A Parallelized Monte Carlo Algorithm for the Nonlinear Poisson-Boltzmann Equation in Two Dimensions

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Abstract – This paper presents the parallelization of a previously-developed two-dimensional floating random walk (FRW) algorithm for the solution of the nonlinear Poisson-Boltzmann (NPB) equation. Historically, the FRW method has not been applied efficiently to the solution of the NPB equation which can be attributed to the absence of analytical expressions for volumetric Green's functions. Stochastic approaches to solving nonlinear equations (in particular the NPB equation) that have been suggested in literature involve an iterative solution of a series of linear problems. As a result, previous applications of the FRW method have examined only the linearized Poisson-Boltzmann equation. In our proposed approach, an approximate (yet accurate) expression for the Green's function for the nonlinear problem is obtained through perturbation theory, which gives rise to an integral formulation that is valid for the entire nonlinear problem. As a result, our algorithm does not have any iteration steps, and thus has a lower computational cost. A unique advantage of the FRW method 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 previously published work, we have presented the fundamentals of our algorithm and in this paper we report the parallelization of this algorithm in two dimensions. The solution of the NPB equation has many interesting applications, including the modeling of plasma discharges, semiconductor device modeling and the modeling of biomolecules.

Key words – Monte Carlo, random walk, stochastic algorithm, nonlinear Poisson-Boltzmann equation, modeling of plasma sheaths, semiconductor device modeling, and modeling of biomolecular structure and dynamics.

I. INTRODUCTION

The solution of the nonlinear Poisson-Boltzmann (NPB) equation has widespread applications in science and engineering. These applications include the modeling of plasma sheaths [1], semiconductor device modeling [2] and the modeling of biomolecular structures and dynamics [3]. In this paper, we address the parallelization of a two-dimensional floating random-walk (FRW) [4-6] algorithm (a sub-class of Monte Carlo algorithms) for the NPB equation, subject to Dirichlet boundary conditions.

The FRW method is based on probabilistic interpretations of deterministic equations. We consider a differential equation, with a differential operator L,

$$L\left[U(\mathbf{r})\right] = f(\mathbf{r}), \tag{1}$$

where 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. Using Green's integral representation [7] $U(\mathbf{r})$ can be written as

$$\begin{aligned} U(\mathrm{r}_\mathrm{o}) = & \iiint_V dv G(\mathrm{r}\,|\,\mathrm{r}_\mathrm{o}) f(\mathrm{r}) \\ & - \oiint_S \left[d\mathbf{s}\cdot\nabla_\mathrm{r} U(\mathrm{r}) \right] \; G(\mathrm{r}|\mathrm{r}_\mathrm{o}) \\ & + \oiint_S \left[d\mathbf{s}\cdot\nabla_\mathrm{r} G(\mathrm{r}|\mathrm{r}_\mathrm{o}) \right] \; U(\mathrm{r}). \end{aligned} \tag{2}$$

The symbol $G(\mathbf{r}|\mathbf{r_o})$ is the volumetric Green's function [7] for equation (1) at $\mathbf{r}$ given an impulse function at $\mathbf{r_o}$ and is given by the solution of the equation $L\left[U(\mathbf{r})\right] = \delta(\mathbf{r}-\mathbf{r_o})$. $\nabla_\mathbf{r} G(\mathbf{r}\,|\,\mathbf{r_o})$, which on the other hand is called the surface Green's function [7]. The first term on the right hand side of equation (2) 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 $d\mathbf{s}$ 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 center of the area

unit. The second integral on the right hand side of equation (2) corresponds to the Neumann [7] boundary condition, whereas the third integral corresponds to the Dirichlet [7] boundary condition.

Equation (2) forms the mathematical basis of the FRW method. To evaluate the solution of equation (1) at a particular point in the domain of interest, we consider maximal spheres, cubes, or any geometrical object for which the volumetric Green's function of equation (1) is known [4-6]. 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 (2). 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 integral, as given by [8],

$$U(\mathrm{r}_0) = \oint_{S_1} ds_1 K(\mathrm{r}_0 \mid \mathrm{r}_1) \times \oint_{S_2} ds_2 K(\mathrm{r}_1 \mid \mathrm{r}_2) \times \oint_{S_n} ds_n K(\mathrm{r}_{n-1} \mid \mathrm{r}_n) U(\mathrm{r}_n), \quad (3)$$

$$K(\mathrm{r}_{n-1} \mid \mathrm{r}_n) = \left| \nabla_{\mathrm{r}_n} G(\mathrm{r}_{n-1} \mid \mathrm{r}_n) \right| \cos(\gamma_{n-1,n}) \ ,$$

