Mathematically Modeling Motion of Cells in Porous Media

Ahaan Rungta
Mentor Dr. Andrew Rzeznik

Fifth Annual MIT-PRIMES Conference

May 16, 2015

Background

- Motion of particles in simple systems

Background

- Motion of particles in simple systems
  - Random free-fluid motion

Background

- Motion of particles in simple systems
  - Random free-fluid motion
  - Random one-dimensional lattice walks

Background

- Motion of particles in simple systems
  - Random free-fluid motion
  - Random one-dimensional lattice walks
- Properties of the truly random infinite walk in $\mathbb{Z}^d$

Goals

- More realistic medium

Goals

- More realistic medium
- Study boundaries

Goals

- More realistic medium
- Study boundaries
- Find parameters that effect asymptotic behavior

Goals

- More realistic medium
- Study boundaries
- Find parameters that effect asymptotic behavior
- Compare analytics to simulations and experiment

Some simple plots

- Walk in $\mathbb{Z}$ without wall

Some simple plots

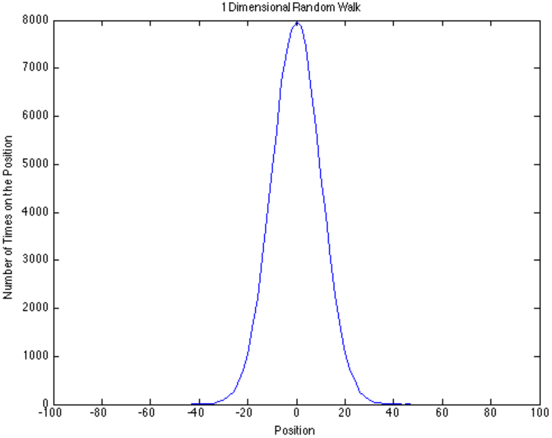
- Walk in $\mathbb{Z}$ without wall
  - t = number of steps in one run
  - r = number of runs

Some simple plots

- Walk in $\mathbb{Z}$ without wall: $p_{\leftarrow} = 0.5$, $t = 100$, $r = 10^5$

Some simple plots

- Walk in $\mathbb{Z}$ without wall: $p_{\leftarrow} = 0.5$, $t = 100$, $r = 10^5$

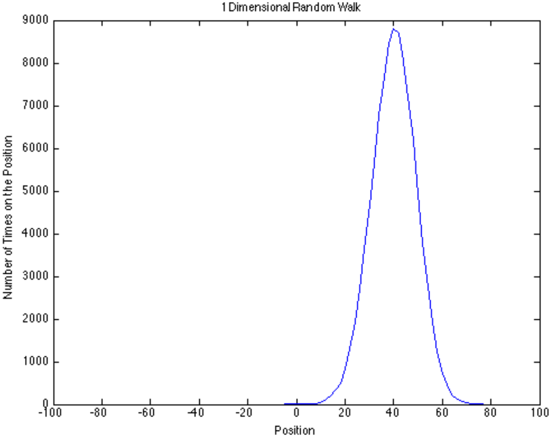


Some simple plots

- Walk in $\mathbb{Z}$ without wall: $p_{\leftarrow} = 0.3$, $t = 100$ $r = 10^5$

Some simple plots

- Walk in $\mathbb{Z}$ without wall: $p_{\leftarrow} = 0.3$, $t = 100$ $r = 10^5$

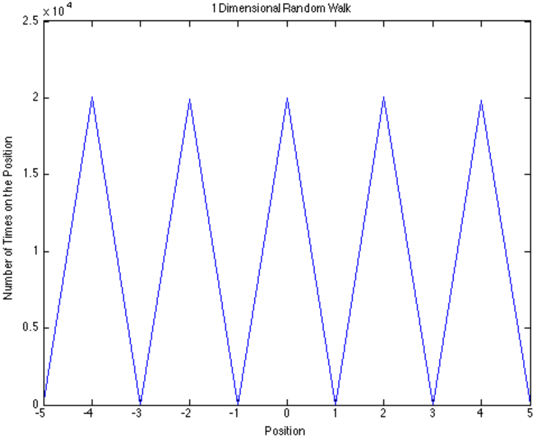


Some simple plots

- Walk in $\mathbb{Z}$ with wall: $p_{\leftarrow} = 0.5$, $t = 100$, $r = 10^5$, $n = 5$

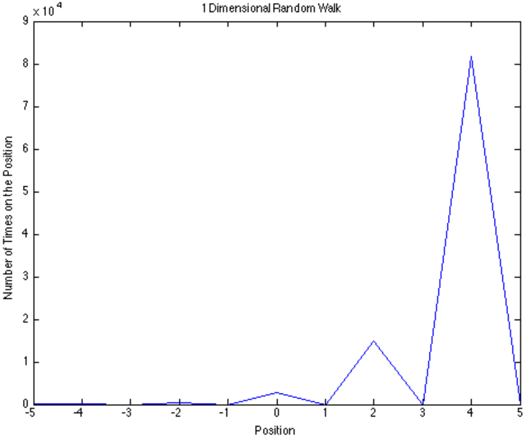
Some simple plots

- Walk in $\mathbb{Z}$ with wall: $p_{\leftarrow} = 0.5$, $t = 100$, $r = 10^5$, $n = 5$



