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A Meshless Stochastic Algorithm for the Solution of the Nonlinear Poisson-Boltzmann Equation in the Context of Plasma Discharge Modeling: 1D Analytical Benchmark

Kausik Chatterjee*
Massachusetts Institute of Technology, Cambridge, MA, 02139

Jonathan Poggie†
Air Force Research Laboratory, Wright-Patterson Air Force Base, OH, 45433

This paper presents a new floating random-walk algorithm for the solution of the nonlinear Poisson-Boltzmann equation in the context of plasma discharge modeling. Previous studies using the floating random-walk method have examined only the linearized Poisson-Boltzmann equation, producing solutions that are only accurate for small values of the potential. This is due to the absence of analytical expressions for volumetric Green's functions for nonlinear equations. In this work, an approximate expression for a volumetric Green's function has been derived with the help of a novel use of iterative perturbation theory, and this expression has been incorporated within the floating random-walk framework. The floating random-walk method is based on probabilistic interpretations of deterministic equations and needs no discretization of either the volume or the surface of the problem domains. Hence the memory requirements are expected to be lower than approaches based on spatial discretization, such as the finite-difference or the finite-element method. Another advantage of this method is that the random-walks are statistically independent, so that the computational procedure is highly parallelizable and a nearly linear increase in computational speed is expected with an increase in the number of processors. In this paper, we present the preliminary results in one dimension where excellent agreement has been obtained with an analytical benchmark solution.

Nomenclature

$\mathbf{E}$ = Electric field
λ_D = Debye length
ε_o = permittivity of vacuum
k = Boltzmann constant
T = Temperature
n_e = number density of electrons
n_i = number density of ions
ρ = charge density
ϕ = potential
m_e = electron mass
m_i = ion mass
e = electronic charge

* Visiting Scientist, Electrical Engineering and Computer Science, Room 10-171, Cambridge, MA 02139, Email: kausik@mit.edu
† Research Aerospace Engineer, Air Vehicles Directorate, 2210 Eighth St, Bldg 146 Room 225, OH 45433, Associate Fellow, AIAA

I. Introduction

In recent years, plasma actuators have shown great promise as a means of flow control in aerospace applications[1-3]. Fundamentally, these flow control systems involve a plasma discharge between electrodes and the transformation of the associated electrical energy into kinetic and thermal energy in the air flow. The addition of such a system to an aerospace vehicle can introduce significant penalties in additional weight and power consumption. Accurate modeling of these systems is thus essential for determining whether the benefits outweigh the penalties[4-6]. However, the modeling of a plasma discharge in an air flow is computationally intensive. This is primarily because of the vast differences in fluid dynamic and electromagnetic time scales[4]. Iterative solutions of the Poisson equation for the electric potential constitute an important part of the computational effort, as this equation has to be converged at each time step.

In this paper, we develop a floating random-walk algorithm[7-9] for the nonlinear Poisson-Boltzmann equation. This method is based on probabilistic interpretations of deterministic equations and is completely meshless requiring no discretization of either the volume or the surface of problem domains. Consequently, the memory requirements for complicated problem geometries are expected to be significantly lower than discretization-based methods. Furthermore, the method is inherently parallelizable and a linear increase in computational speed is expected with an increase in the number of processors. The linearized version of the Poisson-Boltzmann equation and other equations has been studied extensively [10, 11] with the floating random-walk method. However, the floating random-walk method has not been widely applied in the numerical solution of nonlinear partial differential equations. This is because of the absence of analytical expressions for volumetric Green's functions[12] for nonlinear partial differential equations of significance. In this paper, we present a new technique that eliminates this restriction and extends the method to the numerical solution of the nonlinear Poisson-Boltzmann equation. We will describe the fundamentals of the algorithm in one dimension and demonstrate the agreement of this algorithm to an analytical benchmark solution. We believe that with additional work, the algorithm can be extended to two and three dimensions and to other nonlinear equations.

