Using Simple SDEs (Stochastic Differential Equations) to Solve Complicated PDEs (Partial Differential Equations)

Prof. Michael Mascagni

Department of Computer Science & School of Computational Science
Florida State University, Tallahassee, FL 32306 **USA**

E-mail: mascagni@cs.fsu.edu or mascagni@math.ethz.ch
URL: http://www.cs.fsu.edu/∼mascagni

With help from Drs. James Given, Chi-Ok Hwang, Aneta Karaivanova and Nikolai Simonov

Research supported by ARO, DOE/ASCI, NATO, and NSF

Outline of the Talk

Early History of MCMs for PDEs

1. Courant, Friedrichs, and Lewy: Their pivotal 1928 paper has probabilistic interpretations and MC algorithms for linear elliptic and parabolic problems
2. Fermi/Ulam/von Neumann: Atomic bomb calculations were done using Monte Carlo methods for neutron transport, their success inspired much post-War work especially in nuclear reactor design
3. Kac and Donsker: Used large deviation calculations to estimate eigenvalues of a linear Schrödinger equation
4. Forsythe and Leibler: Derived a MCM for solving special linear systems related to discrete elliptic PDE problems

Early History of MCMs for PDEs

5. Curtiss: Compared Monte Carlo, direct and iterative solution methods for $\mathbf{Ax} = \mathbf{b}$
   - General conclusions of all this work (as other methods were explored) is that random walk methods do worse than conventional methods on serial computers except when modest precision and few solution values are required
   - Much of this "conventional wisdom" needs revision due to complexity differences with parallel implementations
6. Muller & Curtiss: Monte Carlo methods for elliptic PDEs

Elliptic PDEs as Boundary Value Problems

1. Elliptic PDEs describe equilibrium, like the electrostatic field set up by a charge distribution, or the strain in a beam due to loading
2. No time dependence in elliptic problems so it is natural to have the interior configuration satisfy a PDE with boundary conditions to choose a particular global solution
3. Elliptic PDEs are thus part of boundary value problems (BVPs) such as the famous Dirichlet problem for Laplace's equation:
$$\frac{1}{2}\Delta u(x) = 0, \quad x \in \Omega, \quad u(x) = f(x), \quad x \in \partial\Omega \qquad (2.1)$$
4. Here $\Omega \subset \mathbb{R}^s$ is a open set (domain) with a smooth boundary $\partial\Omega$ and $f(x)$ is the given boundary condition

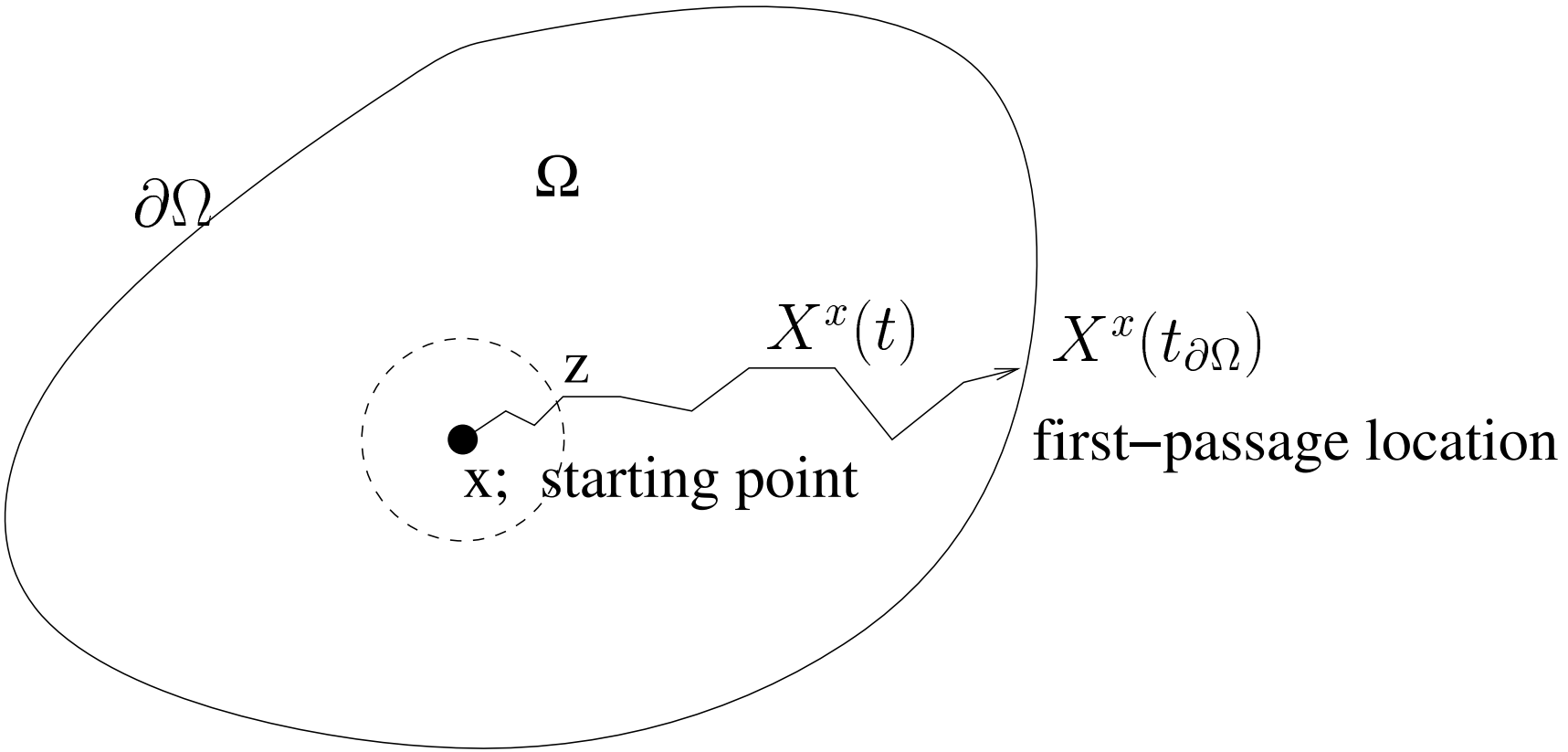
Probabilistic Approaches to Elliptic PDEs

- Early this century probabilists placed measures on different sets including sets of continuous functions
  - **A.** *Called Wiener measure*
  - **B.** *Gaussian based:* $\frac{1}{\sqrt{2\pi t}} e^{-\frac{x^2}{2t}}$
  - **C.** *Sample paths are Brownian motion*
  - **D.** *Related to linear PDEs*
- E.g. $u(x) = \mathbb{E}_x[f(X^{\mathbf{x}}(t_{\partial\Omega}))]$ is the Wiener integral representation of the solution to (2.1), to prove it we must check:
  - **A.** $u(x) = f(x)$ *on* $\partial\Omega$
  - **B.** $u(x)$ *has the MVP*
- Interpretation via Brownian motion and/or a probabilistic Green's function

Probabilistic Approaches to Elliptic PDEs

- Important: $t_{\partial\Omega} =$ first passage (hitting) time of the path $X^{\mathbf{x}}(\cdot)$ started at x to $\partial\Omega$, statistics based on this random variable are intimately related to elliptic problems
- Can generalize Wiener integrals to different BVPs via the relationship between elliptic operators, stochastic differential equations (SDEs), and the Feynman-Kac formula

Probabilistic Approaches to Elliptic PDEs



Probabilistic Approaches to Elliptic PDEs

- E.g. consider the general elliptic PDE:

$$Lu(x) - c(x)u(x) = g(x),\ x \in \Omega,\ c(x) \geq 0,$$
$$u(x) = f(x),\ x \in \partial\Omega \tag{1.1a}$$

where L is an elliptic partial differential operator of the form:

$$L = \frac{1}{2}\sum_{i,j=1}^{s} a_{ij}(x)\frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{s} b_i(x)\frac{\partial}{\partial x_i}, \tag{1.1b}$$

