INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING
Int. J. Numer. Meth. Engng 2006; **66**:72–84
Published online 12 December 2005 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/nme.1539

A two-dimensional stochastic algorithm for the solution of the non-linear Poisson–Boltzmann equation: validation with finite-difference benchmarks§

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SUMMARY

This paper presents a two-dimensional floating random walk (FRW) algorithm for the solution of the non-linear Poisson–Boltzmann (NPB) equation. In the past, the FRW method has not been applied to the solution of the NPB equation which can be attributed to the absence of analytical expressions for volumetric Green's functions. Previous studies using the FRW method have examined only the linearized Poisson–Boltzmann equation. No such linearization is needed for the present approach. Approximate volumetric Green's functions have been derived with the help of perturbation theory, and these expressions have been incorporated within the FRW framework. A unique advantage of this algorithm is that it requires no discretization of either the volume or the surface of the problem domains. Furthermore, each random walk is independent, so that the computational procedure is highly parallelizable. In our previous work, we have presented preliminary calculations for one-dimensional and quasi-one-dimensional benchmark problems. In this paper, we present the detailed formulation of a two-dimensional algorithm, along with extensive finite-difference validation on fully two-dimensional benchmark problems. The solution of the NPB equation has many interesting applications, including the modelling of plasma discharges, semiconductor device modelling and the modelling of biomolecular structures and dynamics. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: floating random walk algorithm; Monte Carlo; stochastic algorithm; non-linear Poisson–Boltzmann equation; modelling of plasma sheaths; semiconductor device modelling; modelling of biomolecular structure and dynamics

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Contract/grant sponsor: Air Force Research Laboratory
Contract/grant sponsor: Air Force Office of Scientific Research
Contract/grant sponsor: National Research Council

Received 26 April 2005
Accepted 15 September 2005

1. INTRODUCTION

The solution of the non-linear Poisson–Boltzmann (NPB) equation has widespread applications in science and engineering. These applications include the modelling of plasma sheaths [1], semiconductor devices [2], and biomolecular structures and dynamics [3]. In this paper, we address the efficient solution of the NPB equation, subject to Dirichlet [4] boundary conditions, by developing a stochastic algorithm based on the floating random walk (FRW) method [5–7].

The FRW method is based on probabilistic interpretations of deterministic equations. The method is completely meshless and requires no discretization of either the volume or the surface of problem domains. As a result, the memory requirements for complicated problem geometries are expected to be significantly lower than for discretization-based methods. Furthermore, each random walk is independent, so that the method is inherently parallelizable. In spite of its many advantages, the FRW method has not been applied to the numerical solution of the NPB equation because analytical expressions for volumetric Green's functions [4] are not available. In particular, previous numerical studies using FRW algorithms [8, 9] have examined only the linearized Poisson–Boltzmann equation, limiting the applicability of the solution to small values of the potential. In our previous work, we have presented the preliminary results for one-dimensional [10] and a quasi-one-dimensional [11] problems subject to Dirichlet boundary conditions. In this paper, we present the detailed formulation of a two-dimensional algorithm, and provide extensive validation through fully two-dimensional benchmark problems. Before presenting the specifics of the algorithm, we will give an overview of the FRW method.

2. OVERVIEW OF THE FRW METHOD

The FRW method is a generalization of the Monte Carlo integration method [12]. The Monte Carlo method is a statistical approach to estimating integrals, which, unlike many other techniques, is well-adapted to evaluating multi-dimensional problems. We will discuss one such method, 'Sample Mean Monte Carlo' [12], and then demonstrate how the technique is modified to form the basis for the FRW method.

Consider a function $f(x)$ defined over the interval $a \leqslant x \leqslant b$. Our problem is to estimate the integral

$$\mathbf{I} = \int_a^b \mathrm{d}x\, f(x) \tag{1}$$

In the event where the integral is improper, absolute convergence [13] is assumed. We select an arbitrary probability density function $p(x)$, with a corresponding random variable ξ. We define another random variable η as

$$\eta = \frac{f(\xi)}{p(\xi)} \tag{2}$$

The expectation value of the random variable η, written as $E(\eta)$, is equal to the integral $\mathbf{I}$, which can be expressed as

$$\mathbf{I} = E(\eta) = \int_a^b \mathrm{d}x \left[\frac{f(x)}{p(x)}\right] p(x) \tag{3}$$

The integral can be evaluated by sampling the integrand with the help of a random-number generator, and averaging over a statistically large number of samples. This approach is particularly suited to evaluating higher-dimensional integrals, because one needs to sample the integrand irrespective of the dimensionality of the integral. We will now describe how this Monte Carlo integration method can be generalized into the FRW method for the solution of boundary-value problems.