II. Problem Formulation

In this section, we present a simplified model for the space-charge boundary layer (plasma-sheath transition) that occurs in an ionized gas in the neighborhood of an electrode. The formation of this layer is attributed to the vast difference in electron and ion mobility and the fact that in the steady-state, the flux of the positive and negative charge carriers to the wall need to be balanced[13].

From Gauss's law, the electric field $\mathbf{E}$ due to a charge density ρ is given by

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_o} \tag{1}$$

The electric field can be expressed as the gradient of a scalar potential, ϕ in the absence of a time-varying magnetic field, and is given by

$$\mathbf{E} = -\nabla \phi. \tag{2}$$

If the electrons are assumed to be in thermodynamic equilibrium, the electron number density $n_e(\mathbf{r})$ follows the Boltzmann distribution[13] given by

$$n_e(\mathbf{r}) = n e^{e\phi(\mathbf{r})/kT}. \tag{3}$$

Above, n represents the number density at a reference point with zero potential. Assuming that the positively charged ions are also in thermodynamic equilibrium and the ions have the same temperature as the electrons, the number density $n_i(\mathbf{r})$ of the ions is given by

$$n_i(\mathbf{r}) = ne^{-e\phi(\mathbf{r})/kT}. \tag{4}$$

As $\rho = e(n_i - n_e)$, substitutions of Eqs. (2)- (4) into Eq. (1) give the governing equation for the scalar potential ϕ, written as

$$\nabla^2\phi = -\frac{ne}{\varepsilon_o}\left(e^{-e\phi(\mathbf{r})/kT} - e^{e\phi(\mathbf{r})/kT}\right), \quad \mathbf{r} \in W \tag{5}$$

where W is the domain of the problem. In this work, a floating random-walk algorithm will be developed for the numerical solution of Eq. (5) in one dimension, subject to Dirichlet boundary condition:

$$\phi = g(\mathbf{r}), \quad \mathbf{r} \in \partial W \tag{6}$$

where ∂W is the boundary of the domain W.

III. The Floating Random-Walk Algorithm

In the one-dimensional test problem, the potential ϕ depends on one independent variable x, and is given by the normalized equation

$$\frac{d^2\hat{\phi}}{d\hat{x}^2} = e^{\hat{\phi}} - e^{-\hat{\phi}}. \tag{7}$$

In Eq. (7) the non-dimensional variables $\hat{\phi}$ and $\hat{x}$ are given by

$$\hat{\phi} = \frac{e\phi}{kT}, \ \hat{x} = \frac{x}{\lambda_D}, \ \lambda_D = \left(\frac{\varepsilon_o kT}{ne^2}\right)^{1/2}, \tag{8}$$

where λ_D is the Debye length[13]. The value of $\hat{\phi}$ is assumed to be known at the two end-points of the problem domain. The development of a floating random-walk algorithm requires the evaluation of the Green's function of Eq. (7) given by the solution of the equation

$$\frac{d^2G(\hat{x} \mid \hat{x}_o)}{d\hat{x}^2} - \left(e^G - e^{-G}\right) = \delta(\hat{x} - \hat{x}_o). \tag{9}$$

Above, $G(\hat{x} \mid \hat{x}_o)$ is a volumetric Green's function at $\hat{x}$, given a delta function at $\hat{x}_o$, and defined on the problem domain $-L \le \hat{x} \le L$. The boundary conditions imposed on this Green's function are: a) $G(L \mid \hat{x}_o) = 0$ and b) $G(-L \mid \hat{x}_o) = 0$. Under these conditions, based on Green's theorem[14] we can write a solution to Eq. (5) at a point $\hat{x}_o$ inside the problem domain given by

$$\hat{\phi}(\hat{x}_o) = \left[\frac{dG}{d\hat{x}}\right]_{\hat{x}=L} \phi(L) - \left[\frac{dG}{d\hat{x}}\right]_{\hat{x}=-L} \phi(-L). \tag{10}$$

