

First Passage Monte-Carlo Simulation for Charge Distribution and Capacitance

Aditya Kumar Singh, Apurva Anand, Anindya Sundar Das

Abstract—A novel scheme has been studied and demonstrated for Monte Carlo simulations of diffusion-reaction processes. The new algorithm skips the traditional small diffusion hops and propagates the diffusing particles over long distances through a sequence of super-hops, one particle at a time. By partitioning the simulation space into non-overlapping protecting domains each containing only one or two particles, the algorithm factorizes the N-body problem of collisions among multiple Brownian particles into a set of much simpler single-body and two-body problems. Efficient propagation of particles inside their protective domains is enabled through the use of time-dependent Green's functions (propagators) obtained as solutions for the first-passage statistics of random walks. The resulting Monte Carlo algorithm is event-driven and asynchronous; each Brownian particle propagates inside its own protective domain and on its own time clock. The algorithm reproduces the statistics of the underlying Monte-Carlo model exactly. The new algorithm is efficient at low particle densities, where other existing algorithms slow down severely. Thus we have analyzed the application of this algorithm in the charge distribution and the capacitance detection.

Index Terms—Monte Carlo Simulation, Charge distribution, capacitance, Markov chain

I. INTRODUCTION

First passage algorithm is a simple and robust computational approach for simulations of systems evolving through random walks. Mathematically, first passage process derives from the theory of Markov processes in which the model evolves from state to state through a sequence of stochastic transitions whose rates depend on the current state alone [1-3]. Random walks are typically simulated as sequences of hops, either from one lattice site to a neighboring one for discrete walks, or through finite displacements for continuum walks. When the system dynamics is defined by collisions among the walkers, the hops themselves are trivial changes of the system's state while significant events take place only when the walkers collide. A serious computational bottleneck is presented for the first passage method by situations when the density of walkers is low. Consider a system of randomly distributed walkers. Many research works have been done on the Monte Carlo simulation (MCS). James A. Given, Chi-Ok Hwang, and Michael Mascagni have shown that Monte Carlo diffusion methods are often the most efficient algorithms for solving certain elliptic boundary value problems [1].

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Melvin H. Kalos, George H. Gilmer and B. Sadigh have introduced a new Monte Carlo simulation method of diffusion-reaction processes where they have eliminated the traditional small diffusion hop and made to propagate the diffusing particles over long distances through a sequence of super-hops, one particle at a time [13-14]. In [4-10] several methods have been discussed for computing the charge distribution and the capacitance by calculating the diffusion of particle. But these methods have several drawbacks which have been discussed in the [11-12]. Some possible solutions were given in [15-19] but as system particles are following the Brownian dynamic model the MCS solutions are getting complex. There are few schemes, discussed in [20-22], which have given the idea of solving the problems by employing MCS scheme with first passage solution.

In this paper we have presented a novel approach for Monte Carlo simulations that is both efficient and exact for a wide class of models involving collisions among multiple Brownian particles, as first proposed in [1]. Based on exact solutions for the first passage statistics of random walks, the new method is referred to as First Passage Kinetic Monte Carlo (First passage Monte Carlo) in the following. In the new algorithm, the particles are propagated over long distances while each walker (particle) is protected (separated from interference by other walkers) within its own spatial region. The N regions are non-overlapping and partition the space into disjoint spatial domains in which the enclosed walkers are propagated individually. The use of first-passage statistics for walker propagation permits an elegant factorization of the N-body problem into a product of N single-body problems. Efficient implementation of the new method leads to an asynchronous event-driven algorithm in which every walker propagates within its personal space and from its own time origin. The resulting speedup is most impressive when the density of diffusing particles is low and particle collisions are rare.

II. THEORY OF FIRST PASSAGE MONTE-CARLO ALGORITHM

In a Monte Carlo Simulation a random value is selected for each of the tasks, based on the range of estimates. This algorithm is based on the first passage (FP) and no passage (NP) propagators to skip numerous small steps and to propagate the walkers to collisions. For the new algorithm to be efficient, Monte Carlo sampling from these propagators should not entail significant computational overhead. In this algorithm FP and NP propagations replace numerous short diffusive hops. The NP propagators are needed when a walker propagates right on or close to the boundary of a neighboring protecting segment. Consequently the new time for FP propagation of the squeezed walker is likely to be so short that the same walker will be selected for the very next propagation

again. Therefore MCS cycle entails one FP and possibly one or few NP propagation, while all other N-1 or N-2 walkers stay inactive. This algorithm allows exact and efficient treatment of particle collisions by protecting and propagating group of walkers. The ultimate purpose of the MCS method is to enable efficient propagation of walkers to the collisions whereas handling of collision events is outside of the method's main scope.

