vxn5
v3(2)=vyn5
v3(3)=vzn5
v4(1)=vxn2
v4(2)=vyn2
v4(3)=vzn2
go to 336

c

336 dummy=2.0
c
c set initial coordinates
c
go to 337
c
x1(1)=0.0
x1(2)=0.0
x1(3)=0.0
x2(1)=1.0
x2(2)=0.0
x2(3)=0.0
x3(1)=0.5
x3(2)=sqrt(0.75)
x3(3)=0.0
x4(1)=0.5
x4(2)=sqrt(0.75)/3.
x4(3)=1.0

set initial velocities

v1(1)=1.0
v1(2)=0.0
v1(3)=0.0
v2(1)=0.0
v2(2)=0.0
v2(3)=0.0
v3(1)=0.0
v3(2)=0.0
v3(3)=0.0
v4(1)=0.0
v4(2)=0.0
v4(3)=0.0

337 dummy=3.0
do 350 ip=1,3
write(10,340) x1(ip),x2(ip),x3(ip),x4(ip)
continue
write(10,341)
format(' ')
do 352 ip=1,3
write(10,342) v1(ip),v2(ip),v3(ip),v4(ip)
continue
337 dummy=3.0
return
end

subroutine initlz(h,f,ep,p)

common/props/den,dref,rmass,vmu,vlamb,eta,phi,rj(3,3)
common/ndata/x1(3),x2(3),x3(3),x4(3),
v1(3),v2(3),v3(3),v4(3),xc(3)
dimension h(3,3),f(3,3),ep(3,3),p(3)

set initial conditions

f(1,1)=1.0
f(1,2)=0.0
f(1,3)=0.0
f(2,1)=0.0
f(2,2)=1.0
f(2,3)=0.0
f(3,1)=0.0
f(3,2)=0.0
f(3,3)=1.0

c detf=denref/den

c f(1,1)=det**(1./3.)
f(2,2)=det**(1./3.)
f(3,3)=det**(1./3.)

c detf=f(1,1)*(f(2,2)*f(3,3)-f(3,2)*f(2,3))-1
2 f(1,2)*(f(2,1)*f(3,3)-f(2,3)*f(3,1))+
c f(1,3)*(f(2,1)*f(3,2)-f(3,1)*f(2,2))

c den=denref/detf

c write(10,103) den
103 format (e20.8)

c ep(1,1)=0.0
ep(1,2)=0.0
ep(1,3)=0.0
ep(2,1)=0.0
ep(2,2)=0.0
ep(2,3)=0.0
ep(3,1)=0.0
ep(3,2)=0.0
ep(3,3)=0.0

c h(1,1)=0.0
h(1,2)=0.0
h(1,3)=0.0
h(2,1)=0.0
h(2,2)=0.0
h(2,3)=0.0
h(3,1)=0.0
h(3,2)=0.0
h(3,3)=0.0

c p(1)=0.0
p(2)=0.0
p(3)=0.0

call ivcalc(h,p)

c xc(1)=0.5
xc(2)=sqrt(0.75)/3.
xc(3)=1.0/4.0

return
end

subroutine fcn(neq,t,y,yprime)

**** subroutine fcn

c common/props/den,denref,rmass,vmu,vlamb,eta,zeta,phi,rj(3,3)
common/ndata/x1(3),x2(3),x3(3),x4(3),
1 v1(3),v2(3),v3(3),v4(3),xc(3)
dimension y(33), yprime(33)

dimension h(3,3), f(3,3), f1(3,3), e(3,3), ep(3,3), p(3),
rji(3,3), rm(3,3,3,3), rk(3,3), rk1(3,3), c(3,3), ci(3,3),
vg(3,3), dd(3,3), rm(3,3,3,3), vkv(3,3), xct(3)

dimension hd(3,3), fd(3,3), ed(3,3), epd(3,3), pd(3), xcd(3)

define variables

do 10 i=1,3
  do 11 j=1,3
    h(i,j) = y(3*(i-1)+j)
  continue
  continue

  do 13 i=1,3
    do 14 j=1,3
      c(i,j)=0.0
    continue
  continue

  do 15 ia=1,3
    c(i,j)=c(i,j)+f(ia,i)*f(ia,j)
  continue
  continue

  ninv=3
  ldc=3
  ldcinv=3

  call linrg(ninv, c, ldc, ci, ldcinv)
  iflag=1
  call matv03(iflag, ninv, c, ci)

  do 12 i=1,3
    p(i) = y(i+27)
    xct(i) = y(i+30)
  continue

  call ecalc(f, e)

  write(10,104)
  format('subroutine fcn')

  call jcalc(den, x1, x2, x3, x4, rj)

  write(10,105)
  format('subroutine fcn jcalc')

  do 201 ii=1,3
    do 202 jj=1,3
      write(10,102) rj(ii,jj)
    continue
  continue