Probabilistic Approaches to Elliptic PDEs

- The Wiener integral representation is:

$$u(x) = \mathbb{E}_x^L \left[\int_0^{t_{\partial\Omega}} \left\{ \frac{f(X^{\mathbf{x}}(t_{\partial\Omega}))}{t_{\partial\Omega}} - g(X^{\mathbf{x}}(t)) \right\} e^{-\int_0^t c(X^{\mathbf{x}}(s))\, ds}\, dt \right] \tag{1.2a}$$

the expectation is w.r.t. paths which are solutions to the following (vector) SDE:

$$dX^{\mathbf{x}}(t) = \sigma(X^{\mathbf{x}}(t))\, dW(t) + b(X^{\mathbf{x}}(t))\, dt, \;\; X^{\mathbf{x}}(0) = x \tag{1.2b}$$

Probabilistic Approaches to Elliptic PDEs

- The matrix $\sigma(\cdot)$ is the Choleski factor (matrix-like square root) of $a_{ij}(\cdot)$ in (1.1b)
- To use these ideas to construct MCMs for elliptic BVPs one must:
  - **A.** *Simulate sample paths via SDEs (1.2b)*
  - **B.** *Evaluate (1.2a) on the sample paths*
  - **C.** *Sample until variance is acceptable*

Different SDEs, Different Processes, Different Equations

- The SDE gives us a process, and the process defines L (note: a complete definition of L includes the boundary conditions)
- We have solved only the Dirichlet problem, what about other BCs?
- Neumann Boundary Conditions: $\frac{\partial u}{\partial n} = g(x)$ on $\partial\Omega$
- If one uses reflecting Brownian motion, can sample over these paths
- Mixed Boundary Conditions: $\alpha\frac{\partial u}{\partial n} + \beta u = g(x)$ on $\partial\Omega$
- Use reflecting Brownian motion and first passage probabilities, together
- In some simple cases, only $X^{\mathbf{x}}(t_{\partial\Omega})$ is needed

Probabilistic Approaches to Parabolic PDEs via Feynman-Kac

- Can generalize Wiener integrals to a wide class of IBVPs via the relationship between elliptic operators, stochastic differential equations (SDEs), and the Feynman-Kac formula
- Recall that $t \to \infty$ parabolic $\to$ elliptic

Probabilistic Approaches to Parabolic PDEs via Feynman-Kac

- E.g. consider the general parabolic PDE:

$$u_t = Lu(x) - c(x)u(x) - f(x),\ x \in \Omega,\ c(x) \geq 0,$$
$$u(x) = g(x),\ x \in \partial\Omega \tag{1.3a}$$

where L is an elliptic partial differential operator of the form:

$$L = \frac{1}{2}\sum_{i,j=1}^{s} a_{ij}(x)\frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{s} b_i(x)\frac{\partial}{\partial x_i}, \tag{1.3b}$$

Probabilistic Approaches to Parabolic PDEs via Feynman-Kac

- The Wiener integral representation is:

$$u(x,t) = \mathbb{E}_x^L \left[g(X^{\mathbf{x}}(\tau_{\partial\Omega})) - \int_0^t f(X^{\mathbf{x}}(t)) e^{-\int_0^t c(X^{\mathbf{x}}(s))\,ds}\,dt \right] \tag{1.4a}$$

the expectation is w.r.t. paths which are solutions to the following (vector) SDE:

$$dX^{\mathbf{x}}(t) = \sigma(X^{\mathbf{x}}(t))\,dW(t) + b(X^{\mathbf{x}}(t))\,dt,\ X^{\mathbf{x}}(0) = x \tag{1.4b}$$

- The matrix $\sigma(\cdot)$ is the Choleski factor (matrix-like square root) of $a_{ij}(\cdot)$ in (1.3b)

The First Passage (FP) Probability is the Green's Function

Back to our canonical elliptic boundary value problem:

$$\frac{1}{2}\Delta u(x) = 0, \quad x \in \Omega$$
$$u(x) = f(x), \quad x \in \partial\Omega$$

- Distribution of z is uniform on the sphere
- Mean of the values of $u(z)$ over the sphere is $u(x)$
- $u(x)$ has mean-value property and harmonic
- Also, $u(x)$ satisfies the boundary condition

$$u(x) = \mathbb{E}_x[f(X^{\mathbf{x}}(t_{\partial\Omega}))] \tag{3.1}$$

The First Passage (FP) Probability is the Green's Function

Reinterpreting as an average of the boundary values

$$u(x) = \int_{\partial\Omega} p(x,y) f(y)\, dy \tag{3.2}$$

Another representation in terms of an integral over the boundary

$$u(x) = \int_{\partial\Omega} \frac{\partial g(x,y)}{\partial \mathbf{n}} f(y)\, dy \tag{3.3}$$

$g(x,y)$ – Green's function of the Dirichlet problem in Ω

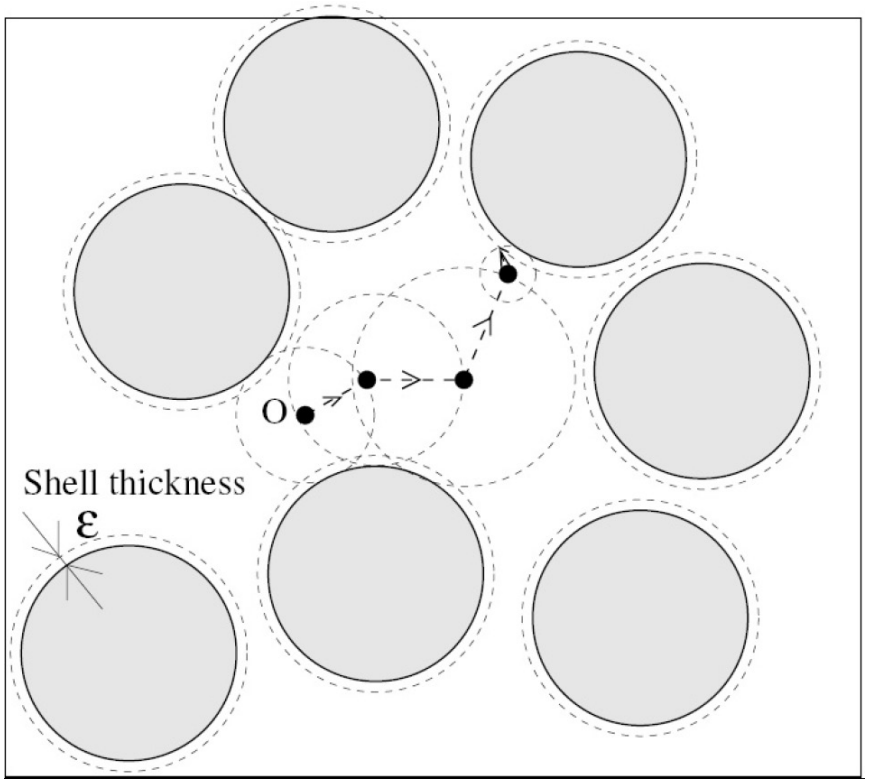
$$\Longrightarrow p(x,y) = \frac{\partial g(x,y)}{\partial \mathbf{n}} \tag{3.4}$$

