Continuous Path Brownian Trajectories for Diffusion Monte Carlo via First- and Last-Passage Distributions

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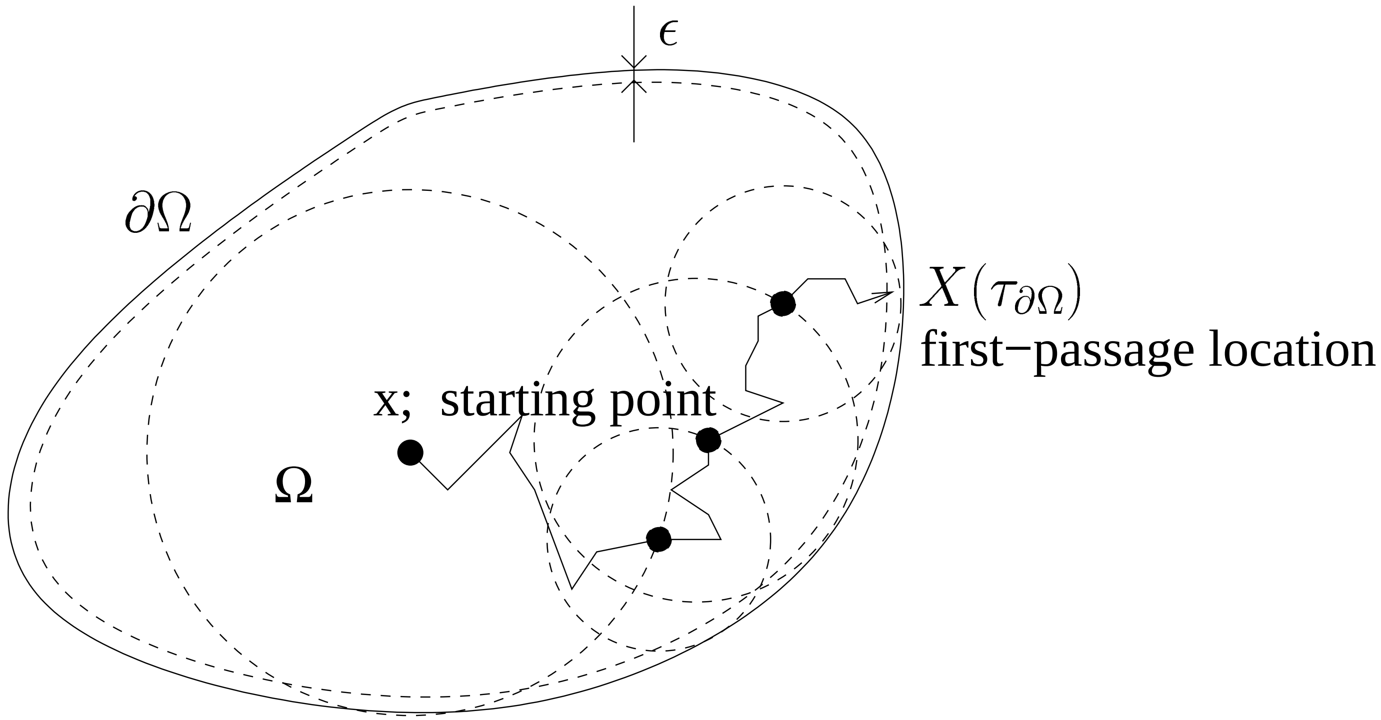
Dirichlet problem for Laplace Equation



First Passage Algorithms

$$\Delta u(\mathbf{x}) = -q(\mathbf{x}), \qquad \mathbf{x} \in \Omega \tag{1}$$

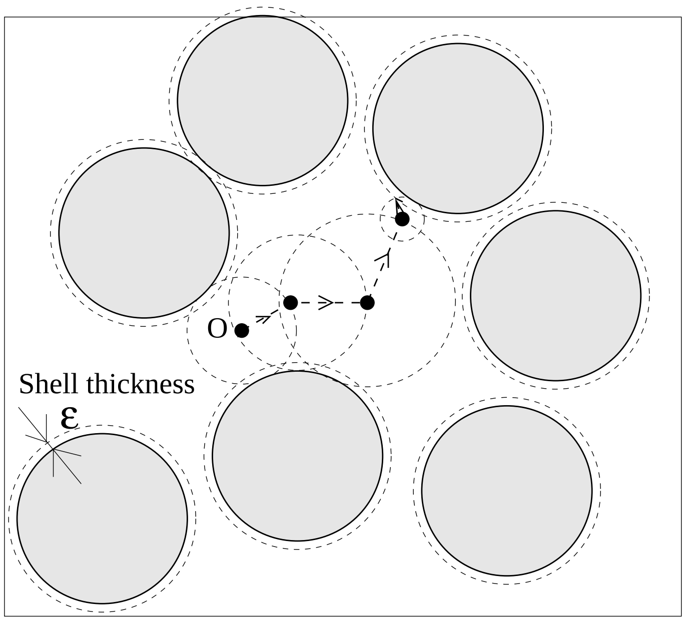
$$u(\mathbf{x}) = f(\mathbf{x}), \qquad \mathbf{x} \in \partial\Omega. \tag{2}$$

$$u(\mathbf{x}) = -\int_s \frac{\partial G(x,y)}{\partial n_y} f(y) dS_y + \int G(x,y) q(y) dy \tag{3}$$

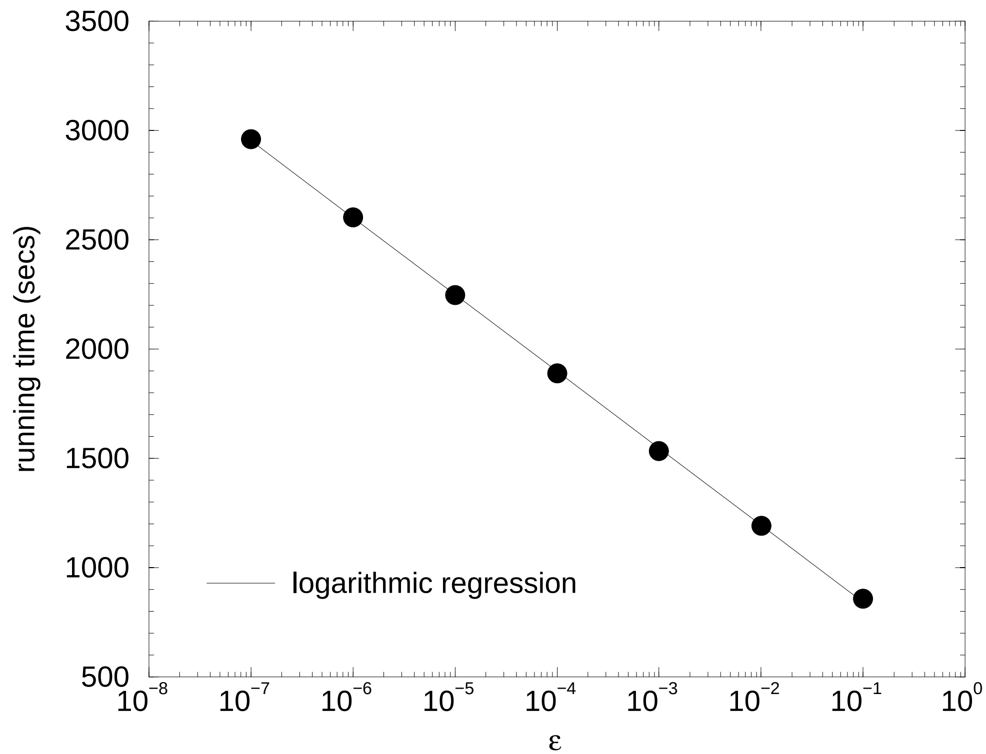
- Isomorphism: First passage probability is exactly the Laplacian surface Green's function for the boundary value problem for the given geometry.
- Electrostatic charge density on a conducting first-passage surface induced by a charge to first-passage probability density on the absorbing first-passage surface surrounding the diffusing particle.