III. CALCULATION OF CHARGE DISTRIBUTION

If Gauss law gives us charge distribution by the equation

$$\sigma(x) = -\frac{1}{4\pi} \frac{d}{d\epsilon} \Big|_{\epsilon=0} V(x+\epsilon) \quad (1)$$

By the probabilistic potential theory $V(x+\epsilon)$ is probability density associated with a diffusing particle initiating at point $(x+\epsilon)$. The point $(x+\epsilon)$ is close to the surface. Diffusing particle performs the random walks from a point on the rod. The particle diffuses to infinity or makes a first passage to the rod. Every point on the rod has probability of first passage simulating number of random walks gives the probability distribution of first passage walks $V(x+\epsilon)$.

Rod is of negligible thickness Length is 1 m maintained at 1V potential. Diffusion particle start at a point on the rod

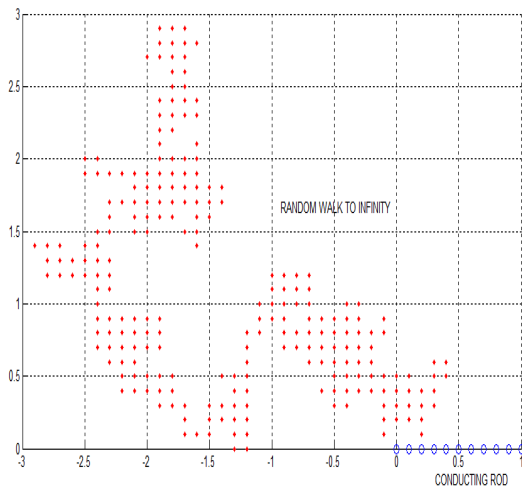


Figure.1 (a)

The walk either goes to infinity or it makes a first passage to the rod.

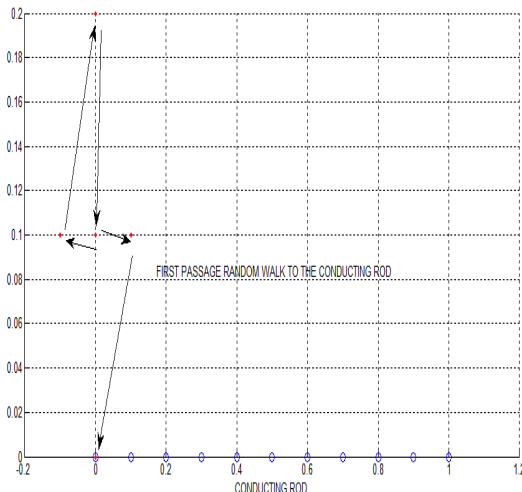


Figure.1 (b)

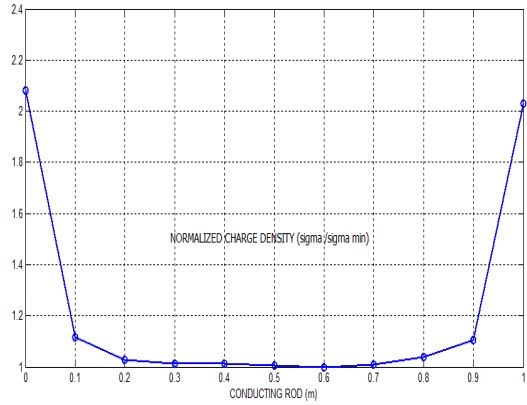


Figure.1 (c)

Figure.1 (a) shows the random walk on the conducting rod; figure.1 (b) shows the graph for first passage random walk to the conducting rod and the figure.1 (c) has shown the plot of varying normalized charge density along the conducting rod due to the first passage MCS.

This charge distribution scheme is also applicable to the square plate surface. We have taken an example of a square conducting plate, which has negligible thickness, area of 1m x 1m and maintained at 1 V potential

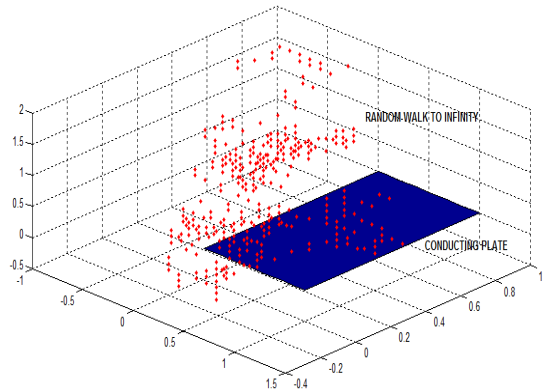


Figure.2 (a)

Figure.2 (a) has shown the random walk of the diffusing particles start from a point on the plate. The random walk either goes to infinity or it makes a first passage on the plate