where $\gamma_{n-1,n}$ is the angle between $\nabla_{\mathbf{r_n}} G(\mathbf{r_{n-1}} \mid \mathbf{r_n})$ and $d\mathbf{s_n}$, being a vector whose magnitude (ds_n) is equal to that of an infinitesimally small area unit on the surface S_n and directed normally outward from the center of the area unit. The successive surface integrals in equation (3) relate to successive random hops across the problem domain and the weight factors of the form $K(\mathbf{r_{n-1}} \mid \mathbf{r_n})$ are derived from the third integral term on the right hand side of equation (2) 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 (1) is obtained by averaging over a statistically large number of such samples.

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. In contrast, deterministic numerical methods require the discretization of either the volume or the surface of the problem domain. Methods such as the finite-difference [9] or the finite-element [10] are based on volume discretization, while methods such as the method of moments [11] require surface discretization. As a result, the FRW method has lower memory requirements compared to deterministic numerical methods.

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. As a result, one can obtain very close to linear rate of parallelization for a large number of processors, which is a very unique advantage that the FRW method enjoys over deterministic methods. In this paper, the superiority of the FRW method over the finite-difference method as regard to parallelization will be demonstrated.

In spite of these unique advantages, the FRW method has not being applied to the NPB equation and other important nonlinear equations. This can be attributed to 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 nonlinear problems might not be possible. In a 1954 paper [12], 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 nonlinear equations (in particular the NPB equation) that have been suggested in literature [13], involve an iterative solution of a series of linear problems and as a result random-walk algorithms that have been presented in literature [14-15], involve prior linearization of the NPB equation. In our proposed approach, an approximate (yet accurate) expression for the Green's function for the nonlinear problem is obtained through perturbation theory, which gives rise to an integral formulation that is valid for the entire nonlinear 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 Prof. K. Chatterjee in Ref. [16-17], where the idea of extending the approach to nonlinear problems was also proposed. Later that idea was extended to develop the fundamentals of a floating random-walk (FRW) algorithm for the NPB equation [18-20]. In this paper,

we present the results of parallelization of the FRW algorithm for the two-dimensional NPB equation.

II. FORMULATION OF THE ALGORITHM

The formulation of the two-dimensional algorithm is presented in detail in [19, 20], along with its validation with the help of finite-difference based benchmarks. In this section, we give a brief description of that formulation before presenting the details of the parallelization.

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

$$\nabla^2\phi = \frac{1}{c^2}\left(e^{k\phi(\mathbf{r})} - e^{-k\phi(\mathbf{r})}\right), \quad \mathbf{r} \in W, \tag{4}$$

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

$$\phi = g(\mathbf{r}), \quad \mathbf{r} \in \partial W \tag{5}$$

where ∂W is the boundary of the domain W. Equation (4) can be normalized to

$$\frac{1}{\hat{r}}\frac{\partial}{\partial \hat{r}}\left(\hat{r}\frac{\partial \hat{\phi}}{\partial \hat{r}}\right) + \frac{1}{\hat{r}^2}\frac{\partial^2 \hat{\phi}}{\partial \hat{\theta}^2} = e^{\hat{\phi}} - e^{-\hat{\phi}}, \tag{6}$$

where $\hat{r} = r/\lambda$, $\hat{\theta} = \theta$, $\hat{\phi} = k\phi$ and $\lambda = c/\sqrt{k}$. 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 $\hat{\rho}_o = \hat{r}_o/R$ in equation (6). The twice-normalized NPB equation is written as,

$$\frac{1}{\hat{\rho}}\frac{\partial}{\partial \hat{\rho}}\left(\hat{\rho}\frac{\partial \hat{\phi}}{\partial \hat{\rho}}\right) + \frac{1}{\hat{\rho}^2}\frac{\partial^2 \hat{\phi}}{\partial \hat{\theta}^2} = R^2\left(e^{\hat{\phi}} - e^{-\hat{\phi}}\right). \tag{7}$$