  call jinv(rj, rji)
calculate transformer modulus

do 20 i=1,3
do 21 j=1,3
do 22 ia=1,3
do 23 ib=1,3
if(i.eq.ib) then
   delib=1.0
else
   delib=0.0
endif
if(j.eq.ib) then
   deljb=1.0
else
   deljb=0.0
endif
rm(i,j,ia,ib)=0.5*(delib*f(ia,j)+f(ia,i)*deljb)
continue
continue
continue
continue
do 30 i=1,3
do 31 j=1,3
if(i.eq.j) then
   delij=1.0
else
   delij=0.0
endif
rk(i,j)=(rmass/denref)*(2.*vmu*(e(i,j)-ep(i,j))+
1 delij*vlamb*((e(1,1)+e(2,2)+e(3,3))-
2 (ep(1,1)+ep(2,2)+ep(3,3)))
rkp(i,j)=-rk(i,j)
call detcal(f,rvl)
rk(i,j)= (rmass/((1.-phi)*denref))*2.*vmu*((e(i,j)-
1 (1./3.)*delij*(e(1,1)+e(2,2)+e(3,3)))-ep(i,j))
2 -(rmass/((1.-phi)*denref))*(vlamb+(2./3.)*vmu)*(1./rvl-1.)
3 *(1./rvl)*ci(i,j)
rkp(i,j)=-(rmass/((1.-phi)*denref))*2.*vmu*((e(i,j)-
1 (1./3.)*delij*(e(1,1)+e(2,2)+e(3,3)))-ep(i,j))
continue
continue
do 50 i=1,3
do 51 j=1,3
fd(i,j)=0.0
fd(i,j)=fd(i,j)+h(i,ia)*rji(ia,j)
continue
continue
continue
ninv=3
ldf=3
ldfinv=3

call linrg(ninv,f,ldf,fi,ldfinv)
iflag=2
call matv03(iflag,ninv,f,fi)

do 300 i=1,3
do 301 j=1,3
vg(i,j)=0.0
do 302 ia=1,3
vg(i,j)=vg(i,j)+fd(i,ia)*fi(ia,j)
302 continue
301 continue
300 continue

do 303 i=1,3
do 304 j=1,3
dd(i,j)=0.5*(vg(i,j)+vg(j,i))
304 continue
303 continue

calculate transformer modulus

do 220 i=1,3
do 221 j=1,3
do 222 ia=1,3
do 223 ib=1,3
if(i.eq.ib) then
  delib=1.0
else
  delib=0.0
endif
if(j.eq.ib) then
  deljb=1.0
else
  deljb=0.0
endif
rn(i,j,ib,ia)=0.5*(delib*fi(ia,j)+fi(ia,i)*deljb)
223 continue
222 continue
221 continue
220 continue

c zeta=1.0
call detcal(f,rvl)

do 231 i=1,3
do 232 j=1,3
vkv(i,j)=0.0
do 233 ia=1,3
do 234 ib=1,3
if(ia.eq.ib) then
  delab=1.0
else
  delab=0.0
endif
c vkv(i,j)=vkv(i,j)+zeta*rn(ia,ib,i,j)*dd(ia,ib)
vkv(i,j)=vkv(i,j)+zeta*(rmax*rvl/((1.-phi)*denref))
*rn(ia,ib,i,j)*
delab*(1./3.)*(dd(1,1)+dd(2,2)+dd(3,3))
delab*(1./3.)*amin(0.0,dd(1,1)+dd(2,2)+dd(3,3))
dd(ia,ib)
*(0.5*(dd(1,1)**2+dd(1,2)**2+dd(1,3)**2)+
  dd(2,1)**2+dd(2,2)**2+dd(2,3)**2+
  dd(3,1)**2+dd(3,2)**2+dd(3,3)**2)**
continue
continue
continue
continue
do 40 i=1,3
do 41 j=1,3
hd(i,j)=0.0
do 42 ia=1,3
do 43 ib=1,3
hd(i,j)=hd(i,j)-rn(ia,ib,i,j)*rk(ia,ib)
continue
continue
hd(i,j)=hd(i,j)-vkv(i,j)
continue
40 continue
do 60 i=1,3
do 61 j=1,3
epd(i,j)=-(1./eta)*rkp(i,j)
continue
continue
do 70 i=1,3
pd(i)=0.0
xcd(i)=(1./rmass)*p(i)
continue
set the vector yprime
do 80 i=1,3
do 81 j=1,3
yprime(3*(i-1)+j) = hd(i,j)
yprime(3*(i-1)+j+9) = fd(i,j)
yprime(3*(i-1)+j+18) = epd(i,j)
continue
continue
do 82 i=1,3
yprime(i+27)= pd(i)
yprime(i+30)=xcd(i)
continue
continue
do 201 ii=1,3
do 202 jj=1,3
write(10,102) f(ii,jj),fd(ii,jj),h(ii,jj),hd(ii,jj)
continue
continue
continue
return
end subroutine ecalc(f,e)

c**** subroutine ecalc

c  dimension f(3,3),e(3,3),c(3,3)

c  calculate e

do 10 i=1,3
  do 11 j=1,3
    e(i,j)=0.0
    c(i,j)=0.0
    if(i.eq.j) then
      delij=1.0
    else
      delij=0.0
    endif
  continue
  do 12 ia=1,3
    c(i,j)=c(i,j)+f(ia,i)*f(ia,j)
  12 continue
  continue
  e(i,j)=0.50*(c(i,j)-delij)
  continue
  continue
  return
end

subroutine jinv(z,zi)

c**** subroutine jinv

c  inverts the symmetric 3x3 matrix z

c  dimension z(3,3),zi(3,3)