Given a differential equation, with a differential operator L,

$$L[U(\mathbf{r})] = f(\mathbf{r}) \tag{4}$$

the solution $U(\mathbf{r})$ is a function of the three-dimensional position vector $\mathbf{r}$. The function $f(\mathbf{r})$ is a source term. The Green's functions for Equation (4) are the solutions of the differential equation

$$L[G(\mathbf{r}|\mathbf{r}_0)] = \delta(\mathbf{r} - \mathbf{r}_0) \tag{5}$$

subject to specified boundary conditions. Above, $G(\mathbf{r}|\mathbf{r}_0)$ is a volumetric Green's function at $\mathbf{r}$ given a dirac-delta function $\delta(\mathbf{r} - \mathbf{r}_0)$ centred at $\mathbf{r}_0$. We assume that the operator L is of the Sturm–Liouville [4] form

$$L = \nabla_{\mathbf{r}} \cdot [p(\mathbf{r})\nabla_{\mathbf{r}}] + q(\mathbf{r}) \tag{6}$$

where $p(\mathbf{r})$ and $q(\mathbf{r})$ are known functions of $\mathbf{r}$, $\nabla_{\mathbf{r}}$ being the gradient operator with respect to $\mathbf{r}$. Using Green's integral representation [4] $U(\mathbf{r})$ can be written as

$$U(\mathbf{r}_0) = \iiint_{\mathrm{V}} \mathrm{d}v G(\mathbf{r}|\mathbf{r}_0) f(\mathbf{r}) - \oiint_S [\mathrm{d}\mathbf{s} \cdot \nabla_{\mathbf{r}} U(\mathbf{r})] p(\mathbf{r}) G(\mathbf{r}|\mathbf{r}_0) + \oiint_S [\mathrm{d}\mathbf{s} \cdot \nabla_{\mathbf{r}} G(\mathbf{r}|\mathbf{r}_0)] p(\mathbf{r}) U(\mathbf{r}) \tag{7}$$

The first term on the right-hand side of Equation (7) is a volume integral involving the source term in the entire volume V of interest. The second and third terms are vector surface integrals over the surface S enclosing V, where $\mathrm{d}\mathbf{s}$ is a vector whose magnitude is equal to that of an infinitesimally small area unit on the surface S and directed normally outward from the centre of the area unit. As mentioned before, $G(\mathbf{r}|\mathbf{r}_0)$ is often referred to as the volumetric Green's function and $\nabla_{\mathbf{r}} G(\mathbf{r}|\mathbf{r}_0)$ is called the surface Green's function. The second integral on the right-hand side of Equation (7) corresponds to the Neumann [4] boundary condition, whereas the third integral corresponds to the Dirichlet [4] boundary condition.

Equation (7) forms the mathematical basis of the FRW method. To evaluate the solution to Equation (4) at a particular point in the domain of interest, we consider [5–7] maximal spheres, cubes, or any geometrical object for which the solution to Equation (5) is known. We then make random hops to the surface of that geometrical object based on any predefined probability density. The weights for such random hops are determined by sampling the various integrands in Equation (7). For example, in the case of a Dirichlet problem with no source term [that is, $f(\mathbf{r}) = 0$], the problem reduces to a Monte Carlo integration of an infinite-dimensional

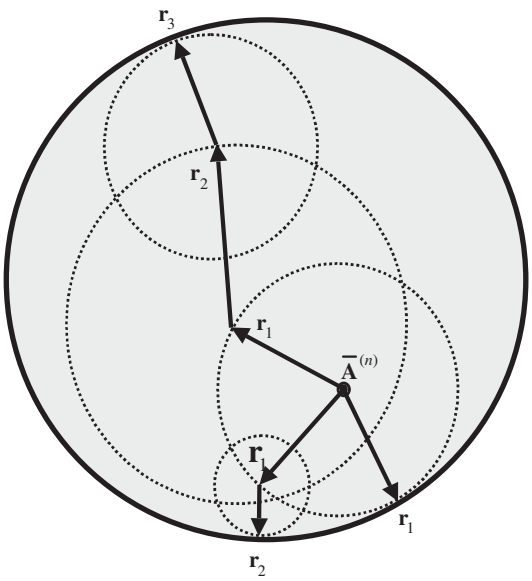

Figure 1. A schematic diagram of circular random walks on a circular problem domain is shown. One-, two- and three-hop random walks are represented.