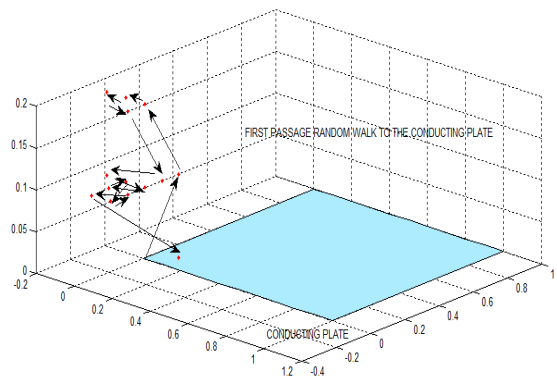


Figure.2 (b)

Figure.2 (b) has shown the plot for first passage random walk to the conducting rod. In figure.2 (c) the plot is shown for random walks simulation in three dimensions. There are 10^5 random walks are simulated for every point. The charge distribution is obtained from the probability distribution.

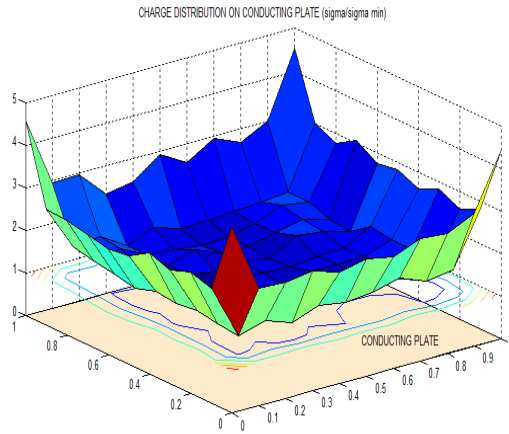


Figure.2 (c)

The charge distribution is obtained in figure.2 (c) by applying the first passage algorithm in the conventional charge distribution scheme (Gauss's law).

IV. CALCULATION OF CAPACITANCE

The computing the capacitance of the unit cube analytically is considered to be one of the major unsolved problems of electrostatic theory [6]. However, due to improvements in computer performance and error analysis for walk on spheres (WOS) Monte Carlo algorithms, we can now calculate the capacitance of the unit cube to many more significant digits than previously possible by using a modified Brownian dynamics algorithm. In our algorithm, there are only two error sources: the error associated with the number of random walks N (sampling error) and the error associated with a ϵ -absorption layer. The sampling error convergence is well-known as $O(N^{1/2})$, and error analysis for WOS, Monte Carlo algorithms enables us to control the error from the ϵ -absorption layer and to get a more accurate capacitance value for the unit cube. Our result supports the calculations given by the conjectured exact value.

Consider the Robin potential, u , inside G . The boundary conditions state that the Robin potential is constant and equal to one in G . The interpretation of this hearkens back to elementary physics where one learns that inside a conductor the electrical potential is constant. Thus we have:

$$\int_{\partial G} \frac{1}{|x-y|} \mu(y) d\sigma(y) = 1 \quad (2)$$

This equation is valid for point $x \in G$ and $[v(y) = 1/|x-y|]$. We get the formula for the capacitance by applying the MCS in every open set in the ∂G region. Thus the capacitance can be calculated using the following formula:

$$C = \left(\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{n=1}^n v(y_n) \right)^{-1} \quad (3)$$

To estimate the computational error, we use a Markov chain version of the central limit theorem. It states that $\frac{1}{n} \sum_{n=1}^n v(y_n)$ Tends to a normally distributed random variable with mean $I[v]$ and variance DN^{-1} . Here

$$D = \lim_{N \rightarrow \infty} \int_{\partial G} \pi_{\infty} \left[\frac{1}{\sqrt{N}} \sum_{n=1}^N (v(y_n) - I[v]) \right]^2 \quad (4)$$

To evaluate D , we use the method of batch means with the number of batches, $k+1$, equal to $(N+1)^{1/2}$ and the batch size m equal to $N^{1/2}$. Thus we have

$$D = \lim_{m \rightarrow \infty, k \rightarrow \infty} \frac{m}{k} \sum_{i=0}^k \left(\frac{1}{m} S_i - \frac{1}{N} S \right)^2 \quad (5)$$

Where

$$S_i = \sum_{j=mi+1}^{m(i+1)} v(y_j), \quad S = \sum_{i=0}^k S_i. \quad (6)$$

Thus equation 3 provide a method to obtain the value of capacitance without explicitly calculating the density,

V. CONCLUSION

In this paper we have studied and analyzed application of first passage MCS theoretically. The calculation of charge distribution and the capacitance is done successfully using the first passage MCS. The scheme is using position of particle absorbed in the surface to calculate the charge distribution and the moment of particles to calculate the capacitance. This first passage MCS can be applicable to solve each and every boundary value problems, Laplace equations, etc.

