# A two-dimensional floating random-walk algorithm for the solution of the nonlinear Poisson–Boltzmann equation: application to the modeling of plasma sheaths

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**Abstract**

This paper presents a new, meshless and inherently parallelizable floating random-walk (FRW) algorithm for the solution of the two-dimensional nonlinear Poisson–Boltzmann (NPB) equation. Historically, the FRW method has not been applied to nonlinear problems of significance, which can be attributed to the absence of Green's functions. This problem has been remedied in our work by a novel use of iterative perturbation theory. Our past work involved the FRW solution of the NPB equation in one dimension. In this work, we extend the algorithm to two dimensions and excellent agreement has been obtained with a finite-difference based solution. The application area of interest is the modeling of plasma sheaths.

*Keywords:* Floating random-walk; Stochastic methods; Nonlinear Poisson–Boltzmann equation; Plasma sheaths

## 1. Introduction

In the last few years, plasma actuators have begun to exhibit great promise as a means of flow control in aerospace applications [1]. These flow control systems are based on a plasma discharge between electrodes and the transformation of the electrical energy into kinetic and thermal energy in the air flow. However, the modeling of a plasma discharge in an air flow is computationally intensive, primarily because of the vast differences in fluid dynamic and electromagnetic time scales. Iterative solutions of the nonlinear Poisson–Boltzmann (NPB) equation for the electric potential constitute a significant part of this computational effort, as this equation has to be converged at each time step.

In this paper, we develop a Floating random-walk (FRW) algorithm [2] for the NPB equation. This method, based on probabilistic interpretations of deterministic equations, is completely meshless and requires no discretization of either the volume or the surface of problem domains. Consequently, the memory requirements are expected to be significantly lower than discretization-based methods. Furthermore, the method is inherently parallelizable and a linear increase in speed is expected with an increase in the number of processors. The linearized version [3] of the NPB equation and other linear equations has been studied extensively with the FRW method. However, the FRW method has not been applied in the numerical solution of nonlinear partial differential equations. This is because of the absence of analytical expressions for Green's functions for nonlinear equations of significance. This problem has been eliminated in our work by a novel use of iterative perturbation theory. In a past work [4], we developed an FRW algorithm for the numerical solution of the one-dimensional NPB equation. In this work, we extend this algorithm to two dimensions.

## 2. Formulation of the two-dimensional floating random-walk algorithm

The assumption of charge neutrality is not valid in an ionized gas in the vicinity of an electrode. A space-charge layer is formed due the difference in mobility of electrons and ions and to the fact that in the steady state, the flux of the positive and negative charge carriers to

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the electrode need to be balanced [5]. The electric potential $\phi$ in the space-charge layer is given by the solution of the NPB equation and written as [5]

$$\nabla^2\phi = -\frac{ne}{\varepsilon_o}\left(e^{+e\phi(\mathbf{r})/kT} - e^{-e\phi(\mathbf{r})/kT}\right) \tag{1}$$

where $n$ is the concentration of electrons and ions in the absence of a potential, $e$ is the electronic charge, $k$ is the Boltzmann constant, $T$ is the temperature and $\varepsilon_0$ is the permittivity of free space. We normalize Eq. (1) in polar coordinates and the normalized potential $\hat{\phi}$ is governed by the equation

$$\frac{1}{\hat{r}}\frac{\partial}{\partial r}\left(\hat{r}\frac{\partial\hat{\phi}}{\partial\hat{r}}\right) + \frac{1}{\hat{r}^2}\frac{\partial^2\hat{\phi}}{\partial\hat{\theta}^2} = e^{\hat{\phi}} - e^{-\hat{\phi}},\ \hat{\phi} = \frac{e\phi}{kT},\ \hat{r} = \frac{r}{\lambda_D},$$
$$\hat{\theta} = \theta,\ \lambda_D = \left(\frac{\varepsilon_o kT}{ne^2}\right)^{1/2} \tag{2}$$