Based on iterative perturbation theory, we can now develop an approximate solution for Eq. (9), and this approximate expression will be used in Eq. (10) to form the basis of our floating random-walk algorithm. The zeroth-order approximation to the solution of Eq. (9), $G^{(0)}(\hat{x} \mid \hat{x}_o)$, is given by the solution to the equation

$$\frac{d^2 G^{(0)}}{d\hat{x}^2} = \delta(\hat{x} - \hat{x}_o) \tag{11}$$

under the same boundary conditions as that of Eq. (9). Eq. (11) represents the Green's function equation for Laplace's equation and its solution is given as[14]

$$G^{(0)}(\hat{x} \mid \hat{x}_o) = \begin{cases} \dfrac{\hat{x}_o - L}{2L}(\hat{x} + L), & \hat{x} < \hat{x}_o \\ \dfrac{\hat{x}_o + L}{2L}(\hat{x} - L), & \hat{x} > \hat{x}_o \end{cases}. \tag{12}$$

Based on the zeroth-order approximation given in Eq. (12), the first-order approximation, $G^{(1)}(\hat{x} \mid \hat{x}_o)$ to Eq. (9) can be expressed as the solution of the equation

$$\frac{d^2 G^{(1)}}{d\hat{x}^2} = \delta(\hat{x} - \hat{x}_o) + \left(e^{G^{(o)}} - e^{-G^{(o)}}\right), \tag{13}$$

the solution to which, based on Green's theorem[14] can be written as

$$G^{(1)}(\hat{x} \mid \hat{x}_o) = G^{(0)}(\hat{x} \mid \hat{x}_o) + \int_{-L}^{+L} d\hat{x}' G^{(0)}(\hat{x} \mid \hat{x}') f\left\{G^{(0)}(\hat{x}' \mid \hat{x}_o)\right\}, \tag{14}$$

where $f\{y\} = e^{y} - e^{-y}$. Using a zero-centered notation, (i.e. $\hat{x}_o = 0$) in Eq. (14) and differentiating both sides of that equation with respect to $\hat{x}$, the derivatives of the volumetric Green's function at $\hat{x} = \pm L$ can be calculated and are given by

$$\left[\frac{dG^{(1)}}{d\hat{x}}\right]_{\hat{x}=L} = -\left[\frac{dG^{(1)}}{d\hat{x}}\right]_{\hat{x}=-L} = \frac{1}{2}\left[1-4L^2\left(e^{\frac{1}{2}}+e^{-\frac{1}{2}}-2\right)\right]. \tag{15}$$

The one-dimensional floating random-walk can now be formulated based on Eqs. (10) and (15). The random walks are started at a point where we want to know the solution to Eq. (7) and with the help of a random-number generator a hop is made either to the left or right with equal probability. Associated with every such hop is a multiplicative weight factor w. Based on Eqs. (10) and (15), this weight factor is given by

$$w = 1-4L^2\left(e^{\frac{1}{2}}+e^{-\frac{1}{2}}-2\right). \tag{16}$$

To maintain the validity of the first-order approximation in the volumetric Green's function in Eq. (14), the size of a hop, L, has to be restricted to a pre-determined upper limit. A particular random-walk terminates at one of the two end-points of the problem domain with the reward for that walk being the known value of $\hat{\phi}$ at that end-point. For any particular walk, the overall weight factor, obtained by multiplying the weight factors of the individual hops, is multiplied by the reward at the end-point to give the contribution for that walk. The estimate of the solution $\overline{\hat{\phi}}$ at a particular point in the problem domain is the average of the contributions, $\hat{\phi}_n$ from a statistically large number (N) of random walks originating from that point and is given by

$$\overline{\hat{\phi}} = \frac{1}{N}\sum_{n=1}^{N}\hat{\phi}_n. \tag{17}$$

In the next section, the random walk solution to this one-dimensional problem will be presented and it will be shown that this random-walk solution is in excellent agreement with an exact, analytical solution of Eq. (7).