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REFERENCES

- [1] James A. Given, Chi-Hwang, Michel Mascagni, "First and last passage Monte Carlo algorithm for charge distribution on a conducting surface", Phys. Rev. 66,0567042002.
- [2] Sydeny Redner, "A Guide to First Passage Process" Cambridge university press, 2001.
- [3] M.Strobel, K.-H. Heinig, and W. Moller. "Three-dimensional domain growth on the size scale of the capillary length: Effective growth exponent and comparative atomistic and mean-field simulations". Phys. Rev. B, 64(24):245422, 2001.
- [4] J. S. Reese, S. Raimondeau, and D. G. Vlachos. Monte Carlo Algorithms for Complex Surface Reaction Mechanisms: Efficiency and Accuracy. J. Comp. Phys. 173(1):302-321, 2001.
- [5] M. Biehl. "Lattice gas models and Kinetic Monte Carlo simulations of epitaxial growth". In Voigt, editor, Int. Series of Numerical Mathematics 149, pages 3-18. Birkhaeuser, 2005.
- [6] S. K. Theiss, M.-J. Caturla, M. D. Johnson, J. Zhu, T. J. Lenosky, B. Sadigh, and T. Diazde la Rubia. Atomic scale models of ion implantation and dopant diffusion in silico. Thin Solid Films, 365:219-230, 2000.
- [7] C. Domain, C. S. Becquart, and L. Malerba. "Simulation of radiation damage in Fe alloys: an object kinetic Monte Carlo approach. Journal of Nuclear Materials", 335(1):121-145, 2004.
- [8] D. P. Tolle and N. Le Novere. "Particle-based stochastic simulation in systems biology". Current Bioinformatics, 1(3):315-320, 2006.
- [9] J. S. van Zon and P. R. ten Wolde. "Green's-function reaction dynamics: A particle-based approach for simulating biochemical networks in time and space". J. Chem. Phys., 123(23):234910, 2005.
- [10] S. J. Plimpton and A. Slepoy. "Microbial cell modeling via reacting diffusive particles". J. Phys.: Conf. Ser., 16:305-309, 2005.
- [11] M. H. Kalos, D. Levesque, and L. Verlet. "Helium at zero temperature with hard-sphere and other forces". Phys. Rev. A, 9(5):2178-2195, 1974.
- [12] J. Dalla Torre, J.-L. Bocquet, N. V. Doan, E. Adam, and A. Barbu. "JERK an event-based Kinetic Monte Carlo model to predict microstructure evolution of materials under irradiation". Philosophical Magazine, 85:549-558, 2005.
- [13] T. Oettelstrup, V. V. Bulatov, G. H. Gilmer, M. H. Kalos, and B. Sadigh. "First-Passage Monte Carlo Algorithm: Diffusion without All the Hops". Phys. Rev. Lett., 97(23):230602, 2006.Donev.

- [14] T. Oppelstrup, V. V. Bulatov, G. H. Gilmer, M. H. Kalos, and B. Sadigh. "Asynchronous event-driven particle algorithms. SIMULATION". Transactions of The Society for Modeling and Simulation International, 85(4):229–242, 2008.
- [15] Daniel Ben Abraham. "Computer simulation methods for diffusion-controlled reactions". J. Chem. Phys., 88(2):941–948, 1988.
- [16] F. Leyvraz and S. Redner. "Spatial organization in the two-species annihilation reaction $A+B \rightarrow 0$ ". Phys. Rev. Lett., 66(16):2168–2171, 1991.
- [17] Y. Shafirir and D. ben Avraham. "Large scale simulations of two-species annihilation, $A+B \rightarrow 0$, with drift". Phys. Lett. A, 278(4):184–190, 2001.
- [18] M. Smith and T. Matsoukas. "Constant-number Monte Carlo simulation of population balances". Chemical Engineering Science, 53(9):1777–1786, 1998.
- [19] D. Zhong, R. Dawkins, and D. Ben Abraham. "Large-scale simulations of diffusion-limited n-species annihilation". Phys. Rev. E, 67(4):040101, 2003.
- [20] S. S. Andrews and D. Bray. "Stochastic simulation of chemical reactions with spatial resolution and single molecule detail". Physical biology, 1(3):137–151, 2004.
- [21] D. Toussaint and F. Wilczek. "Particle–antiparticle annihilation in diffusive motion". J. Chem. Phys., 78(5):2642–2647, 1983.
- [22] H. Kim and K. J. Shin. Exact Solution of the Reversible Diffusion-Influenced Reaction for an Isolated Pair in Three Dimensions. Phys. Rev. Lett., 82(7):1578–1581, 1999



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