'Walk on Spheres' (WOS) and 'Green's Function First Passage' (GFFP) Algorithms

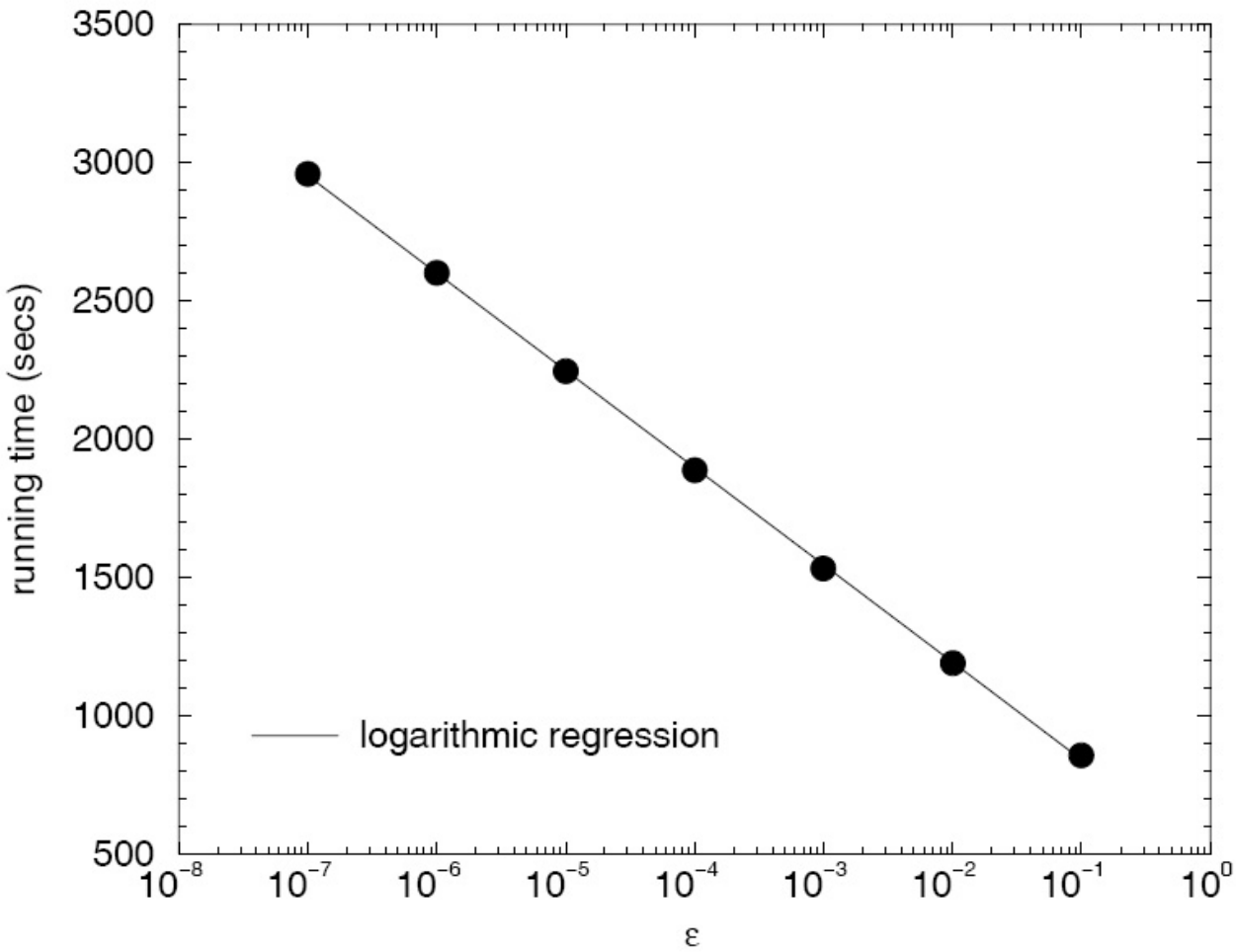
- Green's function is known
  $\Longrightarrow$ direct simulation of exit points and computation of the solution through averaging boundary values
- Green's function is unknown
  $\Longrightarrow$ simulation of exit points from standard subdomains of Ω, e.g. spheres
  $\Longrightarrow$ Markov chain of 'Walk on Spheres' (or GFFP algorithm) $x_0 = x, x_1, \ldots, x_N$
  $x_i \to \partial\Omega$ and hits ε-shell is $N = O(|\ln(\varepsilon)|)$ steps
  x_N simulates exit point from Ω with $O(\varepsilon)$ accuracy

'Walk on Spheres' (WOS) and 'Green's Function First Passage' (GFFP) Algorithms

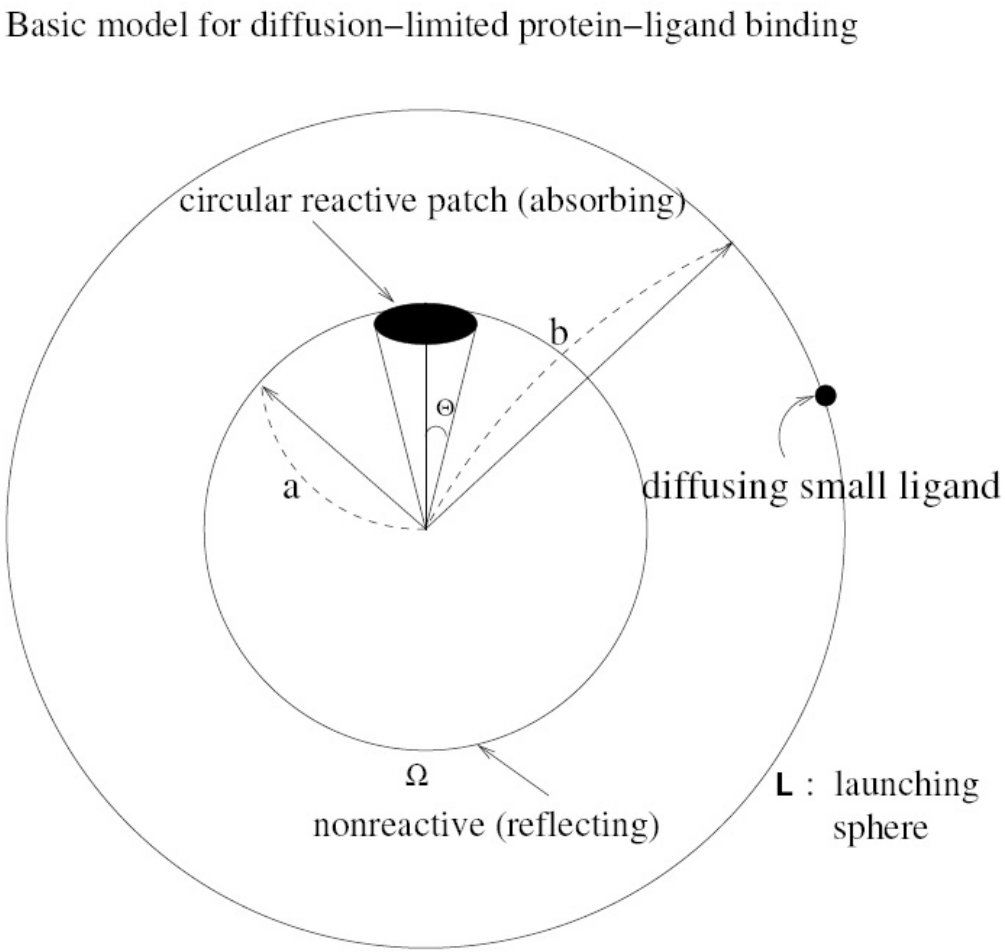
WOS:



Timing with WOS

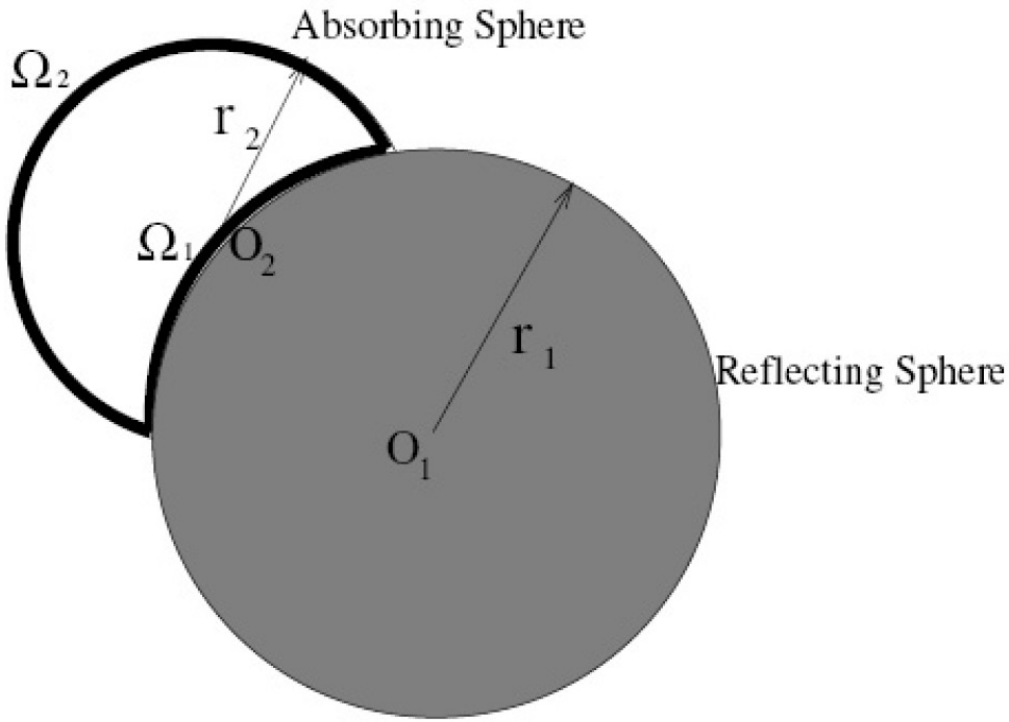


Solc-Stockmayer Model without Potential



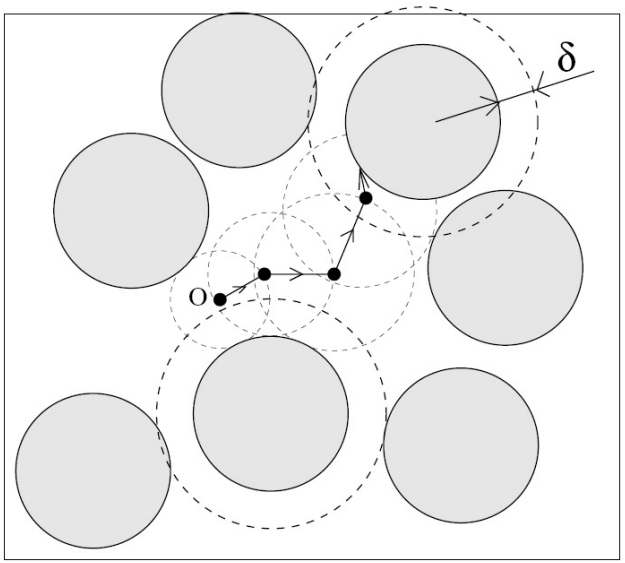
The Simulation-Tabulation (S-T) Method for Generalization

- Green's function for the non-intersected surface of a sphere located on the surface of a reflecting sphere

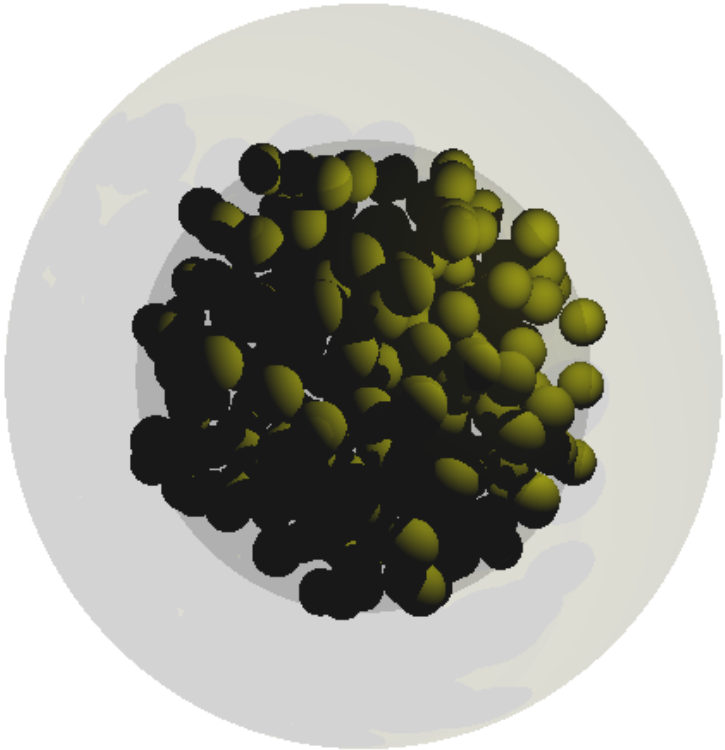


Another S-T Application: Mean Trapping Rate

In a domain of nonoverlapping spherical traps :



Porous Media: Complicated Interfaces



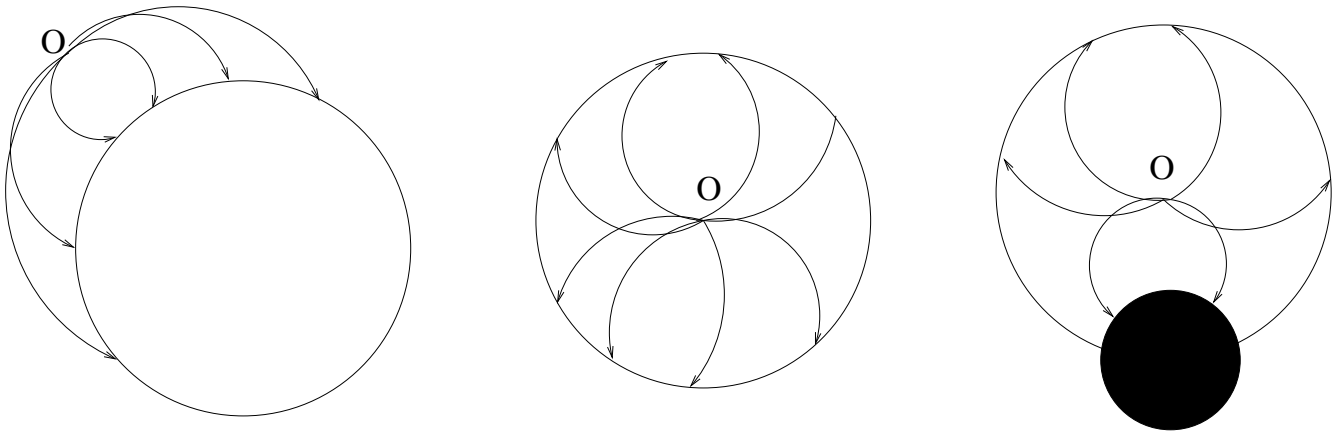
Computing Capacitance Probabilistically

- Hubbard-Douglas: can compute permeability of nonskew object via capacitance
- Recall that $C = \frac{Q}{u}$, if we hold conductor (Ω)at unit potential $u = 1$, then $C =$ total charge on conductor (surface)
- The PDE system for the potential is

$$\Delta u = 0, \quad x \notin \Omega; \quad u = 1, \quad x \in \partial\Omega; \quad u \to 0 \ \text{as} \ x \to \infty \tag{3.5}$$

- Recall $u(\mathbf{x}) = \mathbb{E}_x[f(X^{\mathbf{x}}(t_{\partial\Omega}))] =$ probability of walker starting at $\mathbf{x}$ hitting Ω before escaping to infinity
- Charge density is first passage probability
- Capacitance (relative to a sphere) is probability of walker starting at $\mathbf{x}$ (random chosen on sphere) hitting Ω before escaping to infinity

Various Laplacian Green's Functions for Green's Function First Passage (GFFP)



(a) Putting back (b) Void space (c) Intersecting

Escape to ∞ in A Single Step

- Probability that a diffusing particle at $r_0 > b$ will escape to infinity

$$P_{esc} = 1 - \frac{b}{r_0} = 1 - \alpha \tag{3.6}$$

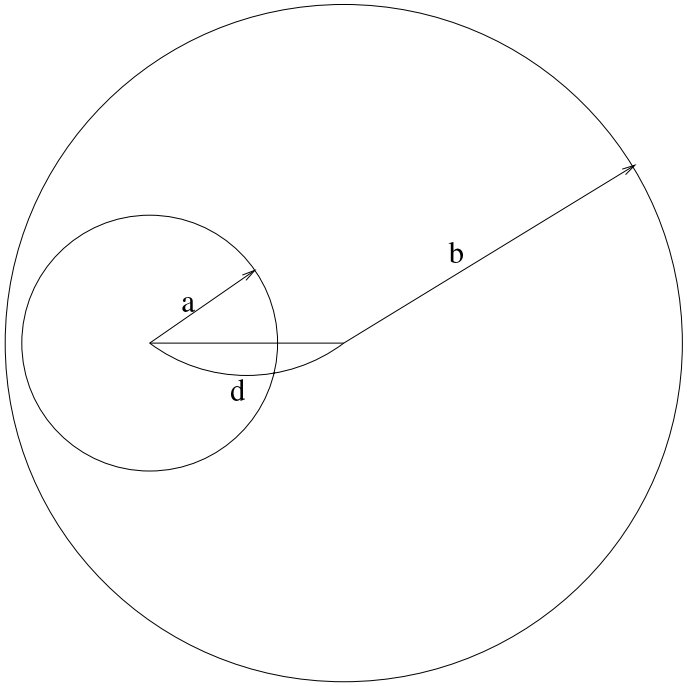
- Putting-back distribution density function

$$\omega(\theta, \phi) = \frac{1 - \alpha^2}{4\pi[1 - 2\alpha\cos\theta + \alpha^2]^{3/2}} \tag{3.7}$$