c  z1=z(1,1)
z2=z(2,2)
z3=z(3,3)
z4=z(1,2)
z5=z(2,3)
z6=z(1,3)
c  det=z1*(z2*z3-z5*z5)-z4*(z4*z3-z5*z6)+z6*(z4*z5-z2*z6)
c  zi(1,1)=+(1./det)*(z2*z3-z5*z5)
  zi(2,1)=-(1./det)*(z4*z3-z5*z6)
  zi(3,1)=+(1./det)*(z4*z5-z2*z6)
  zi(1,2)=-(1./det)*(z4*z3-z5*z6)
  zi(2,2)=+(1./det)*(z1*z3-z6*z6)
  zi(3,2)=-(1./det)*(z1*z5-z4*z6)
  zi(1,3)=+(1./det)*(z4*z5-z2*z6)
  zi(2,3)=-(1./det)*(z1*z5-z4*z6)
G-30

zi(3,3) = +(1./det)*(z1*z2-z4*z4)

return

end

subroutine jref(g,rjp)

subroutine jref

common/props/den, denref, rmass, vmu, vlamb, eta, zeta, phi, rj(3, 3)
common/rdata/xxl (3), xx2 (3), xx3 (3), xx4 (3), xxc (3), vref

dimension g(3,3), rjp(3,3)

detg=g(1, 1)*g(2, 2)*g(3, 3)-g(3, 2)*g(2, 3)-
    g(1, 2)*g(2, 1)*g(3, 3)-g(2, 3)*g(3, 1)]+
    2 g(1, 3)*g(2, 1)*g(3, 2)-g(3, 1)*g(2, 2))

rmass=(1.0-phi)*den*vref*detg
rmass=abs((1.0-phi)*den*vref*detg)

calculate the reference inertia tensor

h1 = sqrt((xxl(1)-xxc(1))**2+(xxl(2)-xxc(2))**2+(xxl(3)-xxc(3))**2)

h2 = sqrt((xx2(1)-xxc(1))**2+(xx2(2)-xxc(2))**2+(xx2(3)-xxc(3))**2)

h3 = sqrt((xx3(1)-xxc(1))**2+(xx3(2)-xxc(2))**2+(xx3(3)-xxc(3))**2)

h4 = sqrt((xx4(1)-xxc(1))**2+(xx4(2)-xxc(2))**2+(xx4(3)-xxc(3))**2)

epl1 = (xxl(1)-xxc(1))/h1
epl2 = (xxl(2)-xxc(2))/h1
epl3 = (xxl(3)-xxc(3))/h1
ep12 = (xx2(1)-xxc(1))/h2
ep22 = (xx2(2)-xxc(2))/h2
ep23 = (xx2(3)-xxc(3))/h2
ep31 = (xx3(1)-xxc(1))/h3
ep32 = (xx3(2)-xxc(2))/h3
ep33 = (xx3(3)-xxc(3))/h3
ep41 = (xx4(1)-xxc(1))/h4
ep42 = (xx4(2)-xxc(2))/h4
ep43 = (xx4(3)-xxc(3))/h4

rjp11=(rmass/20.)*(h1**2)*ep11*ep11+(h2**2)*ep21*ep21
       +(h3**2)*ep31*ep31+(h4**2)*ep41*ep41

rjp12=(rmass/20.)*(h1**2)*ep11*ep12+(h2**2)*ep21*ep22
       +(h3**2)*ep31*ep32+(h4**2)*ep41*ep42

rjp13=(rmass/20.)*(h1**2)*ep11*ep13+(h2**2)*ep21*ep23
       +(h3**2)*ep31*ep33+(h4**2)*ep41*ep43

rjp21=(rmass/20.)*(h1**2)*ep12*ep11+(h2**2)*ep22*ep21
       +(h3**2)*ep32*ep31+(h4**2)*ep42*ep41

rjp22=(rmass/20.)*(h1**2)*ep12*ep12+(h2**2)*ep22*ep22
       +(h3**2)*ep32*ep32+(h4**2)*ep42*ep42

1 + (h3**2)*ep32*ep32+(h4**2)*ep42*ep42
rjp23= (rmass/20.)*((h1**2)*ep12*ep13+(h2**2)*ep22*ep23
1 + (h3**2)*ep32*ep33+(h4**2)*ep42*ep43

c
rjp31= (rmass/20.)*((h1**2)*ep13*ep11+(h2**2)*ep23*ep21
1 + (h3**2)*ep33*ep31+(h4**2)*ep43*ep41
rjp32= (rmass/20.)*((h1**2)*ep13*ep12+(h2**2)*ep23*ep22
1 + (h3**2)*ep33*ep32+(h4**2)*ep43*ep42
rjp33= (rmass/20.)*((h1**2)*ep13*ep13+(h2**2)*ep23*ep23
1 + (h3**2)*ep33*ep33+(h4**2)*ep43*ep43

c
rjp(1,1)=rjp11
rjp(1,2)=rjp12
rjp(1,3)=rjp13
rjp(2,1)=rjp21
rjp(2,2)=rjp22
rjp(2,3)=rjp23
rjp(3,1)=rjp31
rjp(3,2)=rjp32
rjp(3,3)=rjp33

c
return
end

c subroutine jcalc(x1,x2,x3,x4,xc,rj)
c subroutine jcalc(den,x1,x2,x3,x4,xc,rj)
c**** subroutine jcalc