integral, as given by [14]

$$U(\mathbf{r}_0) = \oint_{S_1} \mathrm{d}s_1 K(\mathbf{r}_0|\mathbf{r}_1) \oint_{S_2} \mathrm{d}s_2 K(\mathbf{r}_1|\mathbf{r}_2) \ldots\ldots\ldots \oint_{S_n} \mathrm{d}s_n K(\mathbf{r}_{n-1}|\mathbf{r}_n) U(\mathbf{r}_n)$$

$$K(\mathbf{r}_{n-1}|\mathbf{r}_n) = p(\mathbf{r}_n) |\nabla_{\mathbf{r}_n} G(\mathbf{r}_{n-1}|\mathbf{r}_n)| \cos(\gamma_{n-1,n}) \tag{8}$$

where $\gamma_{n-1,n}$ is the angle between $\nabla_{\mathbf{r}_n} G(\mathbf{r}_{n-1}|\mathbf{r}_n)$ and $\mathrm{d}\mathbf{s}_n$, $\mathrm{d}\mathbf{s}_n$ being a vector whose magnitude ($\mathrm{d}s_n$) is equal to that of an infinitesimally small area unit on the surface S_n and directed normally outward from the centre of the area unit. The successive surface integrals in Equation (8) relate to successive random hops across the problem domain and the weight factors of the form $K(\mathbf{r}_{n-1}|\mathbf{r}_n)$ are derived from the third integral term on the right-hand side of Equation (7) that corresponds to the Dirichlet boundary condition. A particular random walk is terminated at the boundary, where the solution is known, and the samples of successive weight factors multiplied by the solution at the boundary yield a particular sample of the solution. A numerical solution of Equation (4) is obtained by averaging over a statistically large number of such samples. A schematic diagram of circular random walks on a circular problem domain is shown in Figure 1.

At this point, we note that this method does not require any discretization, as the solution can be evaluated at the point of origination of the random walks irrespective of the solution at any other point. We also note that this method is inherently parallelizable, since different random walks can be performed in different processors, and inter-processor communication is required only during the final averaging of the contributions from different walks. In spite of these unique advantages, the FRW method has not being applied to the NPB equation and other

important non-linear equations because of the absence of analytical expressions for volumetric Green's functions of these equations. Early researchers in the area expressed the apprehension that the extension of the stochastic solution methodology to non-linear problems might not be possible. In a 1954 paper [15], J. R. Curtiss wrote: 'So far as the author is aware, the extension of Monte Carlo methods to non-linear processes has not yet been accomplished and may be impossible.' Stochastic approaches to solving non-linear equations (in particular the NPB equation) that have been suggested in the literature [16] involve an iterative solution of a series of linear problems. In our proposed approach, an approximate (yet accurate) expression for the Green's function for the non-linear problem is obtained through perturbation theory, which gives rise to an integral formulation that is valid for the entire non-linear problem. As a result, our algorithm does not have any iteration steps, and thus has a lower computational cost. The validity of such an integral expression is maintained by restricting the size of a random hop and increasing the order of perturbation in the Green's function would allow one to increase the hop size, thus increasing computational speed. An approach utilizing a perturbation-based Green's function was used to develop an FRW algorithm for the Helmholtz equation in heterogeneous problem domains (important for IC interconnect analysis at high frequencies) by the first author in References [17, 18], where the idea of extending the approach to non-linear problems was also proposed. Later that idea was extended to the NPB equation for one-dimensional [10] and quasi-one-dimensional [11] problems. In this work, a two-dimensional volumetric Green's function truncated to the first order (with a correspondingly restricted hop size) has been derived and a detailed description of this derivation is presented in the next section.