“Walk on Spheres” (WOS) and Green’s Function First Passage (GFFP) Algorithms

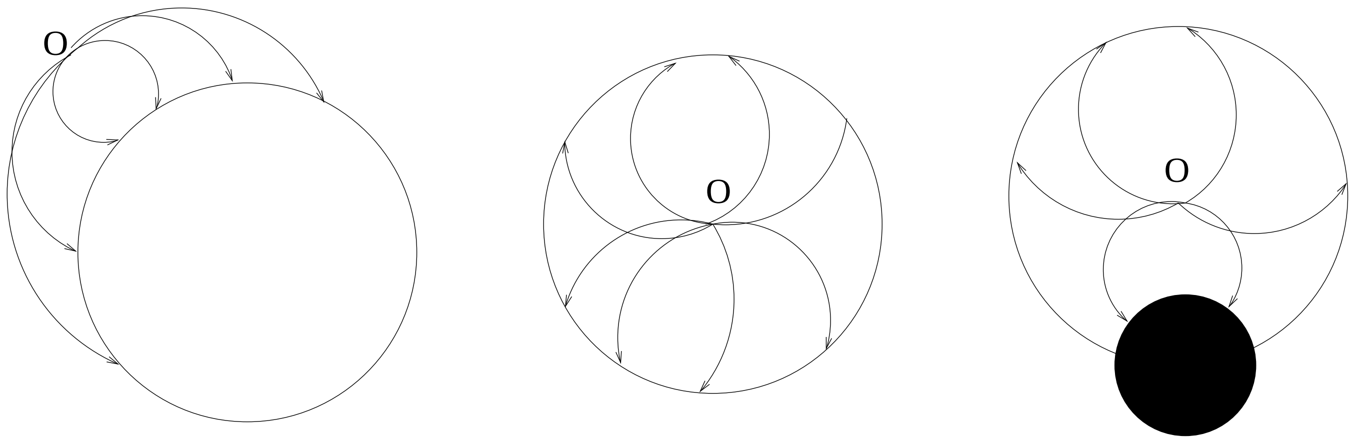
WOS:



Timing with WOS:

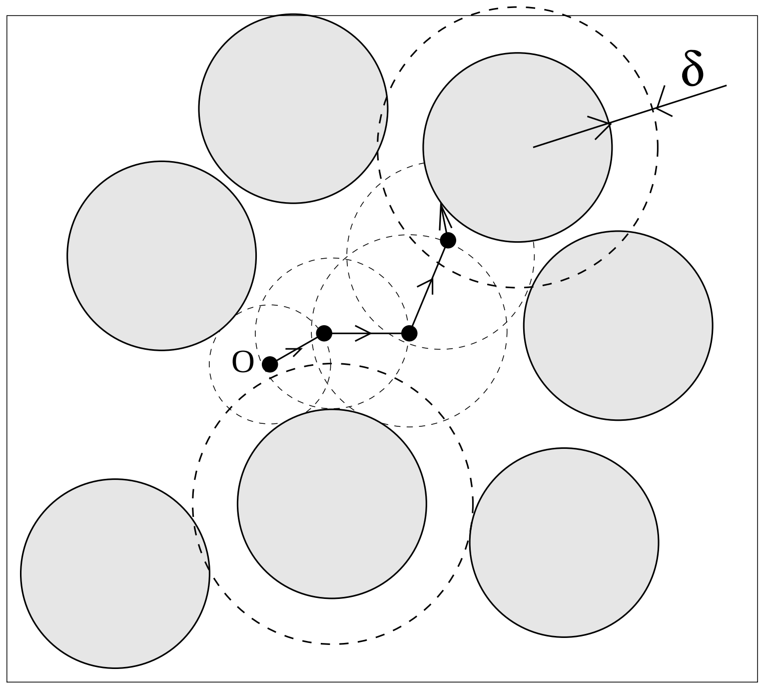


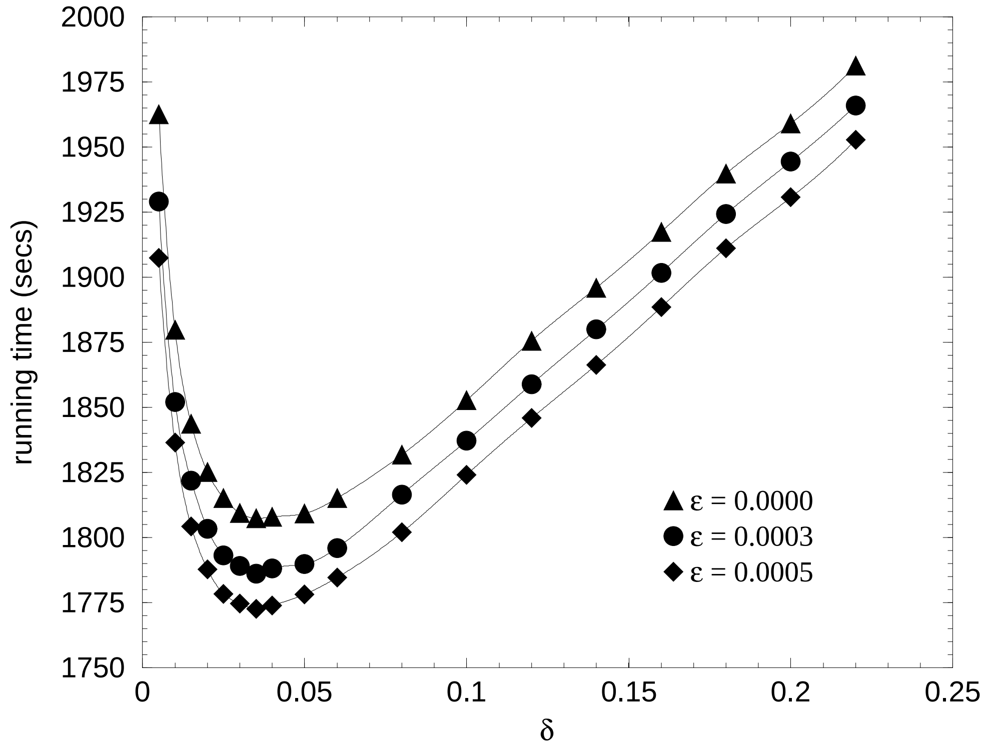
Green's Functions



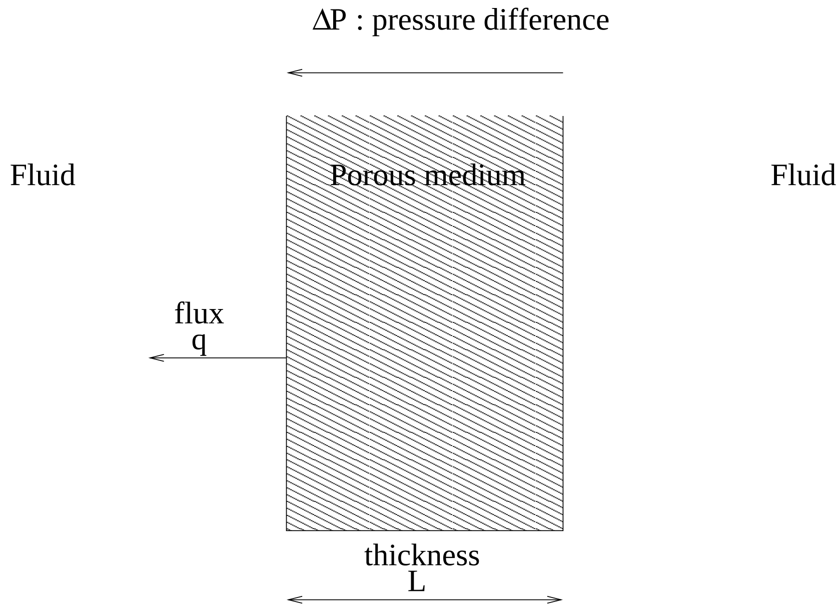
(a) Putting back (b) Void space (c) Intersecting

GFFP:




2000
1975
1950
1925
1900
1875
1850
1825
1800
1775
1750
running time (secs)
0
0.05
0.1
0.15
0.2
0.25
δ
ε = 0.0000
ε = 0.0003
ε = 0.0005

Darcy's Law



$$q = \frac{k \, \Delta P}{\eta \, L}$$

η : dynamic viscosity

Darcy's Law

$$q = \frac{k\Delta P}{\eta L} \tag{4}$$

- A slow steady flow of a single Newtonian fluid through a stationary, inert and isotropic porous medium
- k : fluid permeability
- ΔP : applied pressure difference
- L : thickness of the porous sample
- η : dynamic viscosity
- q : volumetric flow per unit cross-sectional area (flux)

Hubbard-Douglas TFC for an Arbitrary Nonskew Object

- Using angle averaging, Hubbard and Douglas derived: vector or tensor Laplace equations to scalar Laplace equations

$$f = 6\pi\eta C \tag{5}$$

- f : translational friction coefficient
- η : dynamic viscosity
- C : electrical capacitance

Felderhof's TFC for a Macromolecule

- From the Debijf-Brinkman equation for porous flow under pressure:

$$\nabla P = \eta \nabla^2 \mathbf{V} - \frac{\eta}{k}\mathbf{V}, \tag{6}$$

we get:

$$f = 6\pi\eta R G_0(\sigma)\{1 + \frac{3}{2\sigma^2} G_0(\sigma)\}^{-1} \tag{7}$$

  - f : translational friction coefficient
  - η : dynamic viscosity
  - R : macromolecular radius

Felderhof's TFC for a Macromolecule

with:

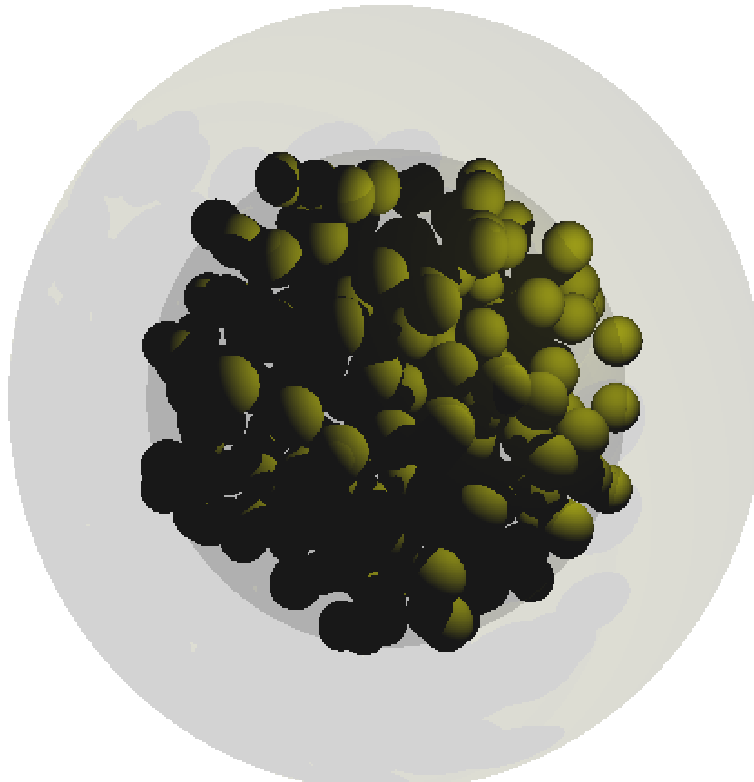
$$G_0(\sigma) = 1 - \frac{1}{\sigma} \tanh \sigma \tag{8}$$

dimensionless quantity:

$$\sigma = \frac{R}{\sqrt{k}} \tag{9}$$

k : fluid permeability

Porous Media



Unit Capacitance Method

- Combining two previous equations

$$\frac{C}{R} = G_0(\sigma)\{1 + \frac{3}{2\sigma^2}G_0(\sigma)\}^{-1} \tag{10}$$

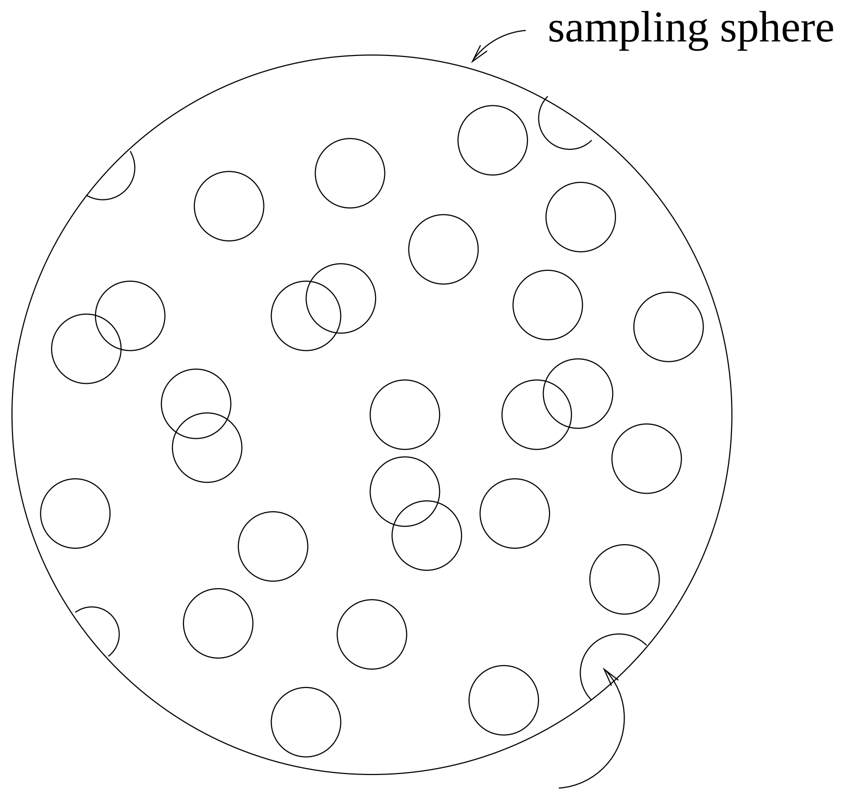
- Getting C/R gives us σ
- From:

$$\sigma = \frac{R}{\sqrt{k}} \tag{11}$$

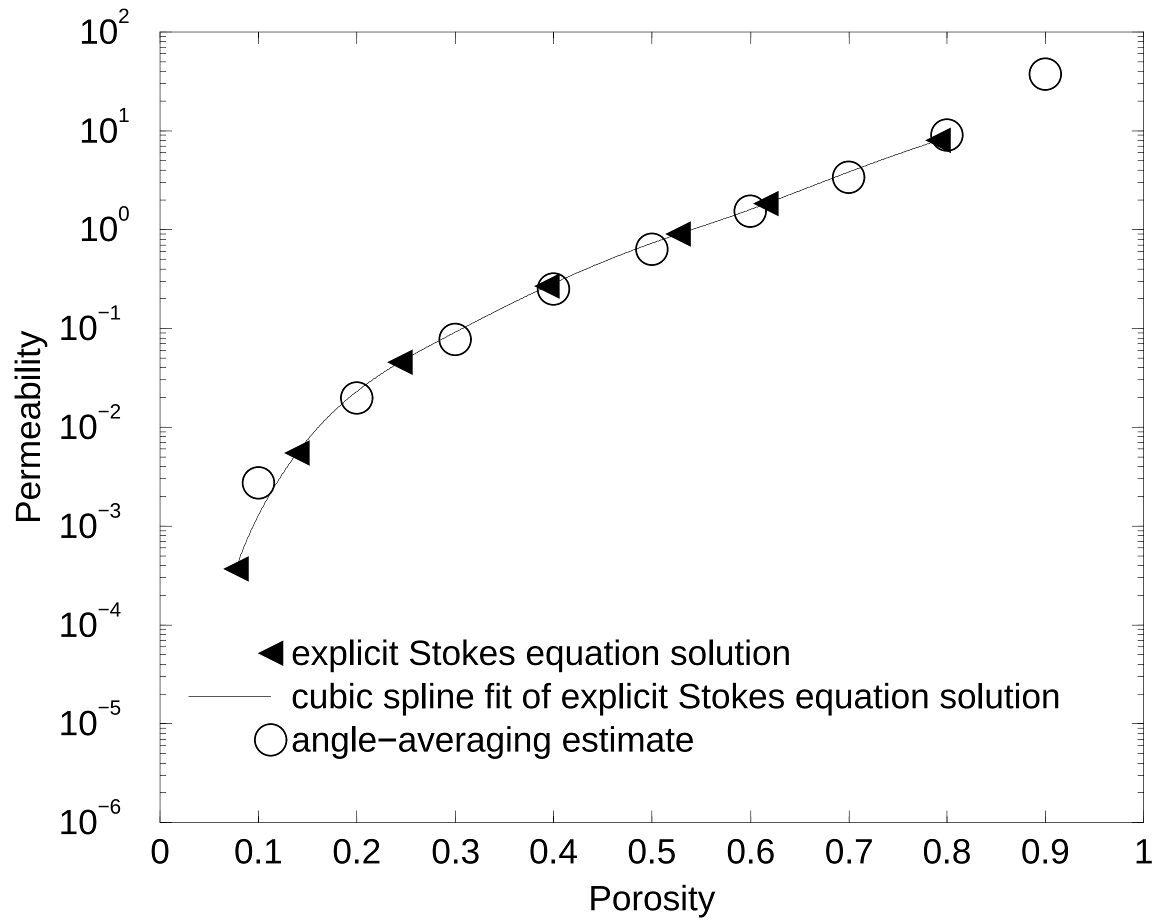
we get permeability

Sampling Methods

Sharp Boundary Method



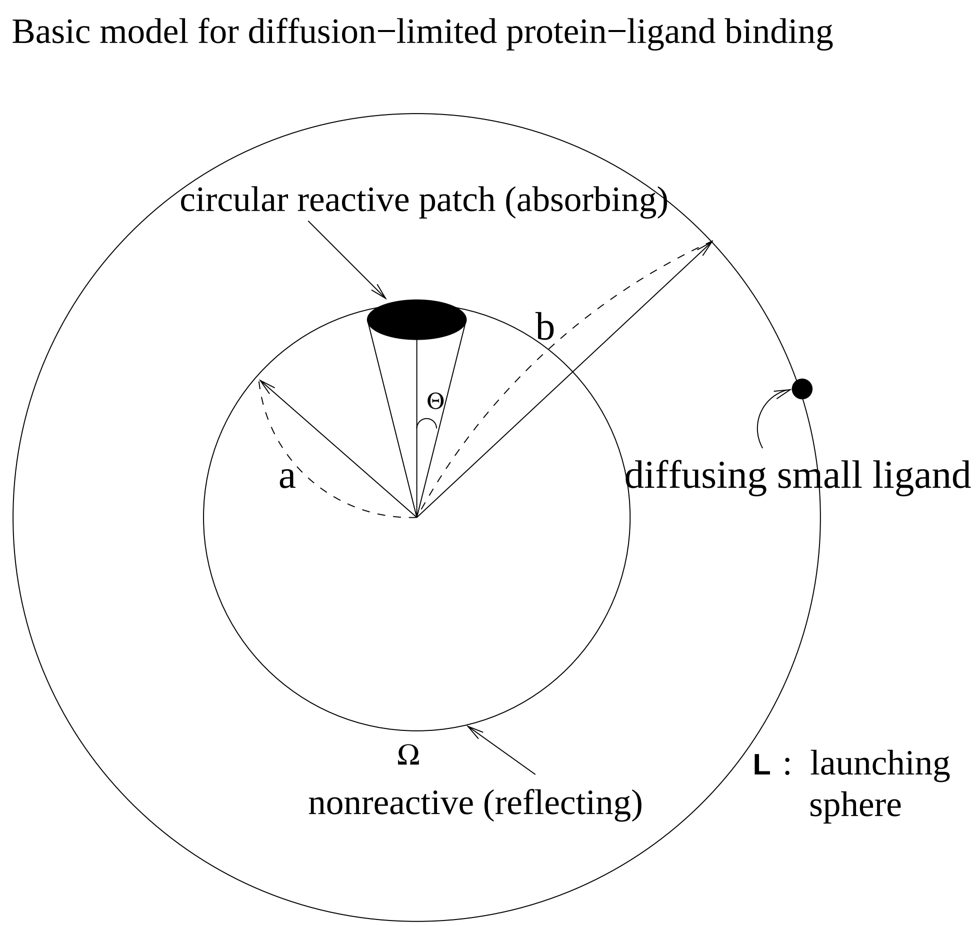
Polydispersed Spheres



Summary and Conclusions for Permeability

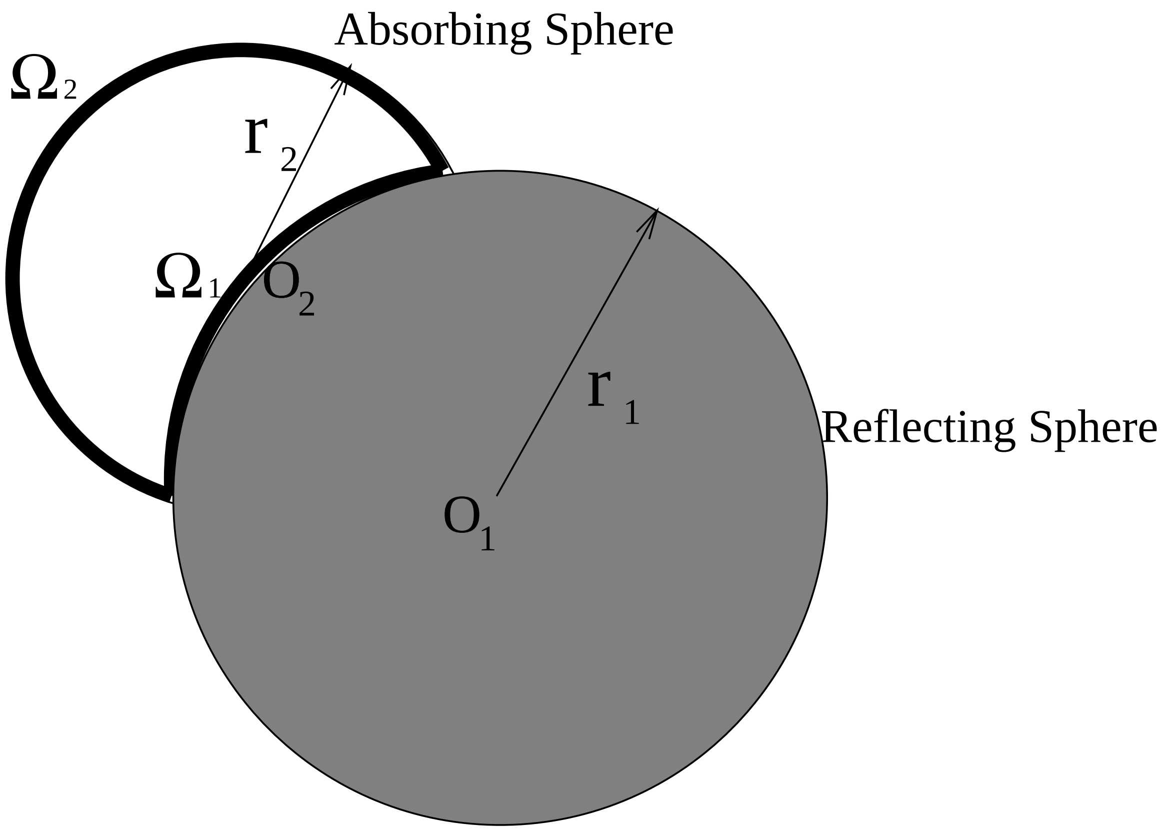
- The two methods with sharp boundary sampling agree well with each other except at very low porosities.
- For overlapping sphere beds, the new estimate is good except at very low porosities ($\phi_0 < 0.2$).
- Each data point used 10^5 trajectories and consumed approximately one minute of 233 Mhz PII CPU time (very fast).
- The actual data set of mono-sized and polydispersed overlapping spheres beds from N. S. Martys agrees well with the sharp boundary simulation data.
- The methods will work for general homogeneous and isotropic porous media.
- Applying the new permeability estimation methods to more realistic porous media models