c common/rdata/xxl(3),xx2(3),xx3(3),xx4(3),xxc(3),vref
c dimension x1(3),x2(3),x3(3),x4(3),rj(3,3),
1 rjp(3,3),a(12,12),b(12),s(12),ainv(12,12),
2 g(3,3),ginv(3,3),xc(3),am1(12,12),am2(12,12)
c set the reference tetrahedron
xx1 (1)=0.0
xx1 (2)=0.0
xx1 (3)=0.0
xx2 (1)=1.0
xx2 (2)=0.0
xx2 (3)=0.0
xx3 (1)=0.5
xx3 (2)=sqrt(0.75)
xx3 (3)=0.0
xx4 (1)=0.5
xx4 (2)=sqrt(0.75)/3.
xx4 (3)=1.0
xxc (1)=0.5
xxc (2)=sqrt(0.75)/3.
xxc (3)=1.0/4.0
vref=(1./3.)*(1./2.)*sqrt(0.75)
c set the right hand side vector
\begin{align*}
\text{set the coefficient matrix} \\

a(1, 1) &= x_{1}(1) - x_{c}(1) \\
(a, 2) &= x_{1}(2) - x_{c}(2) \\
(a, 3) &= x_{1}(3) - x_{c}(3) \\
(a, 4) &= 0.0 \\
(a, 5) &= 0.0 \\
(a, 6) &= 0.0 \\
(a, 7) &= 0.0 \\
(a, 8) &= 0.0 \\
(a, 9) &= 0.0 \\
(a, 10) &= 1.0 \\
(a, 11) &= 0.0 \\
(a, 12) &= 0.0 \\

\text{set the coefficient matrix} \\

a(2, 1) &= 0.0 \\
(a, 2) &= 0.0 \\
(a, 3) &= 0.0 \\
(a, 4) &= x_{1}(1) - x_{c}(1) \\
(a, 5) &= x_{1}(2) - x_{c}(2) \\
(a, 6) &= x_{1}(3) - x_{c}(3) \\
(a, 7) &= 0.0 \\
(a, 8) &= 0.0 \\
(a, 9) &= 0.0 \\
(a, 10) &= 0.0 \\
(a, 11) &= 1.0 \\
(a, 12) &= 0.0 \\

\text{set the coefficient matrix} \\

a(3, 1) &= 0.0 \\
(a, 2) &= 0.0 \\
(a, 3) &= 0.0 \\
(a, 4) &= 0.0 \\
(a, 5) &= 0.0 \\
(a, 6) &= 0.0 \\
(a, 7) &= x_{1}(1) - x_{c}(1) \\
(a, 8) &= x_{1}(2) - x_{c}(2) \\
(a, 9) &= x_{1}(3) - x_{c}(3) \\
(a, 10) &= 0.0 \\
(a, 11) &= 0.0 \\
(a, 12) &= 1.0 \\

\text{set the coefficient matrix} \\

a(4, 1) &= x_{2}(1) - x_{c}(1) \\
(a, 2) &= x_{2}(2) - x_{c}(2) \\
(a, 3) &= x_{2}(3) - x_{c}(3) \\
(a, 4) &= 0.0
\end{align*}
\[
\begin{align*}
a(4,5) &= 0.0 \\
a(4,6) &= 0.0 \\
a(4,7) &= 0.0 \\
a(4,8) &= 0.0 \\
a(4,9) &= 0.0 \\
a(4,10) &= 1.0 \\
a(4,11) &= 0.0 \\
a(4,12) &= 0.0 \\
a(5,1) &= 0.0 \\
a(5,2) &= 0.0 \\
a(5,3) &= 0.0 \\
a(5,4) &= xx2(1) - xxc(1) \\
a(5,5) &= xx2(2) - xxc(2) \\
a(5,6) &= xx2(3) - xxc(3) \\
a(5,7) &= 0.0 \\
a(5,8) &= 0.0 \\
a(5,9) &= 0.0 \\
a(5,10) &= 0.0 \\
a(5,11) &= 1.0 \\
a(5,12) &= 0.0 \\
a(6,1) &= 0.0 \\
a(6,2) &= 0.0 \\
a(6,3) &= 0.0 \\
a(6,4) &= 0.0 \\
a(6,5) &= 0.0 \\
a(6,6) &= 0.0 \\
a(6,7) &= xx2(1) - xxc(1) \\
a(6,8) &= xx2(2) - xxc(2) \\
a(6,9) &= xx2(3) - xxc(3) \\
a(6,10) &= 0.0 \\
a(6,11) &= 0.0 \\
a(6,12) &= 1.0 \\
a(7,1) &= xx3(1) - xxc(1) \\
a(7,2) &= xx3(2) - xxc(2) \\
a(7,3) &= xx3(3) - xxc(3) \\
a(7,4) &= 0.0 \\
a(7,5) &= 0.0 \\
a(7,6) &= 0.0 \\
a(7,7) &= 0.0 \\
a(7,8) &= 0.0 \\
a(7,9) &= 0.0 \\
a(7,10) &= 1.0 \\
a(7,11) &= 0.0 \\
a(7,12) &= 0.0 \\
a(8,1) &= 0.0 \\
a(8,2) &= 0.0 \\
a(8,3) &= 0.0 \\
a(8,4) &= xx3(1) - xxc(1) \\
a(8,5) &= xx3(2) - xxc(2) \\
a(8,6) &= xx3(3) - xxc(3) \\
a(8,7) &= 0.0 \\
a(8,8) &= 0.0 \\
a(8,9) &= 0.0 \\
a(8,10) &= 0.0
\end{align*}
\]
```plaintext
a(8, 11) = 1.0
a(8, 12) = 0.0

c
a(9, 1) = 0.0
a(9, 2) = 0.0
a(9, 3) = 0.0
a(9, 4) = 0.0
a(9, 5) = 0.0
a(9, 6) = 0.0
a(9, 7) = xx3(1) - xxc(1)
a(9, 8) = xx3(2) - xxc(2)
a(9, 9) = xx3(3) - xxc(3)
a(9, 10) = 0.0
a(9, 11) = 0.0
a(9, 12) = 1.0

c
a(10, 1) = xx4(1) - xxc(1)
a(10, 2) = xx4(2) - xxc(2)
a(10, 3) = xx4(3) - xxc(3)
a(10, 4) = 0.0
a(10, 5) = 0.0
a(10, 6) = 0.0
a(10, 7) = 0.0
a(10, 8) = 0.0
a(10, 9) = 0.0
a(10, 10) = 1.0
a(10, 11) = 0.0
a(10, 12) = 0.0

c
a(11, 1) = 0.0
a(11, 2) = 0.0
a(11, 3) = 0.0
a(11, 4) = xx4(1) - xxc(1)
a(11, 5) = xx4(2) - xxc(2)
a(11, 6) = xx4(3) - xxc(3)
a(11, 7) = 0.0
a(11, 8) = 0.0
a(11, 9) = 0.0
a(11, 10) = 0.0
a(11, 11) = 1.0
a(11, 12) = 0.0

c
a(12, 1) = 0.0
a(12, 2) = 0.0
a(12, 3) = 0.0
a(12, 4) = 0.0
a(12, 5) = 0.0
a(12, 6) = 0.0
a(12, 7) = xx4(1) - xxc(1)
a(12, 8) = xx4(2) - xxc(2)
a(12, 9) = xx4(3) - xxc(3)
a(12, 10) = 0.0
a(12, 11) = 0.0
a(12, 12) = 1.0

c

ss

ninv=12
```
lda=12
daINV=12
c
write(10,106)
c106 format('sub jcalt before solver')
c
do 108 iii=1,12
do 109 jjj=1,12
cwrite(10,110) a(iii,jjj)
c110 format(e20.8)
c109 continue
c108 continue
c
call linrg(ninv,a,lda,aINV,ldaINV)
iflag=3
call matv12(iflag,ninv,a,aINV)
c
call amod1(a,am1)
c
call matinv(ninv,am1,am2)
c
call amod2(AM2,aINV)
c
cwrite(10,107)
c107 format('sub jcalt after solver')
c
calculate the solution vector