3. FORMULATION OF THE ALGORITHM

In our problem of interest, the dependent variable ϕ is governed by the NPB equation given as

$$\nabla^2\phi = \frac{1}{c^2}(\mathrm{e}^{k\phi(\mathbf{r})} - \mathrm{e}^{-k\phi(\mathbf{r})}), \quad \mathbf{r} \in W \tag{9}$$

where $\mathbf{r}(r, \theta)$ is the two-dimensional position co-ordinate, c and k are constants, while W is the two-dimensional problem domain. Dirichlet boundary conditions have been imposed:

$$\phi = g(\mathbf{r}), \quad \mathbf{r} \in \partial W \tag{10}$$

where ∂W is the boundary of the domain W. Equation (9) can be normalized to

$$\frac{1}{\hat{r}}\frac{\partial}{\partial\hat{r}}\left(\hat{r}\frac{\partial\hat{\phi}}{\partial\hat{r}}\right) + \frac{1}{\hat{r}^2}\frac{\partial^2\hat{\phi}}{\partial\hat{\theta}^2} = \mathrm{e}^{\hat{\phi}} - \mathrm{e}^{-\hat{\phi}} \tag{11}$$

where $\hat{r} = r/\lambda$, $\hat{\theta} = \theta$ and $\hat{\varphi} = \varphi$; $\hat{\phi} = k\phi$, $\lambda = c/\sqrt{k}$. We further normalize the length scales to the radius R of a circular domain (the chosen geometry for random walks) and substitute $\hat{\rho} = \hat{r}/R$ and $\hat{\rho}_0 = \hat{r}_0/R$ in Equation (11). The twice-normalized NPB equation is written as

$$\frac{1}{\hat{\rho}}\frac{\partial}{\partial\hat{\rho}}\left(\hat{\rho}\frac{\partial\hat{\phi}}{\partial\hat{\rho}}\right) + \frac{1}{\hat{\rho}^2}\frac{\partial^2\hat{\phi}}{\partial\hat{\theta}^2} = R^2(\mathrm{e}^{\hat{\phi}} - \mathrm{e}^{-\hat{\phi}}) \tag{12}$$

A volumetric Green's function, $G(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)$ at $\hat{\boldsymbol{\rho}}$, assuming a dirac-delta function at $\hat{\boldsymbol{\rho}}_0$ inside the circular domain, is given as the solution of the equation

$$\frac{1}{\hat{\rho}}\frac{\partial}{\partial\hat{\rho}}\left(\hat{\rho}\frac{\partial\hat{G}}{\partial\hat{\rho}}\right)+\frac{1}{\hat{\rho}^2}\frac{\partial^2\hat{G}}{\partial\hat{\theta}^2}-R^2(\mathrm{e}^{\hat{G}}-\mathrm{e}^{-\hat{G}})=\delta(\hat{\boldsymbol{\rho}}-\hat{\boldsymbol{\rho}}_0) \tag{13}$$

A zeroth-order approximation for the volumetric Green's function, $G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)$ is the solution of equation

$$\frac{1}{\hat{\rho}}\frac{\partial}{\partial\hat{\rho}}\left(\hat{\rho}\frac{\partial\hat{G}^{(0)}}{\partial\hat{\rho}}\right)+\frac{1}{\hat{\rho}^2}\frac{\partial^2\hat{G}^{(0)}}{\partial\hat{\theta}^2}=\delta(\hat{\boldsymbol{\rho}}-\hat{\boldsymbol{\rho}}_0) \tag{14}$$

which is given as [4]

$$G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)=\frac{1}{4\pi}\times\ln\left[\frac{\hat{\rho}^2+\hat{\rho}_0^2-2\hat{\rho}\hat{\rho}_0\cos(\hat{\theta}-\hat{\theta}_0)}{1+\hat{\rho}^2\hat{\rho}_0^2-2\hat{\rho}\hat{\rho}_0\cos(\hat{\theta}-\hat{\theta}_0)}\right] \tag{15}$$

It can be noted that $\{G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)\}_{\hat{\rho}=1}=0$ along the circumference of the circular domain. Equation (15) can be used to obtain a first-order approximation, $G^{(1)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)$, to the volumetric Green's function and is given as a solution of the equation

$$\frac{1}{\hat{\rho}}\frac{\partial}{\partial\hat{\rho}}\left(\hat{\rho}\frac{\partial\hat{G}^{(1)}}{\partial\hat{\rho}}\right)+\frac{1}{\hat{\rho}^2}\frac{\partial^2\hat{G}^{(1)}}{\partial\hat{\theta}^2}=\delta(\hat{\boldsymbol{\rho}}-\hat{\boldsymbol{\rho}}_0)+R^2(\mathrm{e}^{G^{(0)}}-\mathrm{e}^{-G^{(0)}}) \tag{16}$$