Solc-Stockmayer Model without Potential

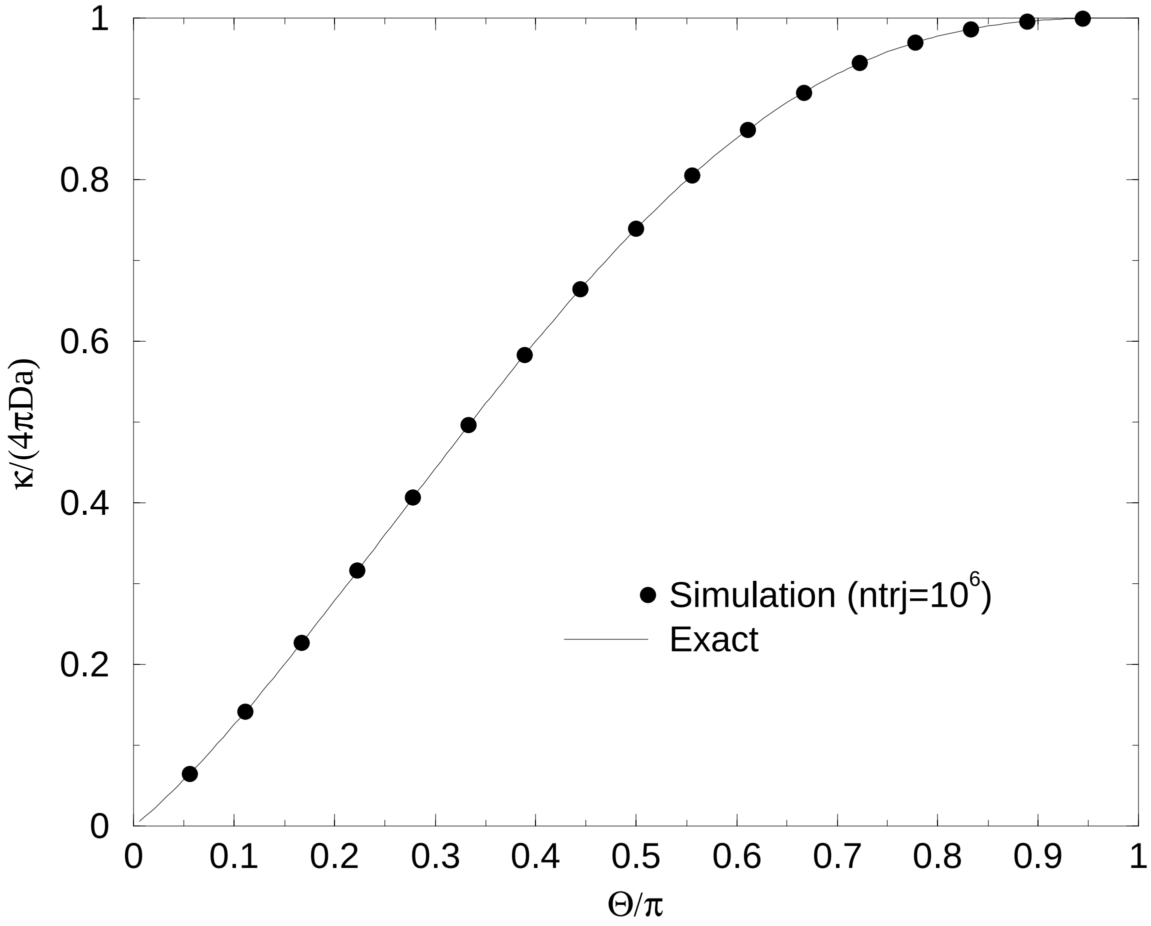


Simulation-Tabulation Method

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

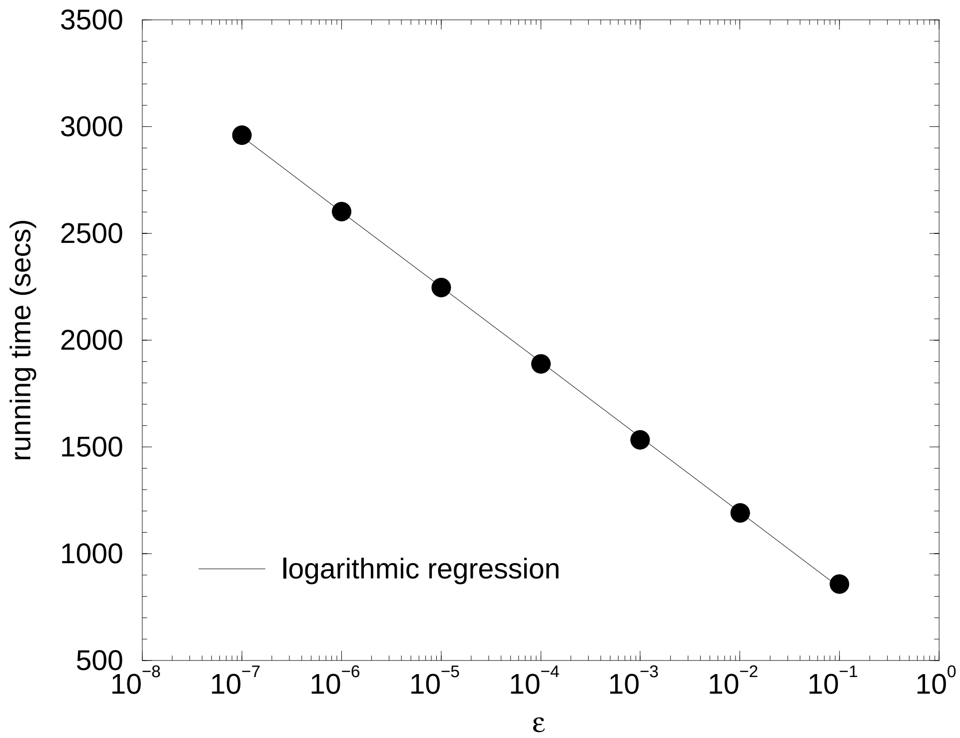


Solc-Stockmayer Model without Potential



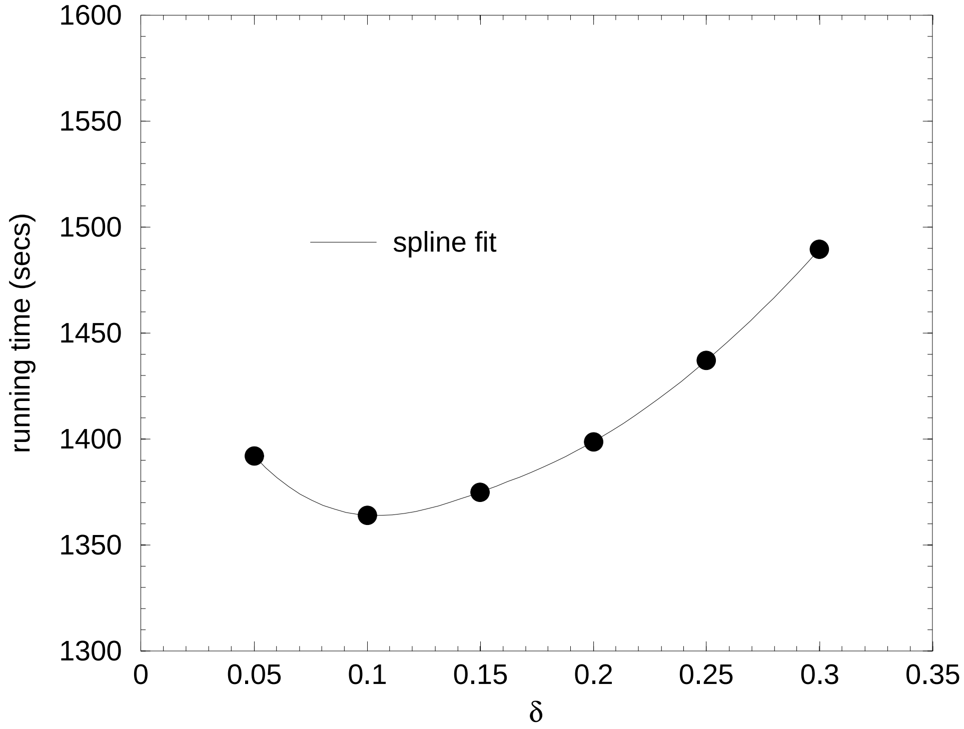
Solc-Stockmayer Model without Potential

Timing with WOS :



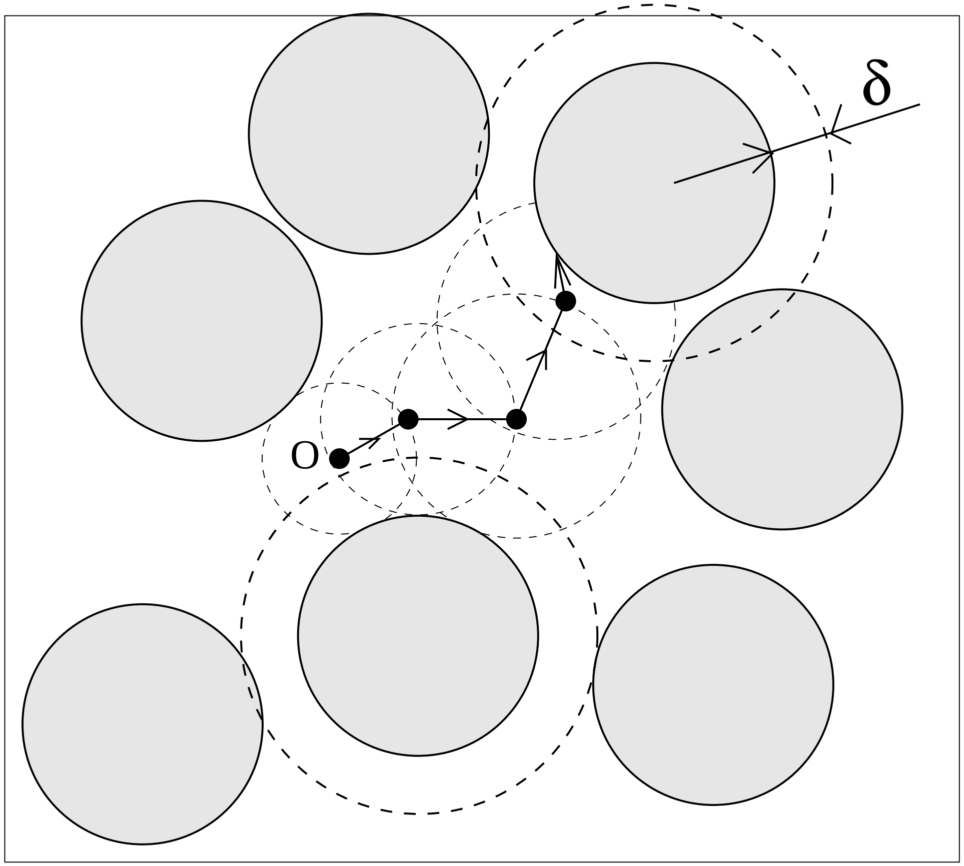
Solc-Stockmayer Model without Potential

Timing with GFFPA :



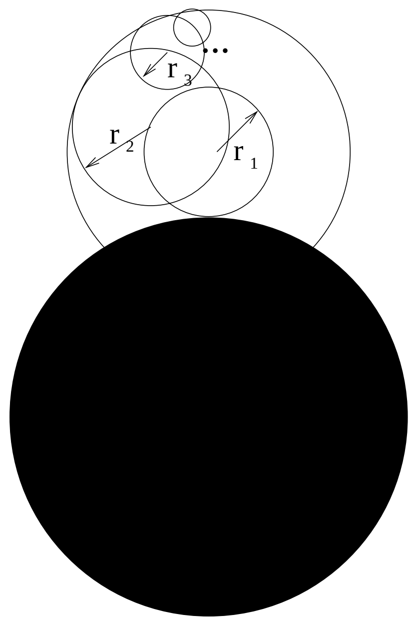
Mean Trapping Rate

In a domain of nonoverlapping spherical traps :