The normalized potential is assumed to be known along the boundary of the problem domain. An approximate expression for a Green's function $G(\hat{\mathbf{r}}|\hat{\mathbf{r}}_0)$ for Eq. (2) on a circular domain is derived given a delta function centered at $\hat{\mathbf{r}}_0$, and boundary conditions such that the Green's function on the circumference of the circular domain is zero. Such a Green's function is given as the solution of the equation

$$\nabla^2 G(\hat{\mathbf{r}}|\hat{\mathbf{r}}_o) - (e^G - e^{-G}) = \delta(\hat{\mathbf{r}} - \hat{\mathbf{r}}_o) \tag{3}$$

Normalizing the length scales to the radius $R$ of the circular problem domain and substituting $\hat{\rho} = \frac{\hat{r}}{R}$ and $\hat{\rho}_o = \frac{\hat{r}_o}{R}$ in Eq. (2), the Green's function equation transforms to

$$\nabla^2_{\hat{\rho}} G - R^2(e^G - e^{-G}) = \delta(\hat{\boldsymbol{\rho}} - \hat{\boldsymbol{\rho}}_o) \tag{4}$$

A zeroth-order approximation for the Green's function is the solution of Laplace's equation

$$\nabla^2_{\hat{\rho}} G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_o) = \delta(\hat{\rho} - \hat{\rho}_o) \tag{5}$$

which is given as [6]

$$G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_o) = \frac{1}{4\pi} \times \ln\left[\frac{\hat{\rho}^2 + \hat{\rho}_o^2 - 2\hat{\rho}\hat{\rho}_o\cos(\hat{\theta} - \hat{\theta}_o)}{1 + \hat{\rho}^2\hat{\rho}_o^2 - 2\hat{\rho}\hat{\rho}_o\cos(\hat{\theta} - \hat{\theta}_o)}\right] \tag{6}$$

Equation (6) in conjunction with Green's theorem [6] can be used to obtain a first-order approximation, $G^{(1)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)$ which is given as

$$G^{(1)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_o) = G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_o) + R^2\int_0^1\int_0^{2\pi}\left[d\hat{\rho}'d\hat{\theta}'\hat{\rho}'G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}'_o)\right.$$
$$\left.\times f\left\{G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_o)\right\}\right],\quad f\{y\} = e^y - e^{-y} \tag{7}$$

Based on Eq. (7) and Green's theorem [6], an expression for normalized potential at a point $\hat{\boldsymbol{\rho}}_0$ is given by an integral expressed as

$$\hat{\phi}(\hat{\boldsymbol{\rho}}_o) = \int_{\theta=0}^{2\pi} d\hat{\theta}\left[\frac{dG^{(1)}}{d\hat{\rho}}\right]_{\hat{\rho}=1}\hat{\phi}\left(1,\hat{\theta}\right) \tag{8}$$

$\left[\frac{dG^{(1)}}{d\hat{\rho}}\right]_{\hat{\rho}=1}$ is obtained by differentiating Eq. (7), and in the zero-centered notation (i.e. $\hat{\rho}_0 = 0$) is given by

$$\left[\frac{dG}{d\hat{\rho}}\right]_{\hat{\rho}=1} = \frac{1}{2\pi} + \frac{R^2}{4\pi}\int_0^1\int_0^{2\pi}\hat{\rho}'d\hat{\rho}'d\hat{\theta}A \times B \tag{9}$$

where $A$ and $B$ are given by

$$A = \left[(\hat{\rho}')^{\frac{1}{2\pi}} - (\hat{\rho}')^{-\frac{1}{2\pi}}\right]$$
$$B = \frac{1 - (\hat{\rho}')^2}{1 + (\hat{\rho}')^2 - 2\hat{\rho}'\cos\left(\hat{\theta} - \hat{\theta}\right)} \tag{10}$$

Equations (8)–(10) form the basis of our two-dimensional FRW algorithm. The random-walks are started at the point, where the potential has to be estimated and a hop is made to the circumference of a circle of radius $R$ according to a pre-determined probability distribution. The radius of such a hop has to be restricted to maintain the validity of the first-order approximation in Eq. (7) and for each hop there is a weight factor obtained by sampling the integrand of Eq. (8). A particular random-walk, composed of several such random hops, is terminated on the boundary of the problem domain, where the value of the potential is known. The overall contribution from a random-walk is obtained by multiplying the overall weight factor for the walk (which is obtained by multiplying the weight factors of the individual hops) with the boundary value, and an estimate of the potential at the original point is obtained by averaging over a statistically large number of random-walks.