Based on Equations (7), (15) and (16), $G^{(1)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)$ is given by the expression

$$G^{(1)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)=G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)+R^2\int_0^1\int_0^{2\pi}[\mathrm{d}\hat{\rho}'\,\mathrm{d}\hat{\theta}'\hat{\rho}'G^{(0)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}')\times f\{G^{(0)}(\hat{\boldsymbol{\rho}}'|\hat{\boldsymbol{\rho}}_0)\}] \tag{17}$$

where $f\{y\}=\mathrm{e}^y-\mathrm{e}^{-y}$. It can again be noted that $\{G^{(1)}(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\rho}}_0)\}_{\hat{\rho}=1}=0$ along the circumference of the circular domain. Based on this approximate expression for the volumetric Green's function and Equation (7), an expression for normalized potential at a point $\hat{\boldsymbol{\rho}}_0$ is given by a line integral over the circumference of the unit circle and is expressed as

$$\hat{\phi}(\hat{\boldsymbol{\rho}}_0)=\int_{\theta=0}^{2\pi}\mathrm{d}\hat{\theta}\left[\frac{\mathrm{d}G^{(1)}}{\mathrm{d}\hat{\rho}}\right]_{\hat{\rho}=1}\hat{\phi}(1,\hat{\theta}) \tag{18}$$

For the development of the FRW algorithm, we need to estimate $[\mathrm{d}G^{(1)}/\mathrm{d}\hat{\rho}]_{\hat{\rho}=1}$ in Equation (18). Such an estimate is obtained by differentiating Equation (17), and in the zero-centred notation (i.e. $\hat{\rho}_0=0$) is given by

$$\left[\frac{\mathrm{d}G}{\mathrm{d}\hat{\rho}}\right]_{\hat{\rho}=1}=\frac{1}{2\pi}+\frac{R^2}{4\pi}\int_0^1\int_0^{2\pi}\hat{\rho}'\mathrm{d}\hat{\rho}'\mathrm{d}\theta' A\times B \tag{19}$$

where A and B are given by

$$A = [(\hat{\rho}')^{1/2\pi} - (\hat{\rho}')^{-1/2\pi}]$$
$$B = \frac{2(1 - (\hat{\rho}')^2)}{1 + (\hat{\rho}')^2 - 2\hat{\rho}' \cos(\hat{\theta} - \hat{\theta}')} \tag{20}$$

Equation (18) in conjunction with Equations (19) and (20) are used to develop the FRW algorithm for the problem under consideration. In order to calculate the normalized potential at a point of interest, we start our random walks at that point and hop to the circumference of a circle of radius R. The random walks have to be restricted to a small fraction of the characteristic length $\lambda(= c/\sqrt{k})$ in order to maintain the validity of the first-order approximation in the perturbation expression for the volumetric Green's function. For every hop there is a weight factor obtained by sampling the multi-dimensional integrand of Equation (18) (with the help of a random-number generator) according to any pre-determined probability distribution for each of the variables. As explained in the previous section, a particular random walk, consisting of several such random hops, is terminated on the boundary of the problem domain, where the value of the potential is known. The contribution from a particular random walk is obtained by multiplying the overall weight factor (which is obtained by multiplying the weight factors of individual hops) with the boundary value. An estimate $\bar{\hat{\phi}}$ of the potential, at the point of origination of the hops, is then obtained by averaging over a statistically large number of random walks and given by

$$\bar{\hat{\phi}} = \frac{1}{N} \sum_{n=1}^{N} \hat{\phi}_n \tag{21}$$

where $\hat{\phi}_n$ is the contribution from the nth random walk and N is the number of random walks. The error in the result has two components:

(1) A deterministic error arising from the truncation of the perturbation-based Green's function in Equation (17), which can be controlled by controlling the radius of the hop.
(2) A statistical 1-σ error σ_{T} given by [19]

$$\sigma_{\mathrm{T}} = \frac{\sigma_{\mathrm{E}}}{\sqrt{N}} \tag{22}$$

where σ_{E} is the standard deviation of the contributions from different random walks. As a result, the statistical error can be controlled by controlling the number of random walks.

4. RESULTS

We have chosen three benchmark problems

1. Problem 1 (Figure 2) is characterized by angular symmetry, where a circle of diameter λ is surrounded by another circle of diameter 3λ. The normalized potential is unity on the inner circle and zero on the outer circle.