Simulation-Tabulation Method

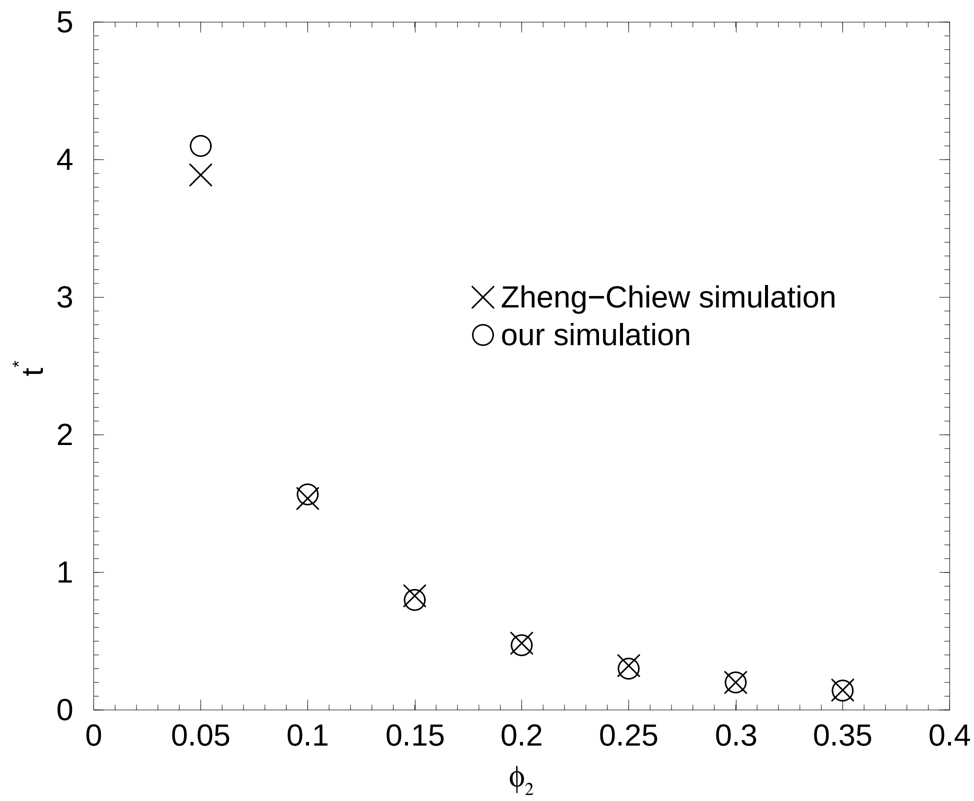
- Average First-passage time



$$\bar{\tau} = \overline{\Sigma\, \tau_i} = \overline{\Sigma\, \frac{r_i^2}{6}}$$

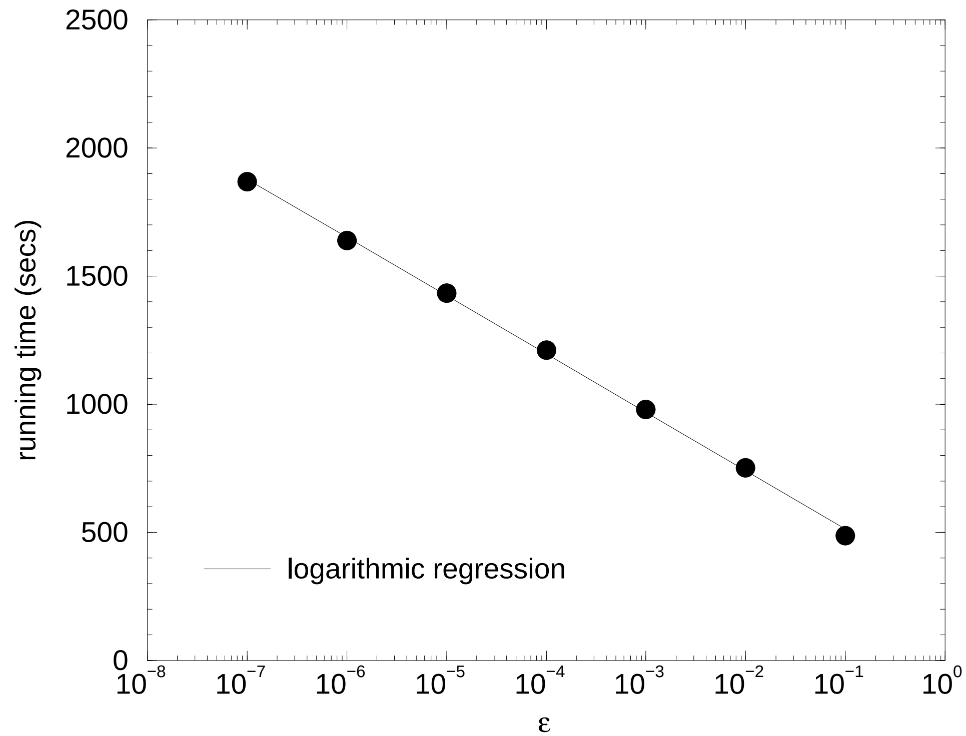
Mean Trapping Rate

In a domain of nonoverlapping spherical traps :



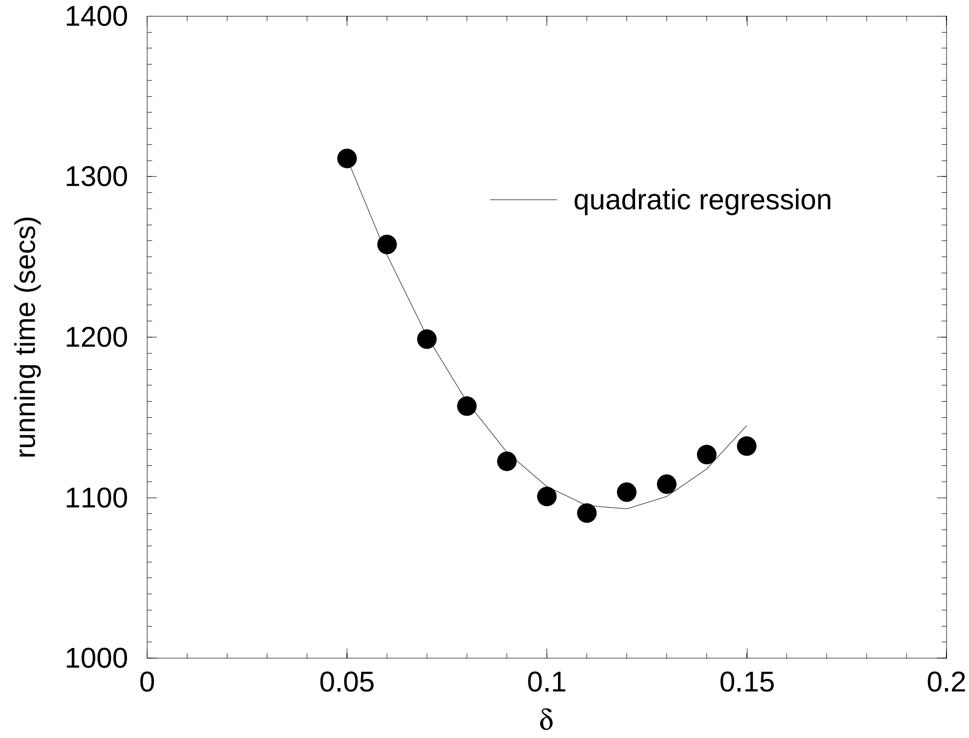
Mean Trapping Rate

In a domain of nonoverlapping spherical traps : Timing with WOS



Mean Trapping Rate

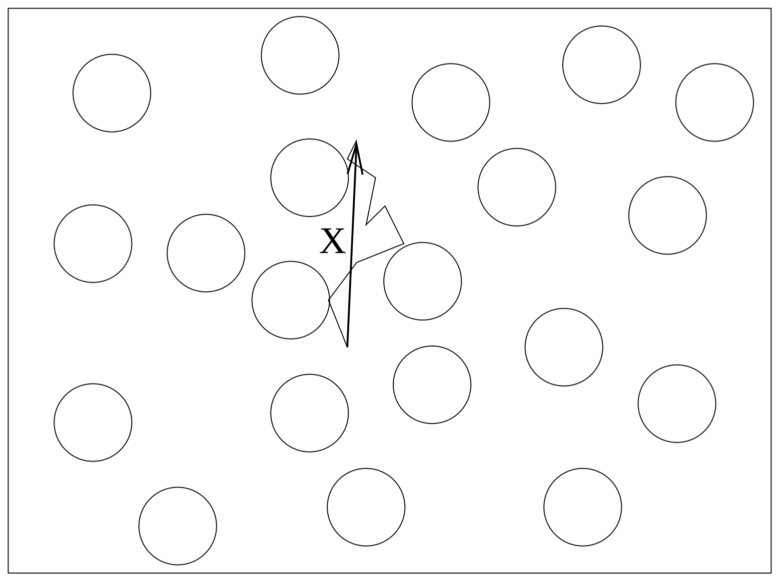
In a domain of nonoverlapping spherical traps : Timing with GFFPA