A volumetric Green's function of equation (7), $\hat{G}(\hat{\boldsymbol{\rho}} \mid \hat{\boldsymbol{\rho}}_{\mathbf{o}})$ at $\hat{\boldsymbol{\rho}}$, assuming a dirac-delta function at $\hat{\boldsymbol{\rho}}_{\mathbf{o}}$ inside the circular domain, is given as the solution of the equation

$$\frac{1}{\hat{\rho}}\frac{\partial}{\partial \hat{\rho}}\left(\hat{\rho}\frac{\partial \hat{G}}{\partial \hat{\rho}}\right) + \frac{1}{\hat{\rho}^2}\frac{\partial^2 \hat{G}}{\partial \hat{\theta}^2} - R^2\left(e^{\hat{G}} - e^{-\hat{G}}\right) = \delta\left(\hat{\rho} - \hat{\rho}_o\right). \tag{8}$$

A zero-order approximation (assuming homogeneous Dirichlet boundary conditions) for the volumetric Green's function, $\hat{G}^{(0)}(\hat{\boldsymbol{\rho}} \mid \hat{\boldsymbol{\rho}}_{\mathbf{o}})$ is the solution of equation

$$\frac{1}{\hat{\rho}}\frac{\partial}{\partial \hat{\rho}}\left(\hat{\rho}\frac{\partial \hat{G}^{(0)}}{\partial \hat{\rho}}\right) + \frac{1}{\hat{\rho}^2}\frac{\partial^2 \hat{G}^{(0)}}{\partial \hat{\theta}^2} = \delta\left(\hat{\rho} - \hat{\rho}_o\right) \tag{9}$$

and is given as [7]

$$\hat{G}^{(0)}\left(\hat{\rho} \mid \hat{\rho}_o\right) = \frac{1}{4\pi} \times \ln\left[\frac{\hat{\rho}^2 + \hat{\rho}_o^2 - 2\hat{\rho}\ \ \hat{\rho}_o\cos\left(\hat{\theta} - \hat{\theta}_o\right)}{1 + \hat{\rho}^2\hat{\rho}_o^2 - 2\hat{\rho}\ \ \hat{\rho}_o\cos\left(\hat{\theta} - \hat{\theta}_o\right)}\right]. \tag{10}$$

Equation (10) can be used to obtain a first-order approximation, $\hat{G}^{(1)}(\hat{\boldsymbol{\rho}} \mid \hat{\boldsymbol{\rho}}_{\mathbf{o}})$ to the volumetric Green's function and is given as a solution of the following equation,

$$\frac{1}{\hat{\rho}}\frac{\partial}{\partial \hat{\rho}}\left(\hat{\rho}\frac{\partial \hat{G}^{(1)}}{\partial \hat{\rho}}\right) + \frac{1}{\hat{\rho}^2}\frac{\partial^2 \hat{G}^{(1)}}{\partial \hat{\theta}^2} = \delta\left(\hat{\rho} - \hat{\rho}_o\right) + R^2\left(e^{G^{(0)}} - e^{-G^{(0)}}\right). \tag{11}$$

Based on equations (2), (10) and (11), $\hat{G}^{(1)}(\hat{\boldsymbol{\rho}} \mid \hat{\boldsymbol{\rho}}_{\mathbf{o}})$ is given by the following expression,

$$G^{(1)}\left(\hat{\boldsymbol{\rho}} \mid \hat{\boldsymbol{\rho}}_{\mathbf{o}}\right) = G^{(0)}\left(\hat{\boldsymbol{\rho}} \mid \hat{\boldsymbol{\rho}}_{\mathbf{o}}\right) + R^2\int_0^1\int_0^{2\pi}\left[d\hat{\rho}'\,d\hat{\theta}'\,\hat{\rho}'\,G^{(0)}\left(\hat{\boldsymbol{\rho}} \mid \hat{\boldsymbol{\rho}}'\right) \times f\{y\}\right], \tag{12}$$

where $f\{y\} = e^y - e^{-y}$ with $y = \hat{G}^{(0)}(\hat{\boldsymbol{\rho}} \mid \hat{\boldsymbol{\rho}}_{\mathbf{o}})$. It can again be noted that $\left\{G^{(1)}\left(\hat{\boldsymbol{\rho}} \mid \hat{\boldsymbol{\rho}}_{\mathbf{o}}\right)\right\}_{\hat{\rho}=1} = 0$ along the circumference of the circular domain. Based on this approximate expression for the volumetric Green's function and equation (2), an expression for normalized potential at a point $\hat{\boldsymbol{\rho}}_{\mathbf{o}}$ is given by a line integral over the circumference of the unit circle and is expressed as,

$$\hat{\phi}\left(\hat{\boldsymbol{\rho}}_{\mathbf{o}}\right) = \int_{\theta=0}^{2\pi} d\hat{\theta}\left[\frac{dG^{(1)}}{d\hat{\rho}}\right]_{\hat{\rho}=1}\hat{\phi}(1,\hat{\theta}). \tag{13}$$

