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Linearized Poisson-Boltzman (TPB) Equation
A Feynman-Kac Formula Implementation for the
First passage time probability distribution

Implementation

Epley-Mihajlov solution and Feynman-Kac representation

"Walk on Spheres" (WOS)

Equation

Dirichlet Problem for the Linearized Poisson-Boltzmann (LPB)

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Future Work

- e-absorption Error Analysis
- Errors from e-absorption Layer
  - Errors
  - Runtime w.r.t. e-absorption Layer

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WOS for 2-D

\[ \partial \Omega \]

\( \epsilon \)

\( x; \) starting point

\[ X(\tau_{\partial \Omega}) \]

first-passage location
(4) \( (\cdot \mathfrak{D}) p = \cdot p \) 
\[ \frac{(y_{I-\cdot} p)}{y_{I-\cdot} p} \left[ \frac{1}{y_{I-\cdot} p} \right] = \cdot p \]
where

\[ (\cdot X)^{0,\cdot} \bigotimes_{N}^{I} = (\cdot x)^{0} \]

\[ \exists \Phi \ni x \quad (\cdot x)^{0} = (\cdot x)^{0} \]

\[ \exists \Phi \ni x \quad (\cdot x)^{0} = (\cdot x)^{0} \]

\textbf{Dirichlet Problem for LFB}
\[
\frac{\frac{\partial \rho}{\partial t}}{\rho} = (p)d
\]

and free diffusion region

\[\text{directed problem for LTP}\]

\[\text{survival probability of a random walker in a continuous}\]

\[\text{radius of the } \text{WOS of the } \text{ith random walker}\]

\[\text{the } \text{absorption layer after } \text{nth WOS steps}\]

\[\text{position where the } \text{ith random walker is absorbed in}\]

\[\text{referred to } \text{ith random walker}\]

\[\text{total number of diffusing random walkers}\]

\[N\] ~ Eppley-Mihailov solution
\( Z(\nu) \) is the free diffusion region using the first moment of the first passage survival probability of a random walker in a continuous and time distribution.

\( \Omega \): the first passage location on the boundary,

\( \Omega \in (\nu) X = \Omega \in (\nu) X : \nu \}

(6) \[
\left\{ \int_{\Omega \nu \gamma}^0 - \exp((\Omega \nu \gamma) X_0 \gamma) \right\} \mathcal{H} = (x) n
\]

\* Feynman-Kac representation of the solution: \* 

\* \* Dirichlet Problem for TPB \* \*
Survival Probabilities

\[ P(d_\kappa) \]

- Feynmann–Kac
- Elepov–Mihailov
$$(\Pi) \quad \frac{\sin \phi}{p^\text{km}} =$$

$$(\Omega) \quad \frac{\frac{\partial \phi}{\partial \theta} (u(1-)) + \int_{\infty}^{1=\infty} \mathcal{F} \cdot \mathcal{G} \cdot \mathcal{H}}{u(1-)} =$$

$$(6) \quad \mathcal{H} \left[ \mathcal{I} \left( \frac{\partial \phi}{\partial \theta} (u(1-)) + \frac{\partial \phi}{\partial \theta} (u(1-)) \right) \right] \cdot \mathcal{E} \int_{\infty}^{1=\infty} \mathcal{F} \cdot \mathcal{G} \cdot \mathcal{H} =$$

$$(8) \quad \mathcal{H} \left[ \mathcal{I} \left( \frac{\partial \phi}{\partial \theta} (u(1-)) \right) \right] \cdot \mathcal{E} \frac{\frac{\partial \phi}{\partial \theta}}{(\mathcal{I})} \int_{\infty}^{0} \mathcal{F} \cdot \mathcal{G} \cdot \mathcal{H}$$

Equivalence of FK to EM
\[(\mathcal{T}_x(t, u)) \exp u(1 - I) \sum_{z=2}^{\infty} z + 1 = (\mathcal{T}_x(t)) D\]

where the first passage time probability distribution, \(\mathcal{T}_x(t)\), is

**Equivalence of FK to EM**

\(\mathcal{T}_x(t)\) is the radius of WOS.
First-passage Time Probability Distribution
For each WOS step,

Peymann-Kac Implementation for LBP

Survival probability, the random walker is removed at this WOS step.

0, 1

and if the random number is greater than the survival probability, the random number is compared with a random number in

\( \text{Corresponding survival probability, } \exp(-\kappa \cdot t) \), is obtained.

Sampling \( t \) using a random number in \((0, 1)\)
An estimate for the solution at \( x^0 \): 

\[ (z^n X)^0 \bigotimes_{\mathcal{N}^1} \mathcal{N} = N S \]

**Dirichlet Problem for TBP**

absorbed after \( n \) WOS steps

\( z^n X \) = final position of the walker on the boundary when it is absorbed

\( ^N \mathcal{N} \) = number of survived and absorbed random walkers

\( ^s \mathcal{N} \) = number of trajectories

Slide 12
Sphere

\[ \frac{\psi}{\psi_0} \]

vs.

\[ r \text{ (in units of } \kappa^{-1}) \]

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Cylinder

$r$ (in units of $\kappa^{-1}$)

$h/h_0$

0 0.5 1 1.5 2 2.5 3 3.5 4

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1
Plate

![Graph showing the relationship between \( r \) (in units of \( \kappa^{-1} \)) and \( \psi/\psi_0 \). The graph demonstrates a decreasing trend as \( r \) increases.](image-url)
Parallel Plates

\[ \psi / \psi_0 \]

\[ r \text{ (in units of } \kappa^{-1}) \]
Runtime \( w.r.t. \ \epsilon \)-absorption Layer

![Graph showing runtime w.r.t. \( \epsilon \)-absorption layer with logarithmic regression line and data points.]

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of trajectories

It is possible to investigate empirically using enough number

• Errors associated with the e-absorption layer

• Errors associated with the number of trajectories – can be reduced by increasing the number of trajectories

• Errors
Errors from $\epsilon$-absorption Layer

![Graph showing absolute error vs. $\epsilon$-absorption layer with linear regression line.]

- absolute error
- $\epsilon$-absorption layer

- simulation error
- linear regression
Question: random walks

Equation

Extension to a method for the time-independent Schrödinger

\[(x)\hat{b} - (x)\hat{\phi} = (x)\hat{\phi} \nabla\]

Solving

Future Work