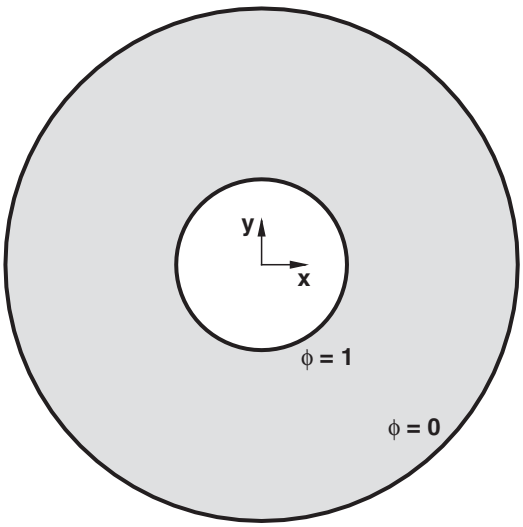

Figure 2. The solution of the NPB equation in the region between two concentric circles maintained at fixed potentials.

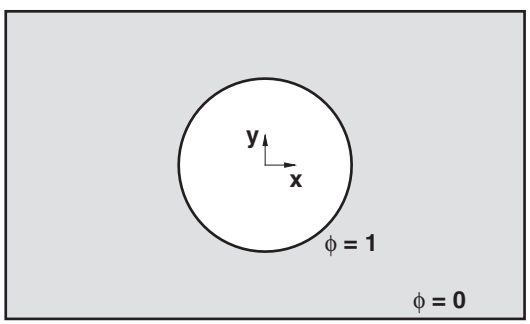

Figure 3. The solution of the NPB equation in the region between a circle (maintained at one potential) surrounded by a rectangular boundary (maintained at another potential).

2. In Problem 2 (Figure 3), a circle λ in diameter is surrounded by a rectangle of dimensions $3\lambda \times 2\lambda$. The normalized potential is unity on the inner circle and zero on the outer rectangle.
3. In Problem 3 (Figure 4), a boundary condition cosinusoidally varying in space is imposed on the left boundary of a square of dimensions $6\lambda \times 6\lambda$. The normalized potential is assumed to be zero on the top, bottom and the right boundaries.

The random-walk algorithms were coded in MATLAB 6.5^{TM}, and run on a 1.8 GHz personal computer, while the finite-difference results were obtained from a FORTRAN-based solver developed at Air Force Research Laboratory at Wright–Patterson Air Force Base and run on

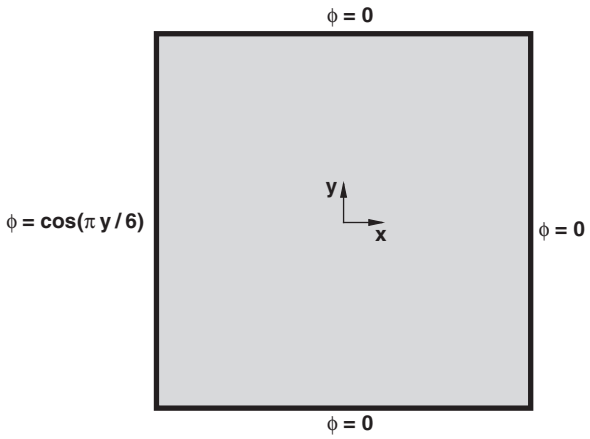

Figure 4. The solution of the NPB equation on a square problem domain. A spatially cosinusoidally varying potential is imposed on the left boundary, while the potential is zero on the left, right and the top boundary.

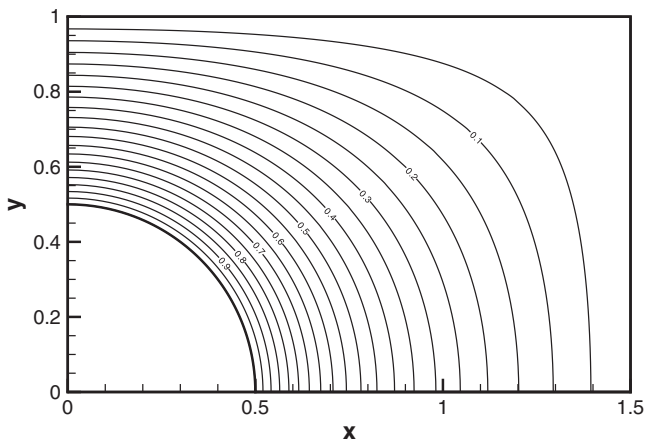

Figure 5. Finite-difference solution for Problem 2.

a Silicon Graphics, Inc. workstation. Because of the relative slowness of an interpreted MATLAB program in comparison to a compiled FORTRAN program, we have not been able to compare these approaches in terms of speed.