The benchmark problem is shown in Fig. (1), where plasma is enclosed between two infinitely long cylinders, maintained at fixed potentials. Due to the absence of an analytical solution, we have carried out finite-difference solutions of the problem and compared them to our random-walk solution. The inner and the outer electrode have been assumed to be equal to $\lambda_D$ and $6\lambda_D$ respectively in radius and we have imposed the boundary condition that $\hat{\phi}(r = \lambda_D) = 1$ and $\hat{\phi}(r = 6\lambda_D) = 0$. The FRW algorithm was coded in MATLAB 6.5TM, and run on a 1.8 GHz personal computer, while the finite-difference algorithm was coded in FORTRAN, and run on a Silicon Graphics, Inc. workstation. Because of the

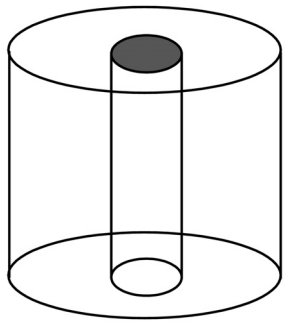

Fig. 1. Plasma enclosed between two infinitely long cylinders maintained at fixed potentials.

relative slowness of an interpreted MATLAB program in comparison to a compiled FORTRAN program, and also the fact that the finite-difference algorithm was in one dimension, it was not possible to compare these approaches in terms of speed. In this work, 20000 random-walks were performed per solution point and the radius of the hops was limited to five percent of the Debye length to maintain the validity of the first-order approximation in the Green's function expression. It was observed that the mean absolute deviation between the random-walk solutions and the finite-difference results was equal to 0.0025. From the solution profile in Fig. (2) and the magnitude of mean absolute error, it can be noted that there is excellent agreement between the FRW and the finite-difference results.

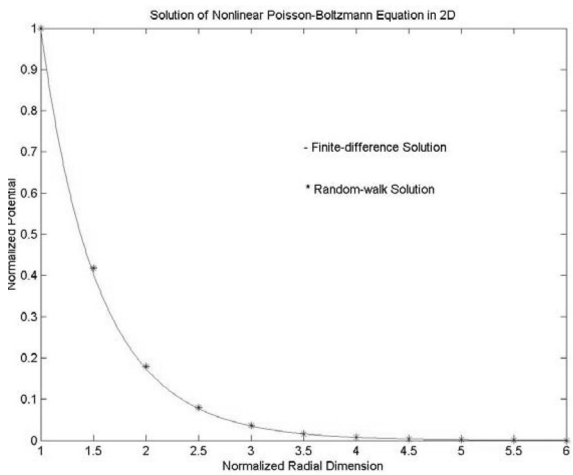


Fig. 2. Potential plotted against position in normalized coordinates.

## 3. Conclusion

Summarizing, we have developed a new FRW algorithm for the solution of the NPB equation in two dimensions. The problem of the absence of an analytical expression for a Green's function has been eliminated by the help of an approximate expression based on a novel use of iterative perturbation theory. Excellent agreement was found between the results of an FRW- and a finite-difference based solution for a Dirichlet benchmark problem. Based on our literature survey, the newly developed algorithm appears to be the first FRW algorithm for an important nonlinear problem. This algorithm is inherently parallelizable and requires no discretization of either the volume or the surface of the problem domain.

The application area of interest is in the modeling of plasma discharges in aerospace applications. Our work in the immediate future will involve the extension of this new FRW algorithm to Dirichlet problems in three dimensions and also to Neumann and mixed-boundary condition problems. The ultimate objective of this research is to develop FRW algorithms for plasma flow equations and the efficient parallelization of these algorithms.

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