For the development of the FRW algorithm, we need to estimate $\left[\frac{dG^{(1)}}{d\hat{\rho}}\right]_{\hat{\rho}=1}$ in equation (13). This estimate is obtained by differentiating equation (12), and in the zero-centered notation (i.e. $\hat{\rho}_o = 0$) is given by,

$$\left[\frac{dG}{d\hat{\rho}}\right]_{\hat{\rho}=1} = \frac{1}{2\pi} + \frac{R^2}{4\pi}\int_0^1\int_0^{2\pi} \hat{\rho}' d\hat{\rho}' d\theta' A \times B, \qquad (14)$$

where A and B are given by,

$$A = \left[\left(\hat{\rho}'\right)^{\frac{1}{2\pi}} - \left(\hat{\rho}'\right)^{-\frac{1}{2\pi}}\right],$$
$$B = \frac{2\left(1-\left(\hat{\rho}'\right)^2\right)}{1+\left(\hat{\rho}'\right)^2 - 2\hat{\rho}'\cos\left(\hat{\theta}-\hat{\theta}'\right)}. \qquad (15)$$

Equation (13) in conjunction with equations (14) and (15) is 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 λ 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 (13) according to a 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 $\overline{\hat{\phi}}$ of the potential, at the point of origination of the hops is then obtained by averaging over a statistically large number of random-walks.

The error in the result has a deterministic component arising from the truncation of the perturbation-based Green's function in equation (12), which can be controlled by controlling the radius of the hop. The error also has a stochastic component, a measure of which is given by the "1-σ error σ_T" given by [21],

$$\sigma_T = \frac{\sigma_E}{\sqrt{N}}, \qquad (16)$$

where σ_E is the standard deviation of the contributions from different random-walks, N being the number of random-walks. As a result, the statistical error can be controlled by controlling the number of random-walks.
The FRW algorithm described previously was parallelized. Two levels of parallelism are inherent in an FRW algorithm. First, the solutions for different points in the domain (different origins for the random walks) are independent of each other. Second, for a given point of origin, each random walk is independent, and inter-processor communication is required only to sum up the contributions of the walks. For this initial parallel implementation, the test points in the domain were handled serially. The walks were distributed in groups across computer processors, with communication and a reduction operation at the completion of the walks. The FRW algorithm was implemented in C, and the serial version of the code was converted to parallel using the Message Passing Interface (MPI) library. The elegance and inherent parallelism of the FRW algorithm is demonstrated in the fact that the serial and parallel versions of the code differ by only four function calls, three of which are merely initialization routines. The results of this parallelization are given in the next section.

III. RESULTS

In our benchmark problem (Fig. 1) [20], 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. When run in a single processor, 20000 random-walks were performed per solution point, while the radii of the hops were restricted to two percent of the characteristic length λ to maintain the validity of the first-order approximation in the derivation of the volumetric Green's function in equation (12). For finite-difference calculations, a grid of 51×51 points, distributed over the first quadrant was used. The finite-difference calculations were carried out using a standard transformation from a curvilinear mesh in physical space to a uniform mesh in computational space, while maintaining second order accuracy. The results are shown in Table 1 and Fig. 2. Excellent agreement is observed between FRW and finite-difference based 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 (12), and also to the truncation errors in the finite-difference based approach.

The parallelized algorithm was implemented on an IBM P4+ machine, running 1.7 GHz Power 4+ chips, with 2 Gigabytes RAM available per processor for as many as 64 processors. The timing results are shown in Fig. 3 for 100000 and 10000 random-walks per solution point. It can be observed that for 100000 random-walks per solution point the speed of computation increases perfectly linearly with the number of processors, particularly for a relatively smaller number of

processors. This can be attributed to the fact that the random-walks per processor needs to be high enough to ensure that the time spent in actual computation is large compared to the communication time between the various processors. For the same reason, the increase in the speed of computation is only sixteen fold for 32 processors with only 10000 random-walks per solution point. It should be borne in mind that the benchmark problems used for validation are relatively simple problems, and for more complicated problems one can expect to see even better scalability, stemming from the increased number of samples per processor. In comparison, the parallelization of the finite-difference algorithm (Fig. 4) for the same problem showed markedly inferior performance (compared to the case where N =100000) with increase in the number of processors. With 32 processors, the speed of computation is only 16 times higher than the speed with a single processor. It can also be concluded that as the finite-difference method (like other deterministic methods based on discretization) reduces the numerical solution of a differential equation to the numerical solution of a matrix equation, our newly-developed algorithm will exhibit superior efficiency of parallelization compared to other discretization-based deterministic methods as well.