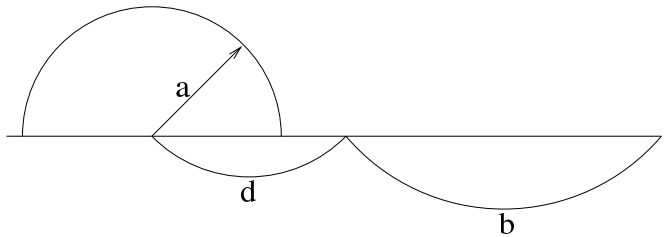
  - (b, θ, ϕ) ; spherical coordinates of the new position when the old position is put on the polar axis

Charge Density on a Circular Disk via Last-Passage

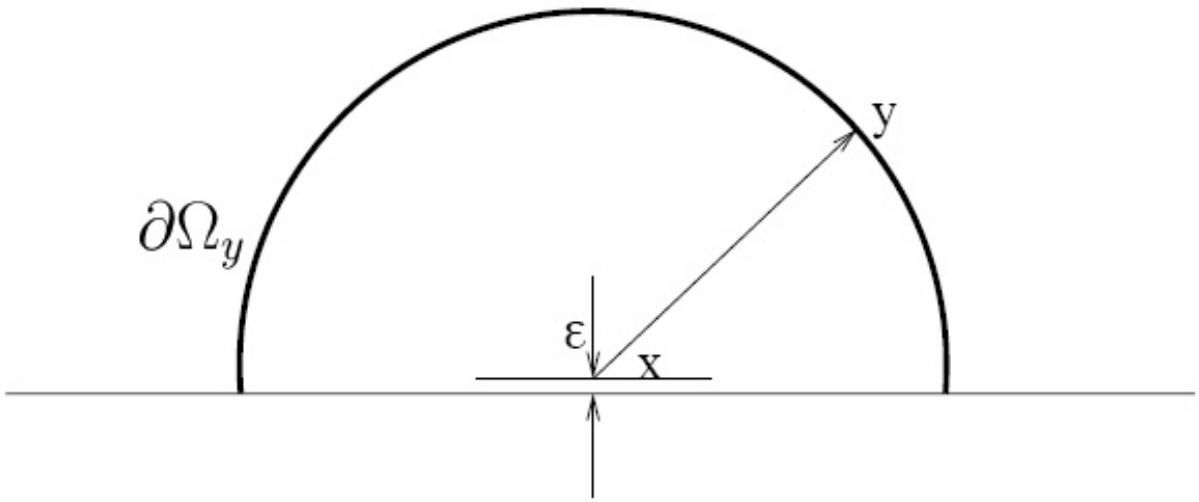
From the top



From the side



Time Reversal Brownian Motion: Approach from the Outside



Approach from the Outside

- $P(x)$: prob. of diffusing from ϵ above lower FP surface to ∞

$$P(x) = \int_{\partial\Omega_y} g(x,y,\epsilon)p(y,\infty)dS \quad (3.8)$$

$$\sigma(x) = -\frac{1}{4\pi}\frac{d}{d\epsilon}\bigg|_{\epsilon=0}\phi(x) = \frac{1}{4\pi}\frac{d}{d\epsilon}\bigg|_{\epsilon=0}P(x) \quad (3.9)$$

$$\sigma(x) = \frac{1}{4\pi}\int_{\partial\Omega_y} G(x,y)p(y,\infty)dS \quad (3.10)$$

where

$$G(x,y) = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} g(x,y,\epsilon) \quad (3.11)$$

- $G(x,y)$ satisfies a point dipole problem

Charge Density on the Circular Disk

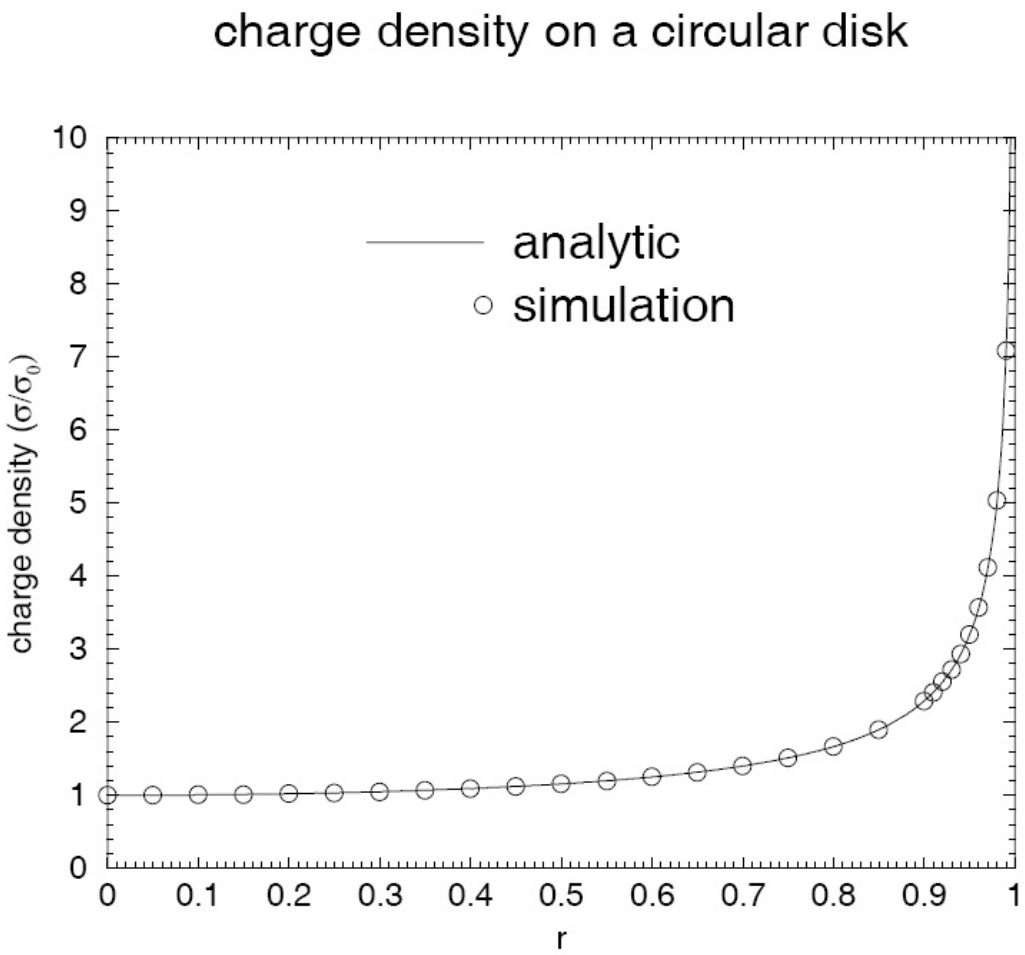
$$G = \frac{3}{4}\frac{\cos\theta}{a^3} \tag{3.12}$$

$$\sigma(x) = \frac{3}{16\pi}\int_{\partial\Omega_{\mathbf{r}}} \frac{\cos\theta}{a^3} p(\mathbf{r},\infty)dS \tag{3.13}$$

where

$$p(\mathbf{r},\infty) = 1 - \frac{2}{\pi}\arctan\left(\frac{\sqrt{2}b}{\sqrt{r^2-b^2+\sqrt{(r^2-b^2)^2+4b^2x^2}}}\right) \tag{3.14}$$

Charge Density on the Circular Disk



Edge Distribution on the Circular Disk

$$\sigma(r) = \frac{1}{4\pi}\frac{1}{\sqrt{1-r^2}} \tag{3.15}$$

Let $r = 1 - x$:

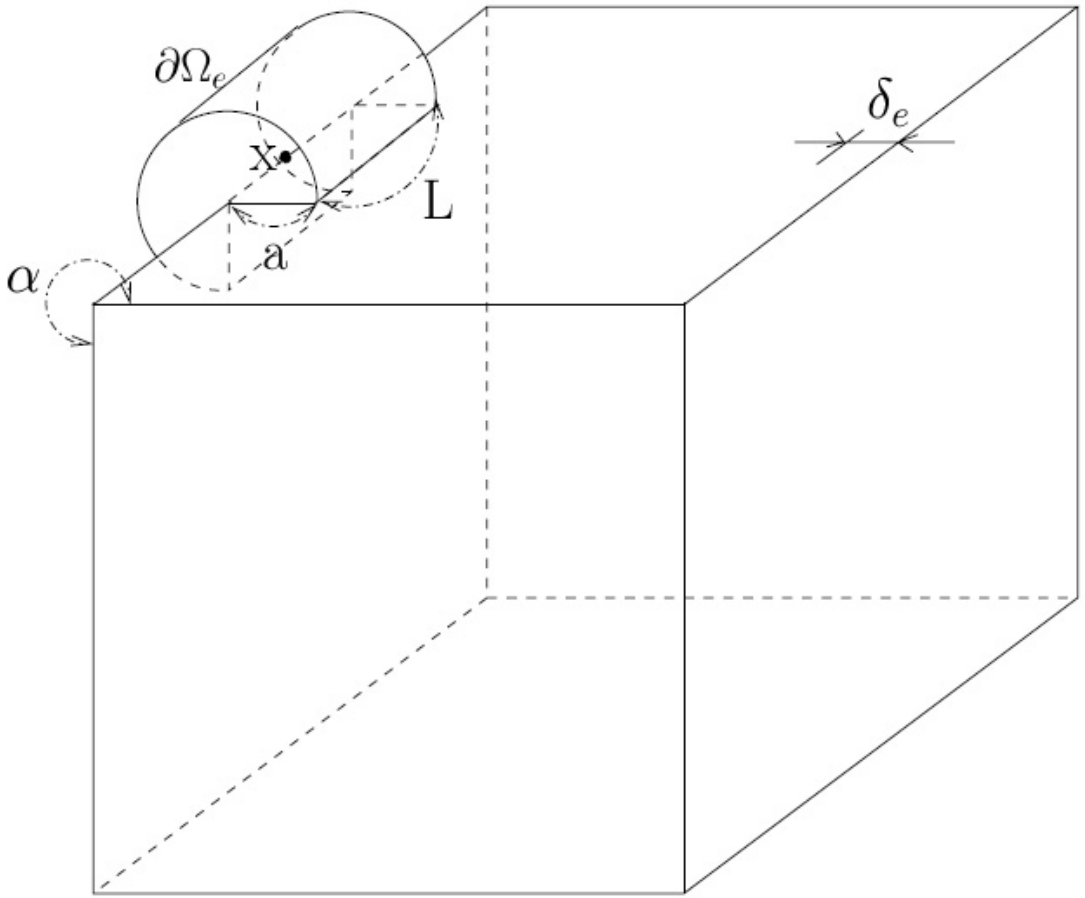
$$\sigma(x) = \frac{1}{4\pi}\frac{1}{\sqrt{2x}}(1 - x/2)^{-1/2} \tag{3.16}$$

when x is small enough,

$$\sigma(x) \simeq \frac{1}{4\sqrt{2}\pi}\frac{1}{\sqrt{x}} \tag{3.17}$$

$$\sigma(x) \simeq \sigma_e\frac{1}{\sqrt{x}} \tag{3.18}$$

Unit Cube Edge Distribution



Unit Cube Edge Distribution

$$\sigma(x, \delta_e) = \delta_e^{\pi/\alpha - 1} \sigma_e(x) \tag{3.19}$$

- $\sigma(x, \delta_e)$: charge on a curve parallel to the edge separated by δ_e
- $\sigma_e(x)$: edge distribution
- α: angle between the two intersecting surfaces, here $\alpha = 3\pi/2$

$$\sigma_e(x) = \frac{1}{4\pi} \lim_{\delta_e \to 0} \delta_e^{1-\pi/\alpha} \int_{\partial\Omega_e} G(x, y) p(y, \infty) dS \tag{3.20}$$

- $\partial\Omega_e$: cylindrical surface that intersects the pair of absorbing surfaces meeting at angle α

Unit Cube Edge Distribution

- $G(x, y)$:

$$G(x, y) = \frac{d}{d\delta_\epsilon}\bigg|_{\delta_\epsilon=0} g(x, y, \delta_\epsilon) \tag{3.21}$$

  - $g(x, y, \delta_\epsilon)$: Laplace Green's function on the surface, $\partial\Omega_e$, with source point x at a distance δ_ϵ from the absorbing surface
- $p(y, \infty)$: probability that a diffusing particle, initiated at point $y \in \partial\Omega_e$, diffuses to infinity without returning to the absorbing surface

Unit Cube Edge Distribution

$$G(\rho = a, \phi, z) = \frac{1}{\Gamma(5/3)2^{2/3}} \frac{4}{9\pi La} \sum_{n=1}^{\infty} \sin\left(\frac{2}{3}\phi\right) \sin\left(\frac{n\pi z}{L}\right) \sin\left(\frac{n\pi z'}{L}\right) \times \left(\frac{n\pi}{L}\right)^{2/3} \frac{1}{I_{2/3}(\frac{n\pi a}{L})}$$

$$G(\rho, \phi, z = 0) = \frac{1}{\Gamma(5/3)2^{2/3}} \frac{4}{9\pi L} \sum_{n=1}^{\infty} \sin\left(\frac{2}{3}\phi\right) \left(\frac{n\pi}{L}\right)^{5/3} \sin\left(\frac{n\pi z'}{L}\right) \times \frac{1}{I_{2/3}(\frac{n\pi a}{L})} \left[I_{2/3}\left(\frac{n\pi a}{L}\right) K_{2/3}\left(\frac{n\pi \rho}{L}\right) - K_{2/3}\left(\frac{n\pi a}{L}\right) I_{2/3}\left(\frac{n\pi \rho}{L}\right) \right]$$