do 10 i=1,12
s(i)=0.0
do 11 j=1,12
s(i)=s(i)+aINV(i,j)*b(j)
11 continue
cwrite(4,876) i,b(i),s(i)
c876 format(ix,i5,2e15.3)
10 continue
c
set the tensor g

g(1,1)=s(1)
g(1,2)=s(2)
g(1,3)=s(3)
g(2,1)=s(4)
g(2,2)=s(5)
g(2,3)=s(6)
g(3,1)=s(7)
g(3,2)=s(8)
g(3,3)=s(9)
c
xc(1)=s(10)
xc(2)=s(11)
xc(3)=s(12)
c
invert the tensor g
c

call inverse solver
c
nINV=3
ldg=3
ldgINV=3
call linrg(ninv,g,ldg,ginv,ldginv)
iflag=4
call matv03(iflag,ninv,g,ginv)
call jref(g,rjp)
calculate the inertia tensor
do 20 i=1,3
do 21 j=1,3
rj(i,j)=0.0
do 22 ia=1,3
do 23 ib=1,3
rj(i,j)=rj(i,j)+ginv(ia,i)*rjp(ia,ib)*ginv(ib,j)
23 continue
22 continue
21 continue
20 continue
return
end

subroutine ivcalc(h,p)
**** subroutine ivcalc
common/props/den,denref,rmass,vmu,vlamb,eta,zeta,phi,rj(3,3)
common/rdata/xxl(3),xx2(3),xx3(3),xx4(3),xxc(3),vref
common/ndata/xl(3),x2(3),x3(3),x4(3),xl(3)
1 v1(3),v2(3),v3(3),v4(3),xc(3)
dimension a(12,12),b(12),s(12),ainv(12,12),
1 g(3,3),h(3,3),p(3),aml(12,12),am2(12,12)
set the right hand side vector
b(1) =v1(1)
b(2) =v1(2)
b(3) =v1(3)
b(4) =v2(1)
b(5) =v2(2)
b(6) =v2(3)
b(7) =v3(1)
b(8) =v3(2)
b(9) =v3(3)
b(10) =v4(1)
b(11) =v4(2)
b(12) =v4(3)
set the coefficient matrix
a(1,1) =xl(1)-xc(1)
a(1,2) =xl(2)-xc(2)
a(1,3) =xl(3)-xc(3)
a(1,4) =0.0
a(1,5) =0.0
a(1,6) =0.0
<table>
<thead>
<tr>
<th></th>
<th>a(1, 7)</th>
<th>a(1, 8)</th>
<th>a(1, 9)</th>
<th>a(1, 10)</th>
<th>a(1, 11)</th>
<th>a(1, 12)</th>
</tr>
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\[
\begin{align*}
a(6, 1) &= 0.0 \\
a(6, 2) &= 0.0 \\
a(6, 3) &= 0.0 \\
a(6, 4) &= 0.0 \\
a(6, 5) &= 0.0 \\
a(6, 6) &= 0.0 \\
a(6, 7) &= x2(1) - xc(1) \\
a(6, 8) &= x2(2) - xc(2) \\
a(6, 9) &= x2(3) - xc(3) \\
a(6, 10) &= 0.0 \\
a(6, 11) &= 0.0 \\
a(6, 12) &= 1.0 \\
a(7, 1) &= x3(1) - xc(1) \\
a(7, 2) &= x3(2) - xc(2) \\
a(7, 3) &= x3(3) - xc(3) \\
a(7, 4) &= 0.0 \\
a(7, 5) &= 0.0 \\
a(7, 6) &= 0.0 \\
a(7, 7) &= 0.0 \\
a(7, 8) &= 0.0 \\
a(7, 9) &= 0.0 \\
a(7, 10) &= 1.0 \\
a(7, 11) &= 0.0 \\
a(7, 12) &= 0.0 \\
a(8, 1) &= 0.0 \\
a(8, 2) &= 0.0 \\
a(8, 3) &= 0.0 \\
a(8, 4) &= x3(1) - xc(1) \\
a(8, 5) &= x3(2) - xc(2) \\
a(8, 6) &= x3(3) - xc(3) \\
a(8, 7) &= 0.0 \\
a(8, 8) &= 0.0 \\
a(8, 9) &= 0.0 \\
a(8, 10) &= 0.0 \\
a(8, 11) &= 1.0 \\
a(8, 12) &= 0.0 \\
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a(9, 4) &= 0.0 \\
a(9, 5) &= 0.0 \\
a(9, 6) &= 0.0 \\
a(9, 7) &= x3(1) - xc(1) \\
a(9, 8) &= x3(2) - xc(2) \\
a(9, 9) &= x3(3) - xc(3) \\
a(9, 10) &= 0.0 \\
a(9, 11) &= 0.0 \\
a(9, 12) &= 1.0 \\
a(10, 1) &= x4(1) - xc(1) \\
a(10, 2) &= x4(2) - xc(2) \\
a(10, 3) &= x4(3) - xc(3) \\
a(10, 4) &= 0.0 \\
a(10, 5) &= 0.0
\end{align*}
\]
a(10,6) =0.0
a(10,7) =0.0
a(10,8) =0.0
a(10,9) =0.0
a(10,10)=1.0
a(10,11)=0.0
a(10,12)=0.0

