BOUNDARY CONDITIONS AND ITERATIVE PROCEDURES FOR PLASMA SHEATH PROBLEMS

Lee W. Parker
Mt. Auburn Research Associates, Inc., Cambridge, Massachusetts

and

Edward C. Sullivan
Goddard Space Flight Center
National Aeronautics and Space Administration, Greenbelt, Maryland

Computer methods have recently been applied to a large class of steady-state collisionless plasma sheath problems, including, for example, moving satellites in the ionosphere,[1-5] stationary plasma probes,[6-8] ion engines,[9] and plasma diodes.[10] These problems involve numerical solutions of the Poisson equation. One aspect of such solutions which can cause difficulties is that in many cases[1-8] one boundary is at infinity, where the potential and net charge density vanish. Because of the limitations of digital computers, the potential and density descriptions are restricted to a finite portion of space, so that the boundary condition corresponding to "infinity" must be simulated by a necessarily artificial finite condition. Another aspect is that the density is generally a non-linear functional of the potential distribution, and that, with specified boundary conditions, an iteration procedure must be used in order to obtain a self-consistent solution. The stability of the iteration procedure depends, not only on the particular algorithm, but also on the artificial boundary condition employed, as will be shown later. Even in finite problems bounded by

electrodes,[9-10] the stability of the iteration is related to the magnitude of the electrode separation.[9-11]

This paper is concerned with the numerical effects of employing certain artificial finite boundary conditions and iterative procedures for self-consistent Poisson problems. Studies have been made with spherical probe and plasma diode models, with the goal of developing economical procedures for more general problems. Results obtained by the use of such models are not expected to depend strongly on their one-dimensionality. A third aspect of the plasma sheath problem, which is numerically non-trivial but will not be discussed, is that of finding the density when the potential distribution is given, in the presence of absorbing boundaries and non-isotropic velocity distributions. Alternative approaches for this calculation in a general problem are suggested in Refs. 2-6 and 12.

A common approach to the artificial finite boundary has been simply to set the potential to zero on a boundary surface as far "out" as possible, within computer limitations.[1-3] "Floating-potential" boundary conditions have also been used,[4-8] in which linear relationships have been assumed between the potential and its gradient. The question of how well a finite boundary condition approximates the "true" infinite boundary condition has been treated recently.[3-8] In these investigations, sequences of Poisson problems with identical boundary conditions were solved, where the boundary was successively moved outward until no further changes occurred, either in the potential distribution in the vicinity of the satellite,[3-4] or in the collected

probe current.[5-8] The solution obtained in this way may be taken to represent that for the "infinite" boundary condition, and will be said to have a "stationary" property with respect to the boundary position.

Computational costs are proportional to the size of the region enclosed by the boundary. If the boundary can be moved inward as a result of changing the boundary condition, without changing the stationary property of the solution, the calculation becomes more economical. In the case of a stationary spherical probe, for example, the potential is known to obey an inverse-square asymptotic law, and computer procedures employing floating boundary conditions based on this law[7-8] have been found to be far more economical than procedures in which the potential is set to zero. In the case of a moving satellite[4] or a circular planar probe,[5-6] where axially symmetric potential distributions occur and no theoretical asymptotic analysis is available, various ad hoc floating-potential relationships, based on intuition, have similarly been found to be more economical than setting the potential to zero. Taylor,[4] for example, has employed an exponential law as well as certain other special relationships, while Parker and Whipple[5-6] have employed a dipole law. In view of these results, it seems worthwhile to look for generally efficient assumptions. For example, for the spherical probe we have found that setting the gradient of the potential to zero at the boundary[13] is as economical as using the asymptotically correct inverse square law. Calculations will be presented which will compare floating conditions with the zero-potential condition.