IV. Results

The one-dimensional benchmark problem is shown in Fig. 1, where a region of plasma is enclosed between two flat plates of infinite area, maintained at fixed potentials. The results of computations with the one-dimensional random-walk algorithm have been compared with an exact analytical solution given by

$$\hat{\phi} = 2\ln\left[\frac{1+\tanh\left(\hat{\phi}_o/4\right)e^{-\sqrt{2}\,\hat{x}}}{1-\tanh\left(\hat{\phi}_o/4\right)e^{-\sqrt{2}\,\hat{x}}}\right]. \tag{18}$$

where the imposed boundary conditions are: a) $\hat{\phi}(\hat{x}=0)=\hat{\phi}_o$ and b) $\hat{\phi}=0, \frac{d\hat{\phi}}{d\hat{x}}=0$ as $\hat{x}\to\infty$. For the verification of the random-walk algorithm, the problem domain has to be finite and is assumed to be equal to $5\lambda_D$. The random-walk results are computed by imposing the boundary conditions: a) $\hat{\phi}(\hat{x}=0)=\hat{\phi}_o$ and b) $\hat{\phi}(\hat{x}=5\lambda_D)=0$.

The random-walk algorithms were coded in MATLAB 6.5™, and run on a 1.8 GHz personal computer. In this work, 20000 random walks were performed per solution point, while the length of the hop has been restricted to five percent of the Debye length to maintain the validity of the first-order approximation in the derivation of the volumetric Green's function. Assuming $\hat{\phi}_o = 1$, it was observed that that the mean absolute deviation between the analytical and random-walk solution points was equal to 0.0019 and the solution profile is plotted in Fig. 2. From the solution profile and the magnitude of mean absolute error, it can be noted that there is excellent agreement between the results from the random-walk algorithm and the exact analytical solution.

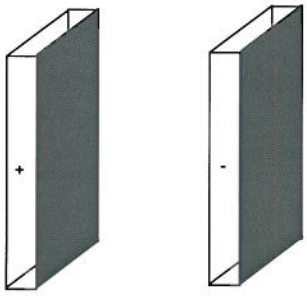

Figure 1. Plasma enclosed between two flat plates of infinite area maintained at fixed potentials.

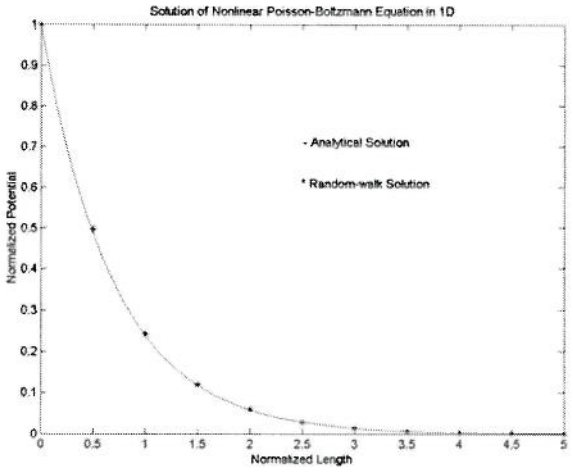

Figure 2. Potential plotted against position in normalized coordinates.

V. Conclusion

In conclusion, we have developed a new floating random-walk algorithm for the solution of the nonlinear Poisson-Boltzmann equation. The problem of the absence of an analytical expression for a volumetric Green's function has been remedied by the help of an approximate (yet accurate) expression based on a novel use of iterative perturbation theory. Excellent agreement was found between the results of random-walk calculations and an exact analytical solution for a one-dimensional benchmark problem. Our literature survey shows that the newly developed algorithm appears to be the first application of the floating random-walk method to a nonlinear problem of physical significance. This algorithm has the advantages of being highly parallelizable and requiring no discretization of the problem domain.

The application area of interest is in the modeling of plasma discharges in aerospace applications, and in particular, the simulation of the space-charge boundary layers (sheaths) that occur near electrode surfaces. Our future work in this area will involve the extension of this new floating random-walk solution to Dirichlet problems in two and three dimensions and also to Neumann and mixed boundary condition problems. The ultimate objective of this research is to develop floating random-walk algorithms for the solution of plasma flow equations and also to address the efficient implementation of the algorithms on parallel processor computer platforms.

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