c
a(11,1) =0.0
a(11,2) =0.0
a(11,3) =0.0
a(11,4) =x4(1)-xc(1)
a(11,5) =x4(2)-xc(2)
a(11,6) =x4(3)-xc(3)
a(11,7) =0.0
a(11,8) =0.0
a(11,9) =0.0
a(11,10)=0.0
a(11,11)=1.0
a(11,12)=0.0

c
call inverse solver
c
ninvs=12
lda=12
ldainv=12

c
write(10,106)
c 106 format('sub jcalc before solver')
c
do 108 iii=1,12
do 109 jjj=1,12
write(10,110) a(iii,jjj)
c 110 format(e20.8)
c 109 continue
c 108 continue
c
 call linrg(ninv,a,lda,ainv,ldainv)
iflag=5
 call matv12(iflag,ninv,a,ainv)
c
 call amod1(a,am1)
c
 call matinv(ninv,am1,am2)
c
 call amod2(am2,ainv)
c
write(10,107)
calculate the solution vector

\[ \text{do } 10 \text{ } i=1,12 \]
\[ s(i)=0.0 \]
\[ \text{do } 11 \text{ } j=1,12 \]
\[ s(i)=s(i)+\text{ainv}(i,j)\cdot b(j) \]
\[ 11 \text{ continue} \]
\[ 10 \text{ continue} \]

set the tensor \( g \)

\[ \text{const}=(\text{denref}/\text{den})^{(1./3.)} \]
\[ g(1,1)=s(1)\cdot \text{const} \]
\[ g(1,2)=s(2)\cdot \text{const} \]
\[ g(1,3)=s(3)\cdot \text{const} \]
\[ g(2,1)=s(4)\cdot \text{const} \]
\[ g(2,2)=s(5)\cdot \text{const} \]
\[ g(2,3)=s(6)\cdot \text{const} \]
\[ g(3,1)=s(7)\cdot \text{const} \]
\[ g(3,2)=s(8)\cdot \text{const} \]
\[ g(3,3)=s(9)\cdot \text{const} \]

\[ p(1)=s(10)\cdot \text{rmass} \]
\[ p(2)=s(11)\cdot \text{rmass} \]
\[ p(3)=s(12)\cdot \text{rmass} \]

calculate the tensor \( h \)

\[ \text{do } 20 \text{ } i=1,3 \]
\[ \text{do } 21 \text{ } j=1,3 \]
\[ h(i,j)=0.0 \]
\[ \text{do } 22 \text{ } ia=1,3 \]
\[ h(i,j)=h(i,j)+g(i,ia)\cdot rj(ia,j) \]
\[ 22 \text{ continue} \]
\[ 21 \text{ continue} \]
\[ 20 \text{ continue} \]

return
end

subroutine ifdcrk(ido, neq, t, tend, tol, param, y)

dimension y(33), yprime(33), param(50)
dimension f1(33), f2(33), f3(33), f4(33), y1(33), y2(33), y3(33),
y4(33)

external fcn

nstep=1000
rnstep=nstep
delt=(tend-t)/rnstep

\[ \text{do } 10 \text{ } i=1, \text{nstep} \]
\[ ri=i \]
t1 = t + (ri - 1.0) * delt
\[ t2 = t1 + \text{delt}/2.0 \]
\[ t3 = t1 + \text{delt}/2.0 \]
\[ t4 = t1 + \text{delt} \]

\[ \text{do } 21 \ j = 1, \text{neq} \]
\[ y1(j) := y(j) \]
\[ \text{continue} \]