Unit Cube Edge Distribution

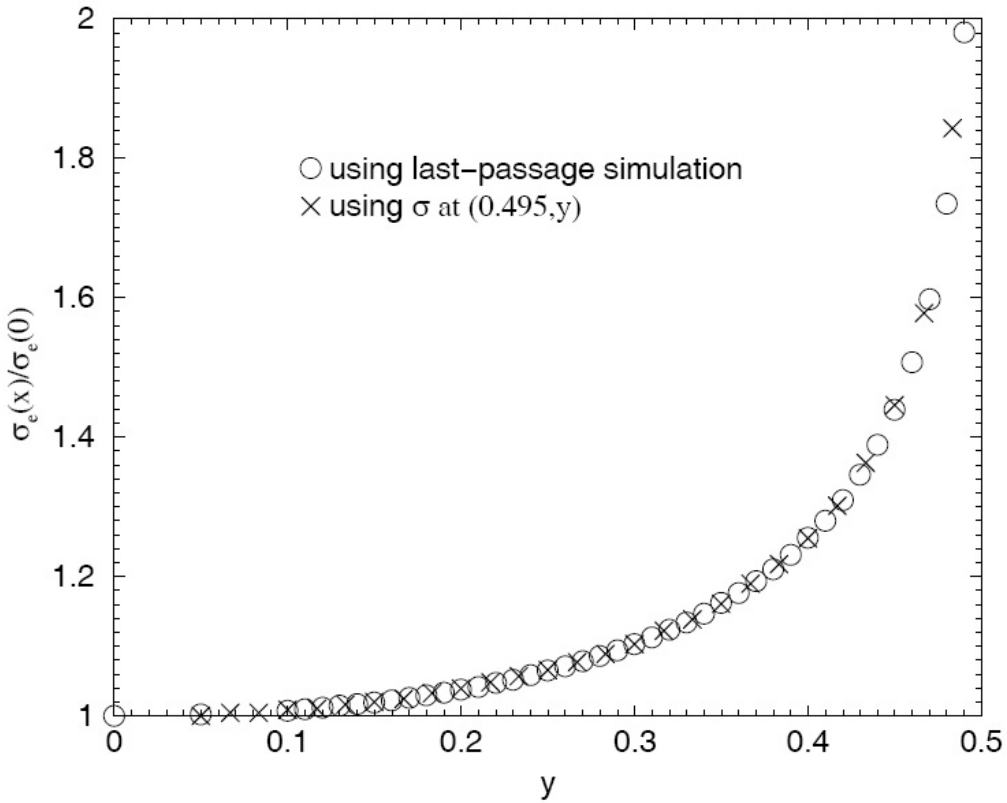


Figure: First- and last-passage edge computations

Unit Cube Edge Distribution

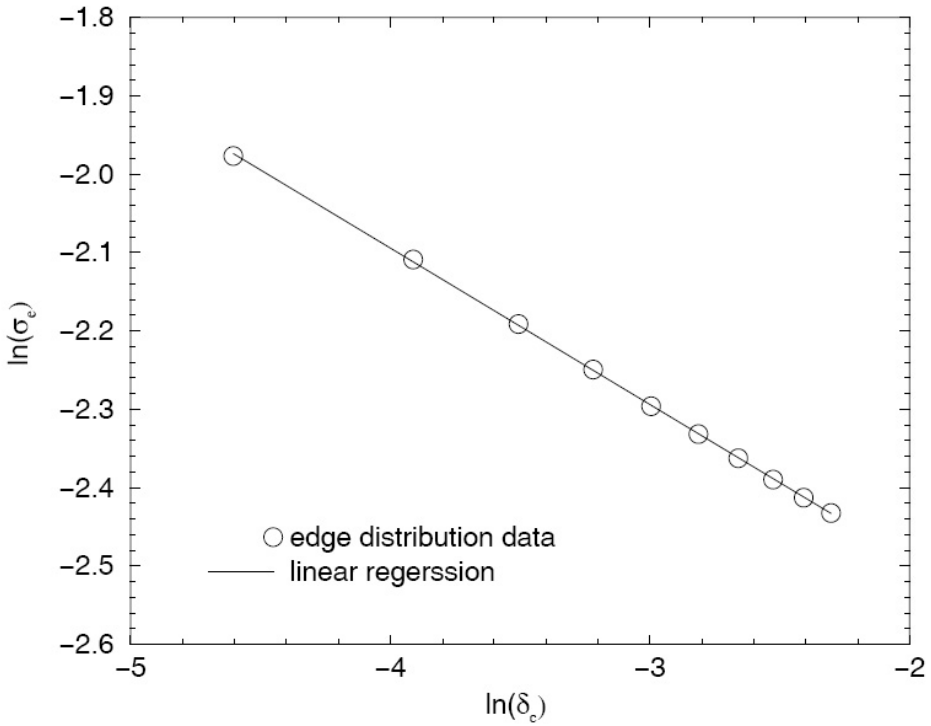


Figure: The slope, that is, the exponent of the edge distribution near the corner is approximately -0.20, that is, $\sigma_e \sim \delta_c^{-1/5}$

Walk on the Boundary Algorithm

- $\mu(y) = -\frac{1}{4\pi}\frac{\partial \phi}{\partial n}(y)$; surface charge density
- $\phi(x) = \int_{\partial\Omega} \frac{1}{|x-y|}\mu(y)d\sigma(y)$; electrostatic potential

Limit properties of the normal derivative ($x \longrightarrow y$ outside of Ω):

$$\mu(y) = \int_{\partial\Omega} \frac{n(y)\cdot(y-y')}{2\pi|y-y'|^3}\mu(y')d\sigma(y')$$

By the ergodic theorem (convex Ω)

$$\int_{\partial\Omega} v(y)\pi_\infty(y)d\sigma(y) = \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N} v(y_n)$$

Walk on the Boundary Algorithm

- π_∞ - stationary distribution of Markov chain $\{y_n\}$ with transition density $p(y_n \to y_{n+1}) = \dfrac{n(y_{n+1}) \cdot (y_{n+1} - y_n)}{2\pi |y_{n+1} - y_n|^3}$
- $\mu = C\pi_\infty$
- C - capacitance if $\phi|_{\partial\Omega} = 1$
- $\phi(x) = 1$ for $x \in \Omega$

$$C = (\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} v(y_n))^{-1} \quad \text{for} \quad v(y) = \frac{1}{x - y}$$

Capacitance of the Unit Cube

Reitan-Higgins (1951)	0.6555
Greenspan-Silverman (1965)	0.661
Cochran (1967)	0.6596
Goto-Shi-Yoshida (1992)	$0.6615897 \pm 5 \times 10^{-7}$
Conjectured Hubbard-Douglas (1993)	0.65946...
Douglas-Zhou-Hubbard (1994)	0.6632 ± 0.0003
Given-Hubbard-Douglas (1997)	0.660675 ± 0.00001
Read (1997)	0.6606785 ± 0.000003
First passage method (2001)	0.660683 ± 0.000005
Walk on boundary algorithm (2002)	0.6606780 ± 0.0000004

Computing Protein Internal Energy

- Poisson equation for the electrostatic potential inside a molecule G (a union of intersecting spherical atoms with: x_m – centers, q_m – charges)

$$-\nabla\epsilon\nabla u(x) = \sum_{m=1}^{M} q_m \delta(x - x_m) \ , \ x \in G$$

- Linearized Poisson-Boltzmann equation outside

$$\Delta u(x) - k^2 u(x) = 0 \ , \ x \in R^3 \setminus \overline{G}$$

- Continuity condition on the boundary

$$u_i = u_e \ , \ \epsilon_i \frac{\partial u_i}{\partial n(y)} = \epsilon_e \frac{\partial u_e}{\partial n(y)} \ , \ y \in \partial G$$

Computing Protein Internal Energy

Free energy of a molecule is defined as:

$$E = \frac{1}{2} \sum_{m=1}^{M} u^{(0)}(x_m) q_m \ ,$$

where $u^{(0)}(x) = u(x) - g(x)$ is the nonsingular part of the electrostatic potential:

$$g(x) = \sum_{m=1}^{M} \frac{q_m}{4\pi\epsilon} \frac{1}{|x - x_m|}$$

Computing Protein Internal Energy

Monte Carlo estimate for E: linear combination (functional) of estimates for $u^{(0)}(x_m)$.

$$\xi[E] = \frac{1}{2}\sum_{m=1}^{M} \xi[u^{(0)}(x_m)]q_m \ , \tag{3.22}$$

$$\xi[u^{(0)}(x_m)] = \xi[u(x_m^{N_m})] - g(x_m^{N_m}) \tag{3.23}$$

- $x_m^0 = x_m, x_m^1, \ldots, x_m^{N_m}$ – Markov chain, every point x_m^i is an exit point of the Brownian motion from the corresponding "atom" (Green's function first passage)
- $y_1^m = x_m^{N_m}$ lies on the boundary, ∂G

Computing Protein Internal Energy

For the grounded (perfect conducting solvent) molecule $u(y_1^m) = 0$ and

$$\xi[E] = -\frac{1}{2}\sum_{m=1}^{M} g(y_1^m)q_m$$

General case:

- Discretization and randomization of the boundary condition

$$u(y) = p_0 u(y - hn) + (1 - p_0)u(y + hn) + O(h^2)$$

$$u(y_1) = E(u(y_2)|y_1) + O(h^2) \qquad (3.24)$$

$y_2 = y - hn$ with probability p_0 (reenter molecule)
$y_2 = y + hn$ with probability $1 - p_0$ (exit to solvent)

$$p_0 = \frac{\epsilon_i}{\epsilon_i + \epsilon_e}$$

Computing Protein Internal Energy

- y_2 inside: $y_3 \in \partial G$ is the last point of Markov chain (exit of the Brownian motion starting at y_2)

$$u(y_2) = E(u(y_3) - g(y_3) + g(y_2)|y_2) \tag{3.25}$$

- y_2 outside: Walk on spheres algorithm ($y_{2,0} = y_2$)
  $y_{2,i+1} = y_{2,i} + \omega \times d_i$, $d_i =$distance$(y_{2,i}, \partial G)$
  Terminates with probability $\dfrac{kd_i}{\sinh(kd_i)}$ on every step, or when $d_N < \varepsilon$.
  y_3 – the nearest to $y_{2,N}$ on the boundary

$$u(y_2) = E(u(y_3)|y_2) + O(\varepsilon) \tag{3.26}$$

Computing Protein Internal Energy

For $\varepsilon = h^2$ relations (3.22), (3.23) and the recurrence (3.24), (3.25), (3.26) define an $O(h)$-biased Monte Carlo estimator. Mean number of steps in the algorithm is $O(h^{-1} \log(h)\ f(k))$, f is a decreasing function.