Effective Conductivity

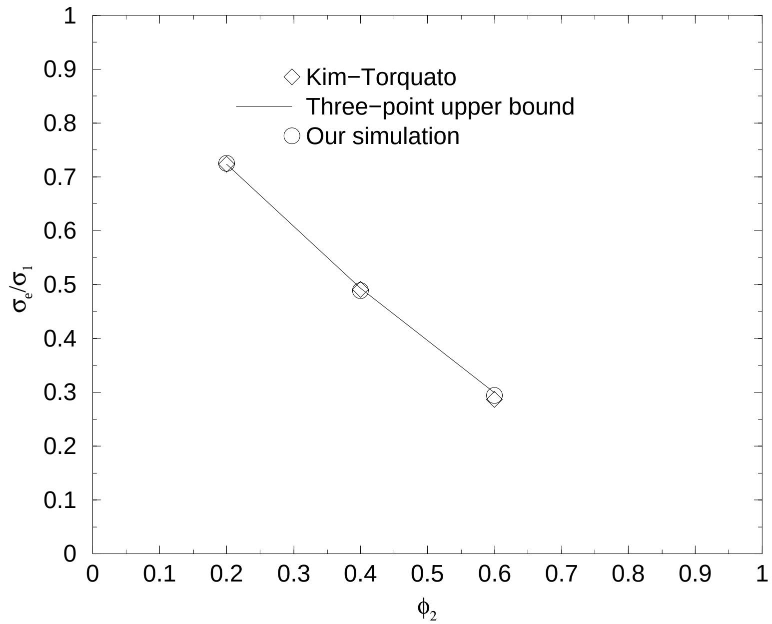
Perfectly insulating, nonoverlapping spherical inclusions :

$$\sigma_e = \frac{\overline{X^2}}{6\,\tau_e(X)}$$



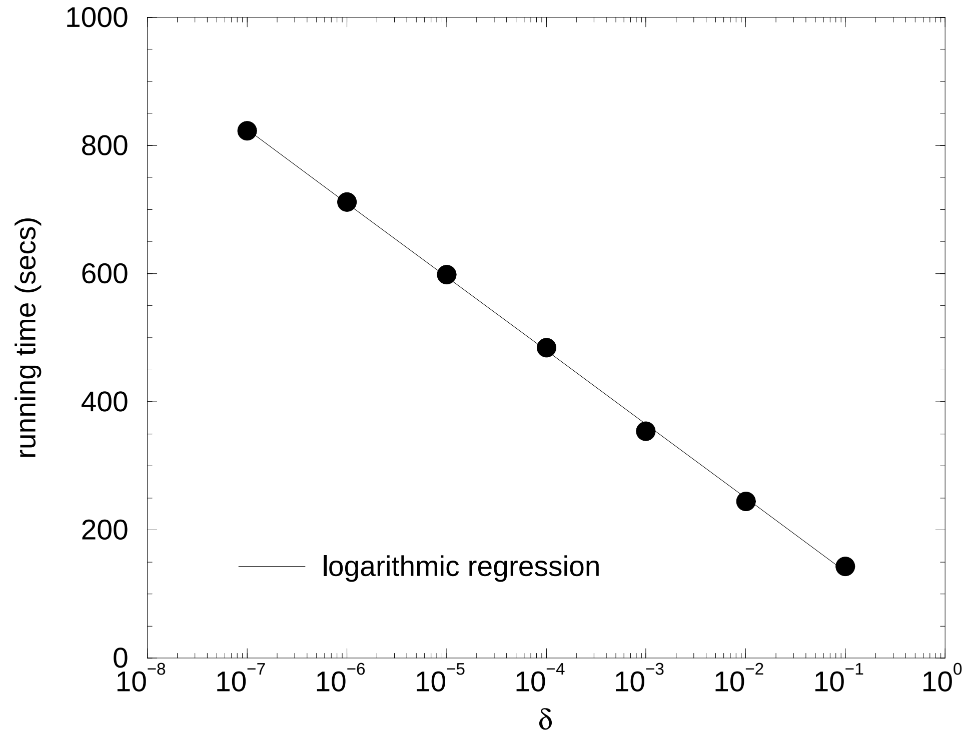
Effective Conductivity

Perfectly insulating, nonoverlapping spherical inclusions :



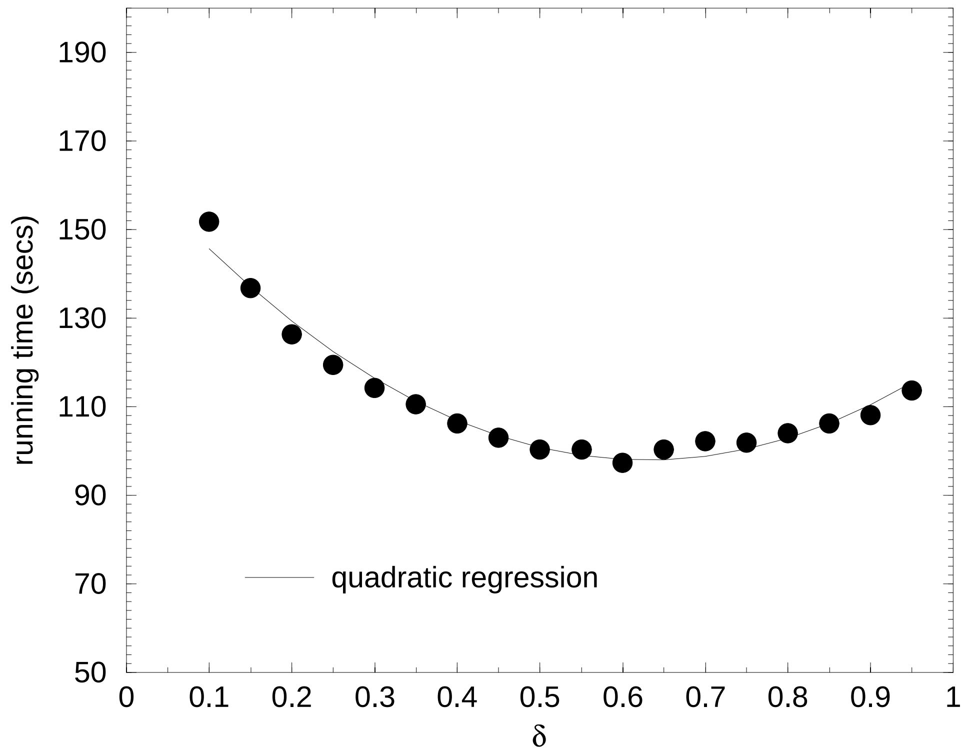
Effective Conductivity

Perfectly insulating, nonoverlapping spherical inclusions : Timing with WOS



Effective Conductivity

Perfectly insulating, nonoverlapping spherical inclusions : Timing with GFFPA



Feynman-Kac Formula

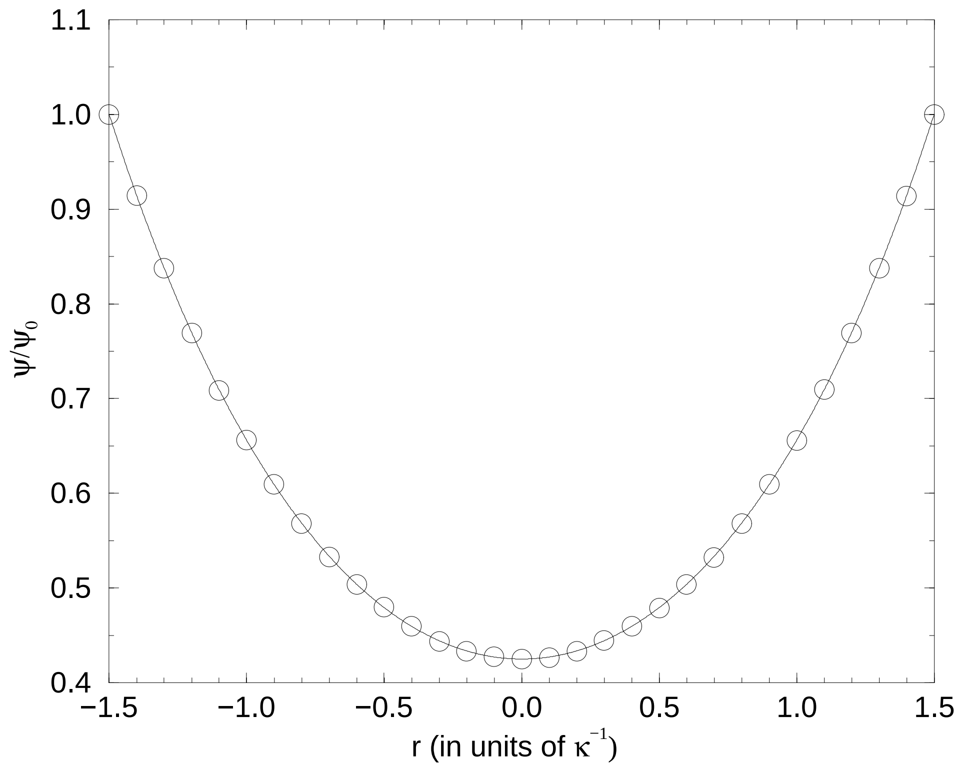
Linearized Poisson-Boltzmann Equation:

$$\Delta\Psi - \kappa^2\Psi = 0, \qquad \mathbf{x} \in \Omega \tag{12}$$

$$\Psi(\mathbf{x}) = \Psi_0(\mathbf{x}), \qquad \mathbf{x} \in \partial\Omega \tag{13}$$

$$\Psi(\mathbf{x}) = E[\Psi_0(X^x_{\tau^{\mathbf{x}}_D})\exp\{-\int_0^{\tau^{\mathbf{x}}_D} \kappa^2 dt\}], \tag{14}$$