\[ \text{call fcn}(\text{neq}, t1, y1, f1) \]

\[ \text{do } 22 \ j = 1, \text{neq} \]
\[ y2(j) := y(j) + (\text{delt}/2.0) \times f1(j) \]
\[ \text{continue} \]

\[ \text{call fcn}(\text{neq}, t2, y2, f2) \]

\[ \text{do } 23 \ j = 1, \text{neq} \]
\[ y3(j) := y(j) + (\text{delt}/2.0) \times f2(j) \]
\[ \text{continue} \]

\[ \text{call fcn}(\text{neq}, t3, y3, f3) \]

\[ \text{do } 24 \ j = 1, \text{neq} \]
\[ y4(j) := y(j) + \text{delt} \times f3(j) \]
\[ \text{continue} \]

\[ \text{call fcn}(\text{neq}, t4, y4, f4) \]

\[ \text{do } 30 \ j = 1, \text{neq} \]
\[ y(j) := y(j) + (\text{delt}/6.0) \times (f1(j) + 2.0 \times f2(j) + 2.0 \times f3(j) + f4(j)) \]
\[ \text{continue} \]

\[ \text{return} \]

\[ \text{end} \]

\[ \text{subroutine ivdcrk}(\text{ido, neq, tbeg, tend, tol, param, y}) \]

\[ \text{common/intpar/epsint, ymxref} \]

\[ \text{dimension y(33), yw(33), ymax(33), param(50), err(33)} \]
\[ \text{dimension f1(33), f2(33), f3(33), f4(33), y1(33), y2(33), y3(33), y4(33)} \]

\[ \text{eps}=1.0 \times 10^{-6} \]
\[ \text{ymxref}=1.0 \times 10^{-6} \]

\[ \text{eps}=\text{epsint} \]

\[ \text{delmin}=1.0 \times 10^{-24} \]
\[ \text{nstep}=1000000 \]

\[ \text{rnstep}=\text{nstep} \]
\[ \text{delt}=(\text{tend-tbeg})/\text{rnstep} \]
\[ \text{delmin}=\text{delt}/10.0 \]
do 11 i=1,neq
  ymax(i)=amax1(ymxref,abs(y(i)))
11 continue

  t=tbeg

  t1=t
  if(t+delt.gt.tend) delt=tend-t
  t2=t+delt/2.0
  t3=t+delt

  do 91 i=1,neq
    yl(i)=y(i)
 91 continue

  call rkstep(ido,neq,t1,t3,tol,param,yl,y2)
call rkstep(ido,neq,t1,t2,tol,param,yl,y3)
call rkstep(ido,neq,t2,t3,tol,param,y3,y4)

  errmax=0.0
  do 12 i=1,neq
    err(i)=abs(y4(i)-y2(i))/(eps*ymax(i))
    errmax=amax1(errmax, err(i))
12 continue

  if(errmax.le.0.0) delt=2.0*delt
  if(errmax.gt.1.0) go to 101
  if(errmax.gt.0.0) delt=0.99*delt*errmax*(-1.0/5.0)

  do 21 i=1,neq
    y(i)=y4(i)
    ymax(i)=amax1(ymax(i),abs(y(i)))
 21 continue

  t=t3
  if(t.ge.tend) go to 99
  if(delt.lt.delmin) go to 98
  go to 100

101 delt=delt/2.0
  if(delt.lt.delmin) go to 98
  go to 100

98 ido=98
  write(10,110) ido, t, delt
110 format(1x,i5,2e15.3)

110 format(1x,'time step less than minimum, ido=',i5)
return

99 ido=99
  write(10,120) ido, t, delt
120 format(1x,i5,2e15.3)
return

end

subroutine rkstep(ido,neq,tbeg,tend,tol,param,y,yout)


dimension y(33), param(50), yout(33)
dimension f(33), f2(33), f3(33), f4(33), y(33), y2(33), y3(33), y4(33)

c
delt=tend-tbeg
t1=tbeg
t2=t1+delt/2.0
t3=t1+delt/2.0
t4=t1+delt
c
do 21 j=1, neq
   y1(j)=y(j)
21 continue
c
call fcn(neq, t1, y1, f1)
c
do 22 j=1, neq
   y2(j)=y(j)+(delt/2.0)*f1(j)
22 continue
c
call fcn(neq, t2, y2, f2)
c
do 23 j=1, neq
   y3(j)=y(j)+(delt/2.0)*f2(j)
23 continue
c
call fcn(neq, t3, y3, f3)
c
do 24 j=1, neq
   y4(j)=y(j)+delt*f3(j)
24 continue
c
call fcn(neq, t4, y4, f4)
c
do 30 j=1, neq
   yout(j)=y(j)+(delt/6.0)*((f1(j)+2.0*f2(j)+2.0*f3(j)+f4(j))
30 continue
c
return
end