In this work, 20 000 random walks were performed per solution point, while the radii of the hops were restricted to 2 per cent of the characteristic length $\lambda(= c/\sqrt{k})$ to maintain the validity of the first-order approximation in the derivation of the volumetric Green's function. For Problem 1, the finite-difference solver exploited the angular symmetry in the problem and the radial dimension was discretized into 101 points. A grid of 51×51 points was used for Problem 2 (Figure 5), distributed over the first quadrant. For Problem 3 (Figure 6), the

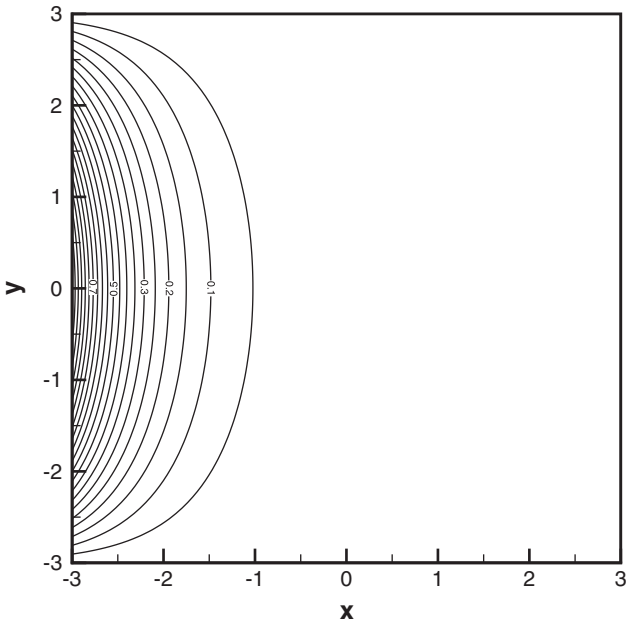

Figure 6. Finite-difference solution for Problem 3.

Table I. Statistical error and mean absolute error between FRW and finite-difference-based results.

Benchmark problem	Mean absolute error	Statistical error
Problem 1 (along the centreline positive x-axis)	0.0035	0.0020
Problem 2 (along the centreline positive x-axis)	0.0033	0.0028
Problem 2 (along the centreline positive y-axis)	0.0067	0.0025
Problem 3 (along the centreline positive x-axis)	0.0044	0.001
Problem 3 (along the centreline positive y-axis)	0.0024	0.0007

In order to compute the error for Problems 2 and 3, the finite-difference-based results were interpolated to a mesh corresponding to the random walk solution.

finite-difference calculations were carried out over a 101×51 grid distributed over the half-plane above the centreline x-axis.

Table I tabulates the statistical error and also the mean absolute error between the random walk and finite-difference-based results for each of the benchmark problems. Solution profiles

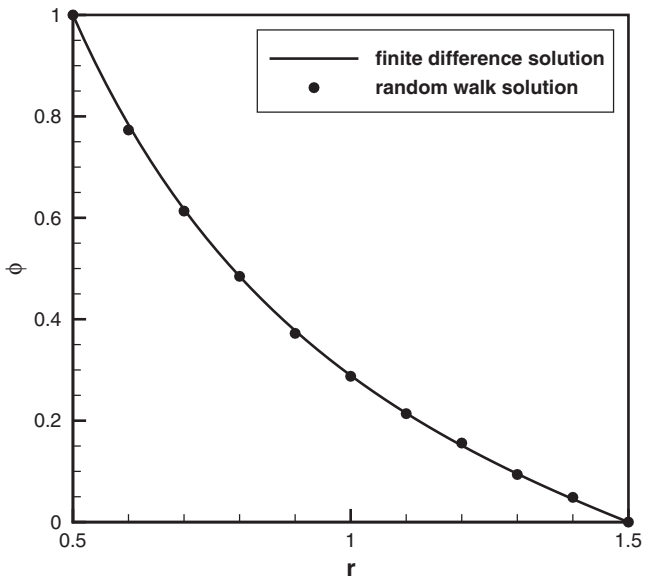

Figure 7. Normalized potential plotted against position in normalized co-ordinates for Problem 1.