The iterative phase of the procedure for obtaining self-consistent numerical solutions may be discussed in terms of the Poisson matrix equation in dimensionless form, namely:

$$L\,\vec{\phi} = -\,\vec{\rho}(\vec{\phi}) \qquad (1)$$

In (1), L is the Laplacian matrix operator resulting from the differencing of the Laplacian on a grid in configurational space. The components of the vectors $\vec{\phi}$ and $\vec{\rho}$ are the values of the potential and the net charge density, respectively, at the grid points. A general iterative procedure may be based on the mixing or coupling of density iterates, namely:

$$L\,\vec{\phi}_{n+1} = -\sum_{m=0}^{n} b_m \vec{\rho}(\vec{\phi}_m) \qquad (2)$$

where $\vec{\phi}_n$ denotes the n-th iterate for $\vec{\phi}$. Alternatively, of course, one may instead couple the potential iterates. The coefficients b_m determine the stability of the iteration.

Using the spherical probe model, we find that the iteration converges when the boundary radius R is less than a certain critical value R_c, and diverges when R is greater than R_c. Let R_s denote the boundary radius such that the probe current is stationary when $R > R_s$. The iteration will converge to the desired solution (with respect to the current) when $R_c > R_s$. With "direct" (uncoupled) iteration, in which $b_m = \delta_{mn}$ (Kronecker delta), R_c is usually less than R_s. Now R_s is fixed by the chosen boundary condition, but R_c can be made to become greater than R_s by a suitable choice of the coupling coefficients b_m.

In the iteration scheme with mixing parameter $\alpha < 1$, defined by

$$L\vec{\phi}_{n+1} = \vec{F}_{n+1} = -\alpha\vec{\rho}(\vec{\phi}_n) + (1 - \alpha)\,\vec{F}_n \qquad (3)$$

(where $\vec{F}_o \equiv 0$ so that $\vec{\phi}_o$ is the Laplace solution), the stability of the iteration (3) is found to increase as α decreases. For any value of R_s, one can apparently force convergence, i.e., cause R_c to exceed R_s, if one chooses a sufficiently small value of α. Equation (3) implies that b_m in (2) is given by $\alpha(1 - \alpha)^{n-m}$, so that for small α the coupling is approximately equally distributed over a large number of past iterates. The use of such an iteration corresponds to replacing the problem by an equivalent time-dependent parabolic heat-diffusion problem in difference form, in which the time index is analogous to the iteration index, and the steady-state solution is the desired one.[2] The use of a small value for α corresponds to the introduction of high damping in the heat-diffusion problem. The required number of iterations, and therefore computer time, is roughly inversely proportional to α.

Various versions of the iteration scheme (3) have been used.[1-3, 5-6, 8-11] Laframboise[8] has found that significant gains can result from additional sophistication, such as the use of an empirical diagonal matrix for α rather than a scalar, that is, a different mixing parameter for each grid point. We are pursuing this promising approach and hope to report new results.

One-dimensional plasma diode problems also afford convenient models for studying iterative stability.[10-11] Numerical instability seems to be connected with the existence of an extended region of space

where the charge density is small, in the vicinity of the point where it changes sign. As the electrode spacing increases, the extent of the regime of small charge density grows, and the parameter α must be reduced for convergence. If, in the plasma diode problem, we restrict attention to a region in the vicinity of the point where the charge density changes sign, and if we assume a linear relation between $\vec{\rho}$ and $\vec{\phi}$ in this region, then it can be shown analytically that α must be smaller than a number proportional to λ^2/D^2, where λ is the Debye length, and D is the extent of the region of linearity. If D is taken to be the electrode separation in an empirical formula, the data of Prince and Jeffries[10] indicates a constant of proportionality between 1 and 10 for large values of D/λ. It is interesting to note that in satellite problems with high ion Mach numbers,[2-3] iterative stability is found to increase with increasing Mach number. One can probably define in this case an effective Debye length, which is based on the ion energy and is therefore large.

In our experiments with the spherical probe model we have found that, for interesting values of the physical parameters, the scheme of Eq. (3) requires α to be of the order of 1/100. This small value implies that many iterations will be required, i.e., of the order of hundreds.[14] Details of these experiments will be presented.

Based on the parabolic nature of the iteration problem, it should be possible to devise more sophisticated iteration schemes which will reduce the number of iterations required and thereby reduce computer time.

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13. Suggested for the satellite wake problem by A. H. Davis (private communication)

14. As compared with the order of 10 iterations for the satellite wake problem[1, 3] and the circular planar probe problem[6]