c subroutine matv12(iflag, n, rm, rmi)
c
gauss-jordon elimination
c
dimension rm(12,12), rmw(12,12), rmi(12,12), chk(12,12),
1 v(12), vw(12), itrak(12)
c
c open(1, file='gauss.inp')
c
c open(2, file='gauss.out')
c
c write(10, 101) n
c 101 format(/'n=', i5)
c
c do 40 i=1, n
c do 41 j=1, n
c write(10, 422) rm(i, j)
c 422 format(e15.3)
c 41 continue
c 40 continue
c c do 42 i=1,n
c read(1,423) v(i)
c 423 format (el5.3)
c vw(i)=v(i)
c 42 continue
c c do 20 i=1,n
itrak(i)=i
c do 21 j=1,n
rmw(i,j)=rm(i,j)
chk(i,j)=0.0
rmi(i,j)=0.0
if(i.eq.j) rmi(i,j)=1.0
21 continue
c 20 continue
c c do 10 i=1,n
isav=i
pmag=abs(rmw(i,i))
c do 301 irow=1,n
tmpnum=abs(rmw(irow,i))
if(tmpnum.gt.pmag) isav=irow
301 continue
itrak(i)=isav
c do 302 jcol=1,n
hold=rmw(i,jcol)
rmw(i,jcol)=rmw(isav,jcol)
rmw(isav,jcol)=hold
hold=rmi(i,jcol)
rmi(i,jcol)=rmi(isav,jcol)
rmi(isav,jcol)=hold
302 continue
pivot=rmw(i,i)
vw(i)=vw(i)/pivot
 c do 11 jj=1,n
rmi(i,jj)=rmi(i,jj)/pivot
rmw(i,jj)=rmw(i,jj)/pivot
11 continue
c c do 12 k=1,n
if(k.eq.i) go to 12
scale=rmw(k,i)
vw(k)=vw(k)-scale*vw(i)
c do 13 j=1,n
rmi(k,j)=rmi(k,j)-scale*rmi(i,j)
rmw(k,j)=rmw(k,j)-scale*rmw(i,j)
13 continue
c 12 continue
c c 10 continue
c c go to 99
chksum=0.0
do 50 i=1,n
do 51 j=1,n
do 52 k=1,n
   chk(i,j)=chk(i,j)+rm(i,k)*rmi(k,j)
52 continue
   if(i.eq.j) chk(i,j)=chk(i,j)-1.0
   chksum=chksum+chk(i,j)**2
51 continue
50 continue

   if(iflag.ne.4) go to 99
   ichk=0
   if(chksum.ge.1.0e-12) ichk=-999
   write(4,222) ichk,iflag,n,chksum
222 format(1x,3i5,e15.3)
   do 30 i=1,n
do 31 j=1,n
   write(4,223) i,j,rm(i,j),rmw(i,j),rmi(i,j),chk(i,j)
223 format(1x,2i5,4e15.3)
31 continue
30 continue

99 dummy=1.0
   do 44 i=1,n
   write(2,223) i,v(i),vw(i)
223 format(1x,i5,2e15.3)
44 continue

return
end

subroutine matv03(iflag,n,rm,rmi)
   gauss-jordon elimination
   dimension rm(3,3),rmw(3,3),rmi(3,3),chk(3,3),
   1 v(3),vw(3),itrak(3)
   open(1,file='gauss.inp')
   open(2, file='gauss.out')
   write(10,101) n
101 format(/'n = ',i5)
do 40 i=1,n
do 41 j=1,n
   write(10,422) rm(i,j)
422 format(e15.3)
41 continue
40 continue
   do 42 i=1,n
   read(1,423) v(i)
423 format(e15.3)
vw(i) = v(i)
continue

do 20 i=1,n
itrak(i) = i
do 21 j=1,n
rmw(i, j) = rm(i, j)
chk(i, j) = 0.0
rmi(i, j) = 0.0
if (i .eq. j) rmi(i, j) = 1.0
continue
20 continue

do 10 i=1,n
isav = 1
pmag = abs(rmw(i, i))
do 301 irow = i, n
tmpnum = abs(rmw(irow, i))
if (tmpnum .gt. pmag) isav = irow
301 continue
itrak(i) = isav
do 302 jcol = 1, n
hold = rmw(i, jcol)
rmw(i, jcol) = rmw(isav, jcol)
rmw(isav, jcol) = hold
hold = rmi(i, jcol)
rmi(i, jcol) = rmi(isav, jcol)
rmi(isav, jcol) = hold
302 continue

pivot = rmw(i, i)
vw(i) = vw(i) / pivot

do 11 jj = 1, n
rmi(i, jj) = rmi(i, jj) / pivot
rmw(i, jj) = rmw(i, jj) / pivot
11 continue

do 12 k = 1, n
if (k .eq. i) go to 12
scale = rmw(k, i)
vw(k) = vw(k) - scale * vw(i)
do 13 j = 1, n
rmi(k, j) = rmi(k, j) - scale * rmi(i, j)
rmw(k, j) = rmw(k, j) - scale * rmw(i, j)
13 continue
12 continue

10 continue

go to 99

chksum = 0.0
do 50 i = 1, n
do 51 j = 1, n
do 52 k = 1, n
chk(i, j) = chk(i, j) + rm(i, k) * rmi(k, j)
52 continue
   if(i.eq.j) chk(i,j)=chk(i,j)-1.0
   checksum=checksum+chk(i,j)**2
51 continue
50 continue
   if(iflag.ne.4) go to 99
   ichk=0
   if(checksum.ge.1.0e-12) ichk=-999
   write(4,222) ichk,iflag,n,checksum
222 format(1x,3i5,e15.3)
   do 30 i=1,n
   do 31 j=1,n
      write(4,223) i,j,rm(i,j),rmw(i,j),rmi(i,j),chk(i,j)
223 format(1x,2i5,4e15.3)
31 continue
30 continue
99 dummy=1.0
   do 44 i=1,n
   write(2,223) i,v(i),vw(i)
223 format(1x,i5,2e15.3)
44 continue
return
end