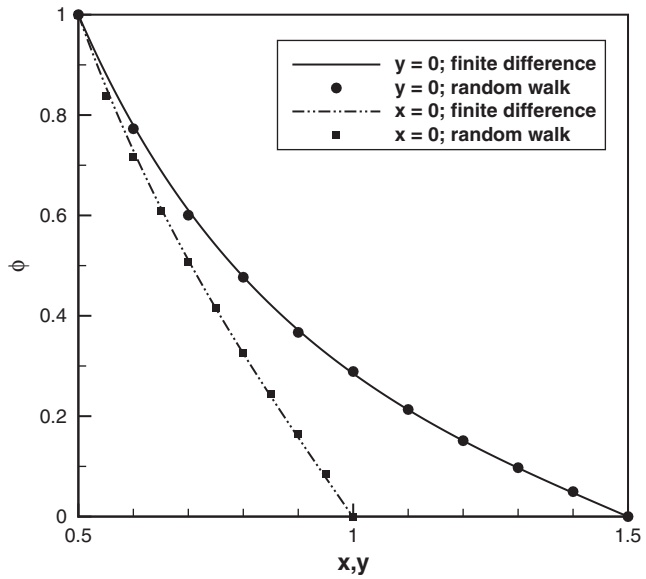

Figure 8. Normalized potential plotted against position in normalized co-ordinates for Problem 2.

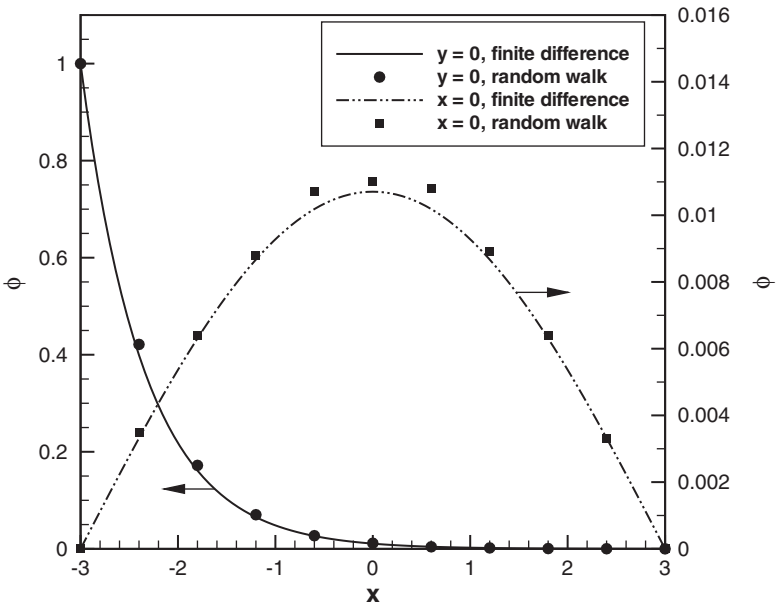

Figure 9. Normalized potential plotted against position in normalized co-ordinates for Problem 3.

for the benchmark problems are plotted in Figures 7–9. Excellent agreement is obtained between random-walk solutions and finite-difference results. It can also be observed that the absolute errors are consistently larger than the statistical errors, which can be attributed to the truncation of the perturbation-based Green's function in Equation (17), and also to the truncation errors in the finite-difference-based approach.

5. CONCLUSION

In summary, we have developed a new FRW algorithm for the solution of the NPB equation in two dimensions. This algorithm is based on an approximate volumetric Green's function, derived using perturbation theory. Excellent agreement was found between the results of random walk calculations and finite-difference results. Our literature survey indicates that the newly developed algorithm is the first application of the FRW method to the NPB equation. This algorithm has the advantages of being highly parallelizable and requiring no discretization of the problem domain. The approach is general, and can be applied to the numerical solution of other important non-linear equations. Our future work in this area will involve the extension of this new FRW algorithm to Neumann and mixed boundary condition problems, and will address the efficient implementation of the algorithms on parallel processor computer platforms.

ACKNOWLEDGEMENTS

Support for Dr K. Chatterjee was provided under a National Research Council Summer Faculty Fellowship at the Air Force Research Laboratory, Wright–Patterson Air Force Base. Additional support was provided by the Air Force Office of Scientific Research, under grants monitored by Dr J. Schmisseur and Dr F. Fahroo. We would like to acknowledge valuable discussions with Dr M. D. White and Dr D. V. Gaitonde.

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