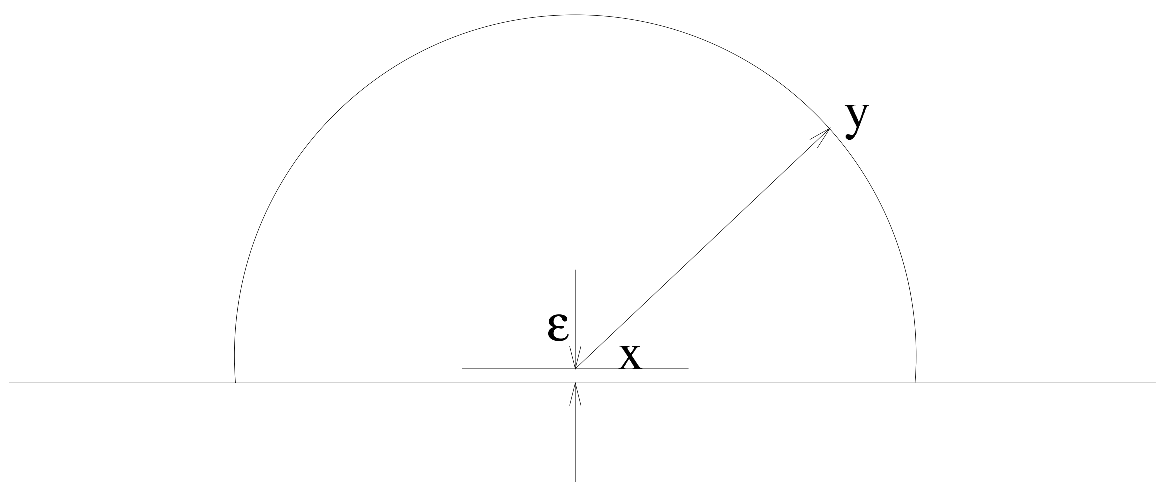
$$E[\exp(-\kappa^2 t)] = \frac{d\kappa}{\sinh d\kappa} \tag{15}$$


1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
ψ/ψ0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
r (in units of κ−1)

Last Passage Algorithms

- Charge distribution on a conducting object with edges and corners.
- Problems in which a large fraction of the absorption takes place on a very small fraction of the surface.
- Problems in which more than one conducting object is present, at close proximity, and at different voltages.

Approach from Outside



Approach from Outside

- probability of diffusing to infinity of a diffusing particle initiated at x ϵ-distant (very near) to the lower FP surface

$$P(x) = \oint d^2y g(x,y,\epsilon) p(y,\infty) \tag{16}$$

$$\sigma(x) = -\frac{1}{4\pi}\frac{d}{d\epsilon}\Big|_{\epsilon=0} \phi(x) = \frac{1}{4\pi}\frac{d}{d\epsilon}\Big|_{\epsilon=0} P(x) \tag{17}$$

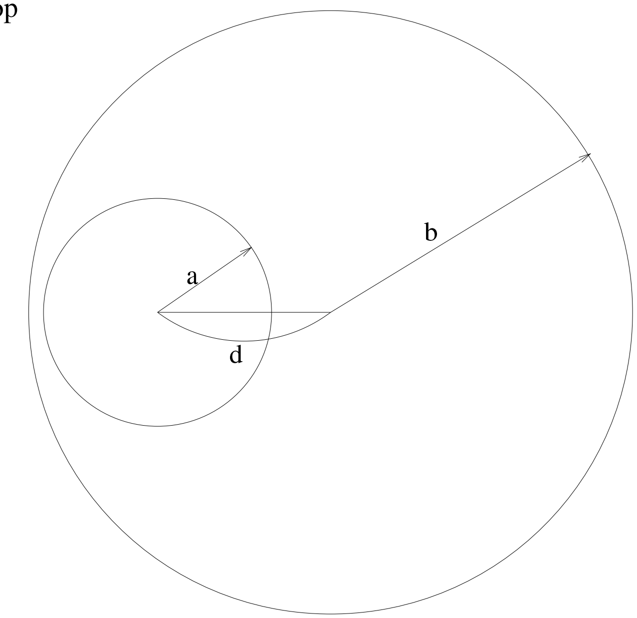
$$\sigma(x) = \frac{1}{4\pi}\oint d^2y \bar{g}(x,y) p(y,\infty), \tag{18}$$

where

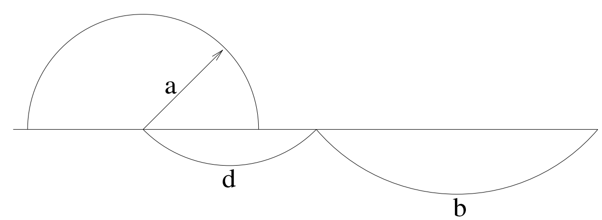
$$\bar{g}(x,y) = \frac{d}{d\epsilon}\Big|_{\epsilon=0} g(x,y,\epsilon) \tag{19}$$

Charge Density on a Circular Disk

From the top



From the side



Charge Density on a Circular Disk

$$\bar{g} = \frac{3}{4}\frac{\cos\theta}{a^3} \tag{20}$$

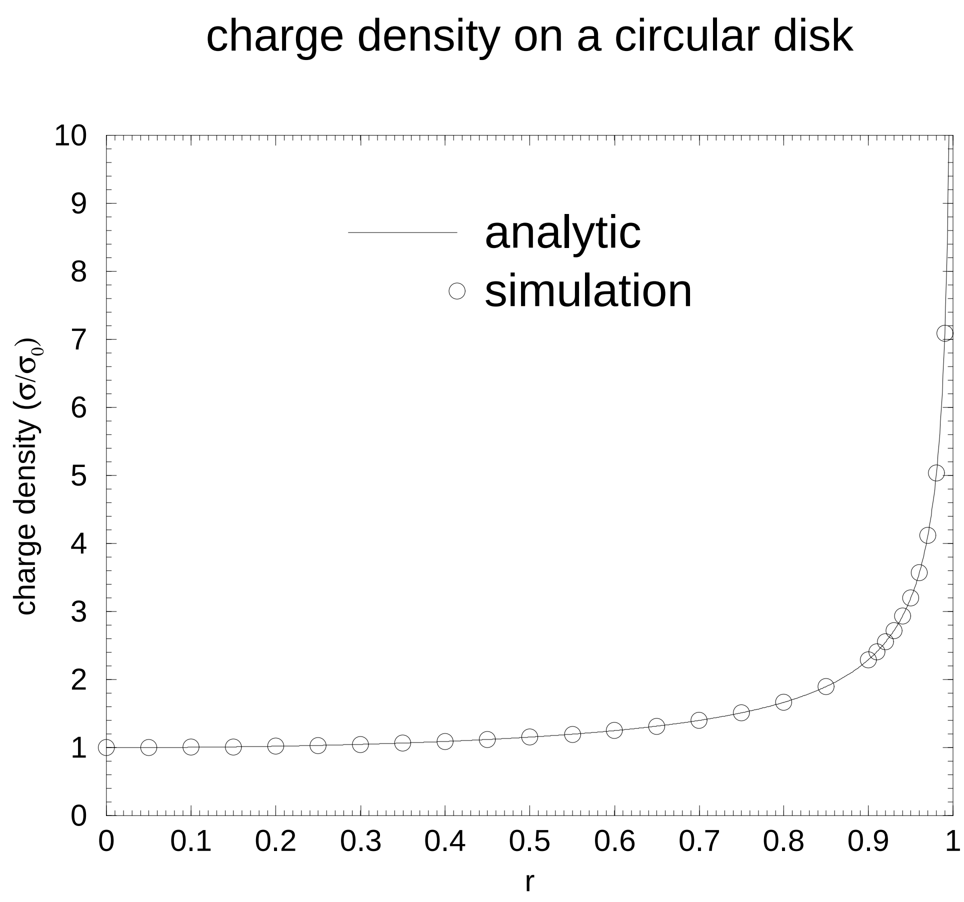
$$\sigma(x) = \frac{3}{16\pi}\oint dS \frac{\cos\theta}{a^3} p(\mathbf{r},\infty), \tag{21}$$

where

$$p(\mathbf{r},\infty) = 1 - \frac{2}{\pi}\arctan\left(\frac{\sqrt{2}b}{\sqrt{r^2 - b^2 + \sqrt{(r^2-b^2)^2 + 4b^2x^2}}}\right), \tag{22}$$

where $r^2 = x^2 + y^2 + z^2$

Charge Density on a Circular Disk



Future Work

- Extension of the Green's function library
  - Using analytic solutions
  - Sampling new Green's functions
- Extension of these methods to other PDEs
  - Poisson equation
  - Linearized Poisson Boltzmann equation
  - Time-independent Schrödinger equation
- More applications such as biological problems
  - Material Science
  - Biomolecular Science
- Quasirandom walks