Exit Points Using Walk on Subdomains

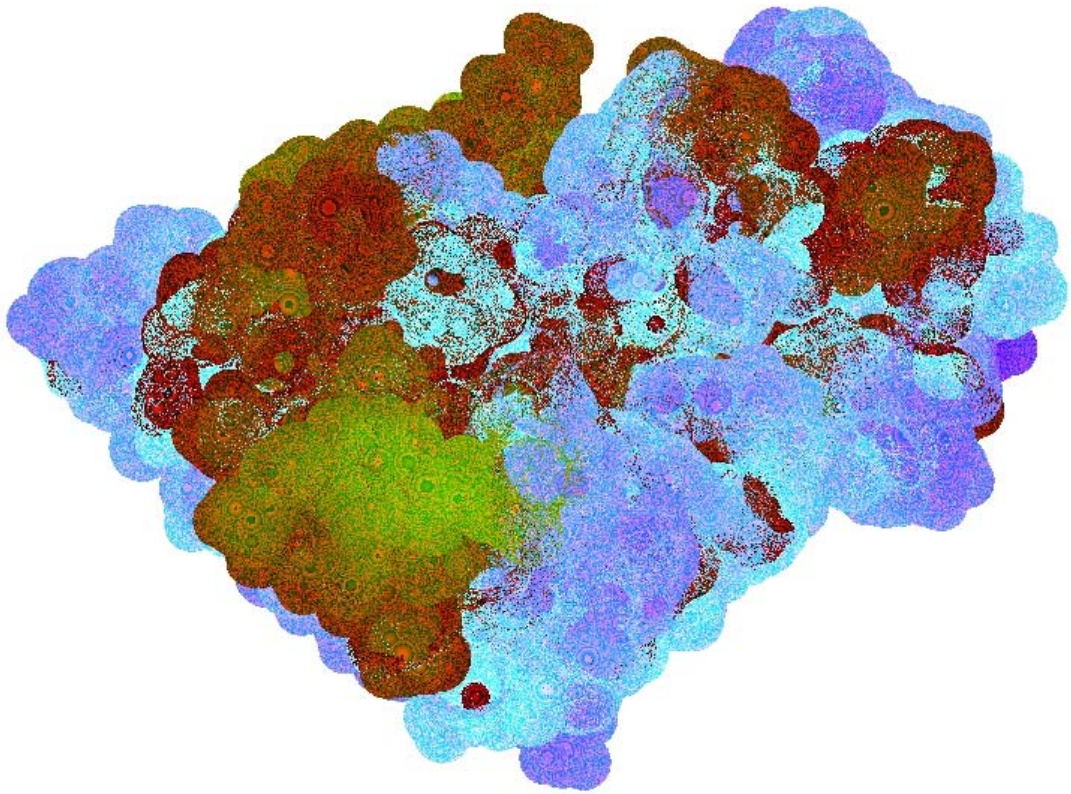


Figure: Exit points on the van der Waals surface of Barnase

MCMs for Hyperbolic PDEs

- We have constructed MCMs for both elliptic and parabolic PDEs but have not considered MCMs for hyperbolic PDEs except for Berger's equation (was a very special case)
- In general MCMs for hyperbolic PDEs (like the wave equation: $u_{tt} = c^2 u_{xx}$) are hard to derive as Brownian motion is fundamentally related to diffusion (parabolic PDEs) and to the equilibrium of diffusion processes (elliptic PDEs), in contrast hyperbolic problems model distortion free information propagation which is fundamentally nonrandom

MCMs for Hyperbolic PDEs

- A famous special case of an hyperbolic MCM for the telegrapher's equation (Kac, 1956):

$$\frac{1}{c^2}\frac{\partial^2 F}{\partial t^2} + \frac{2a}{c^2}\frac{\partial F}{\partial t} = \Delta F,$$

$$F(\mathbf{x}, 0) = \phi(\mathbf{x}), \quad \frac{\partial F(\mathbf{x}, 0)}{\partial t} = 0$$

- The telegrapher's equation approaches both the wave and heat equations in different limiting cases
  - **A.** *Wave equation:* $a \to 0$
  - **B.** *Heat equation:* $a, c \to \infty, 2a/c^2 \to \frac{1}{D}$
- Consider the one-dimensional telegrapher's equation, when $a = 0$ we know the solution is given by $F(x,t) = \frac{\phi(x+ct)+\phi(x-ct)}{2}$

MCMs for Hyperbolic PDEs

- If we think of a as the probability per unit time of a Poisson process then $N(t) = \#$ of events occurring up to time t has the distribution $P\{N(t) = k\} = e^{-at}\frac{(at)^k}{k!}$
- If a particle moves with velocity c for time t it travels $ct = \int_0^t c\, d\tau$, if it undergoes random Poisson distributed direction reversal with probability per unit time a, the distance traveled in time t is $\int_0^t c(-1)^{N(\tau)}\, d\tau$

MCMs for Hyperbolic PDEs

- If we replace ct in the exact solution to the 1D wave equation by the randomized distance traveled average over all Poisson reversing paths we get:

$$F(x,t) = \frac{1}{2}E\left[\phi\left(x + \int_0^t c(-1)^{N(\tau)}\, d\tau\right)\right.$$

$$\left.\frac{1}{2}E\left[\phi\left(x - \int_0^t c(-1)^{N(\tau)}\, d\tau\right)\right]\right.$$

  which can be proven to solve the above IVP for the telegrapher's equation

MCMs for Hyperbolic PDEs

- In any dimension, an exact solution for the wave equation can be converted into a solution to the telegrapher's equation by replacing t in the wave equation ansatz by the randomized time $\int_0^t (-1)^{N(\tau)}\, d\tau$ and averaging
- This is the basis of a MCM for the telegrapher's equation, one can also construct MCMs for finite-difference approximations to the telegrapher's equation
- Used in particle-based multiphase flow algorithm: diffusion adds stability

Applications and Methods Derived

- Application: Electrostatics
  1. Capacitance computations
  2. Charge density computations
  3. Biological electrostatics
  4. Semiconductor mutual capacitance
- Application: Materials science of random media
- Permeability computations (didn't show penetration depth method)
  1. Green's function first-passage algorithm (GFFP)
  2. Simulation-Tabulation method (S-T)
  3. Last-passage techniques
  4. Random walk on the boundary (WOB)
  5. Walk on subdomains method
  6. New boundary conditions

Conclusions

Conclusions

- New conventional wisdom about Monte Carlo methods (MCMs)
  1. MCMs can be used in low dimensions where geometry is complex
  2. MCMs can be used to solve linear functionals of PDEs and integral equations
  3. Some high-accuracy situations are amenable to MCMs

Future Work

Future Work

- Molecular Electrostatics
  1. More complicated functionals of the solution
  2. Derivatives (forces)
  3. Nonlinear problem via branching processes and expansions
- Anisotropic permeability (penetration depth)
- Multiscale Monte Carlo
- MCM solutions on surfaces

Bibliography I


[M. Mascagni and N. A. Simonov (2004)]
Monte Carlo Methods for Calculating Some Physical Properties of Large Molecules
SIAM Journal on Scientific Computing, **26(1)**: 339-357.


[N. A. Simonov and M. Mascagni (2004)]
Random Walk Algorithms for Estimating Effective Properties of Digitized Porous Media
Monte Carlo Methods and Applications, **10**: 599-608.


[M. Mascagni and N. A. Simonov (2004)]
The Random Walk on the Boundary Method for Calculating Capacitance
Journal of Computational Physics, **195**: 465-473.

Bibliography II


[C.-O. Hwang, J. A. Given and M. Mascagni (2001)]
The Simulation-Tabulation Method for Classical Diffusion Monte Carlo
Journal of Computational Physics, **174**: 925-946.


[C.-O. Hwang, J. A. Given and M. Mascagni (2000)] On the Rapid Calculation of Permeability for Porous Media Using Brownian Motion Paths
Physics of Fluids, **12**: 1699-1709.