Table 1. Statistical error and mean absolute error between FRW and finite-difference based results.

Benchmark Problem (20000 Random Walks per Solution Point)	***Mean Absolute Error***	***Statistical Error***
Along the centerline positive x-axis	0.0033	0.0028
Along the centerline positive y-axis	0.0067	0.0025

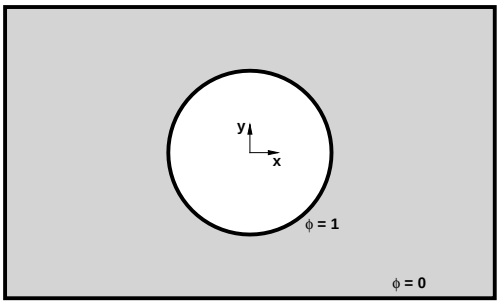

Fig. 1. The solution of the NPB equation in the region between a circle surrounded by a rectangular boundary. Problem dimension is $3\lambda \times 2\lambda$.

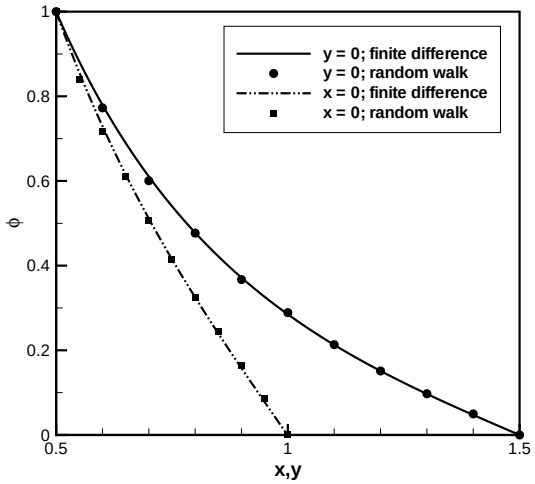

Fig. 2. Normalized potential plotted against position in normalized coordinates.

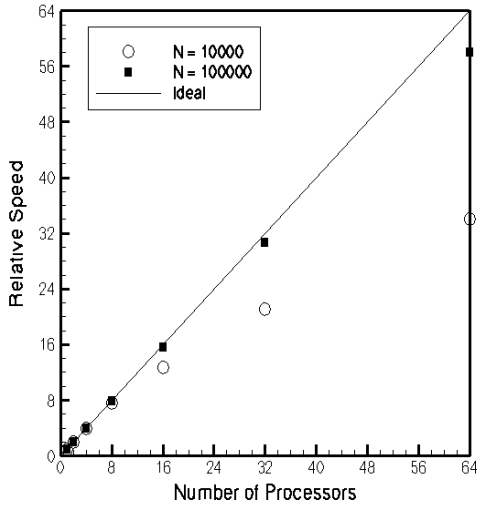

Fig.3. Parallelization results for the FRW algorithm.

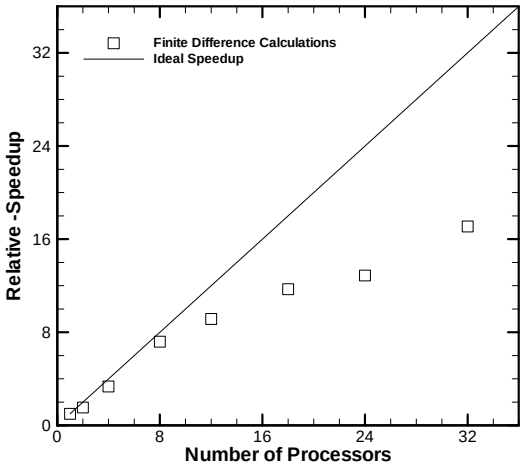

Fig. 4. Parallelization results for the finite-difference algorithm.

IV. CONCLUSION

In summary, we have parallelized a previously-developed 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 random walk and finite-difference results, while the FRW algorithm exhibited vastly superior (almost linear) efficiency of parallelization for a statistically significant number of random-walks per processor. The FRW algorithm also has the advantage of not requiring any discretization of the volume or the surface of problem domains. The approach is general, and can be applied to the numerical solution of other important nonlinear equations. Our work in the immediate future will involve the extension of this new FRW algorithm to Neumann and mixed boundary condition problems. The ultimate objective of this work is the extension of the perturbation-based approach to flow problems.

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