Some simple plots

- Walk in $\mathbb{Z}$ with wall: $p_{\leftarrow} = 0.3$, $t = 10^5$, $r = 10^4$



Framework

- Represent the porous medium as an array of points

Framework

- Represent the porous medium as an array of points
- Convert the lattice grid to a graph

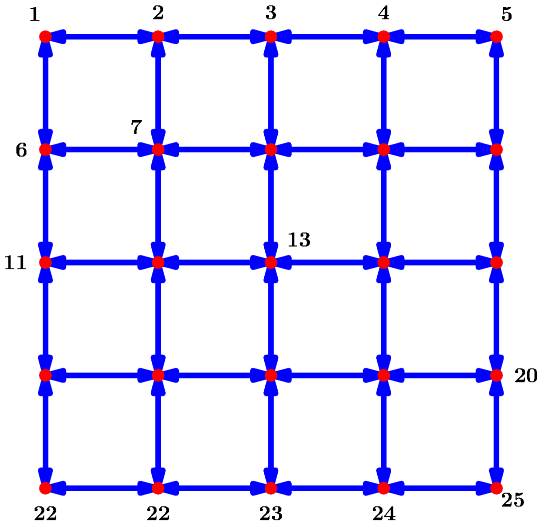
Framework

- Represent the porous medium as an array of points
- Convert the lattice grid to a graph
- Assign probabilities to the edges

Framework

- Represent the porous medium as an array of points
- Convert the lattice grid to a graph
- Assign probabilities to the edges
- Run the walk and graph a histogram

Framework



Extra dimension

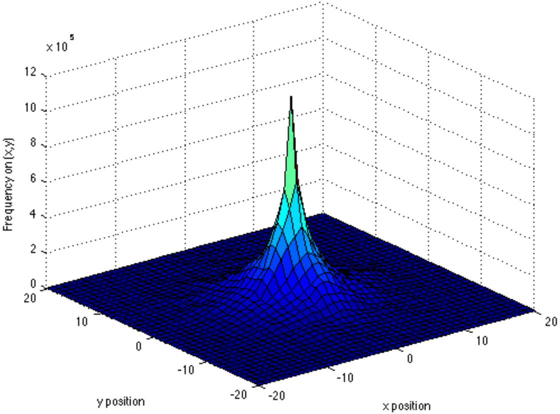
- Walk in $\mathbb{Z}^2$ with a negligible wall

Extra dimension

- Walk in $\mathbb{Z}^2$ with a negligible wall: persistency 0, $t = 100$, $r = 1000$, and $n = 20$.

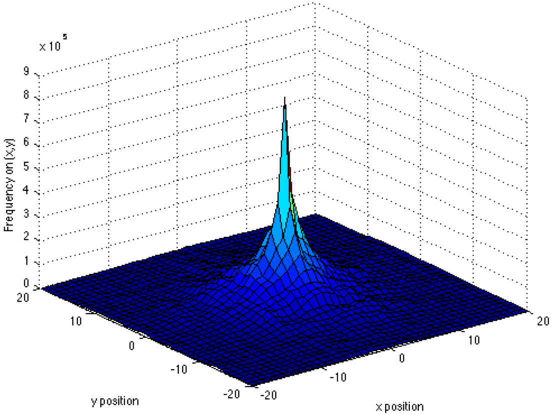
Extra dimension

- Walk in $\mathbb{Z}^2$ with a negligible wall: persistency 0, $t = 100$, $r = 1000$, and $n = 20$.



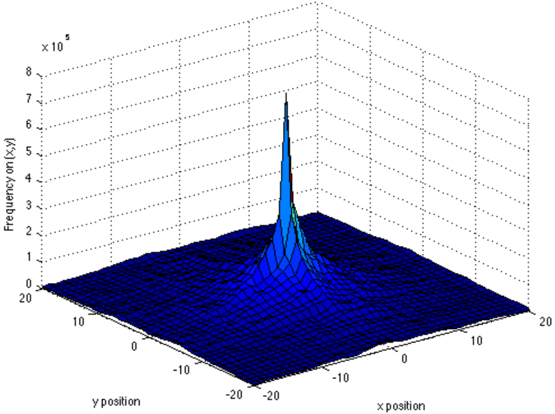
Extra dimension

- Walk in $\mathbb{Z}^2$ with a negligible wall: persistency 0.5, $t = 100$, $r = 1000$, and $n = 20$.



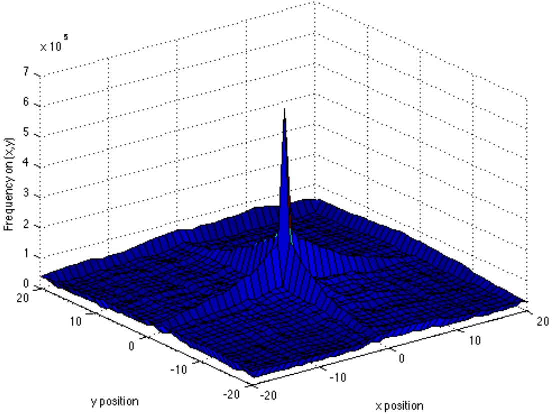
Extra dimension

- Walk in $\mathbb{Z}^2$ with a negligible wall: persistency 0.7, $t = 100$, $r = 1000$, and $n = 20$.



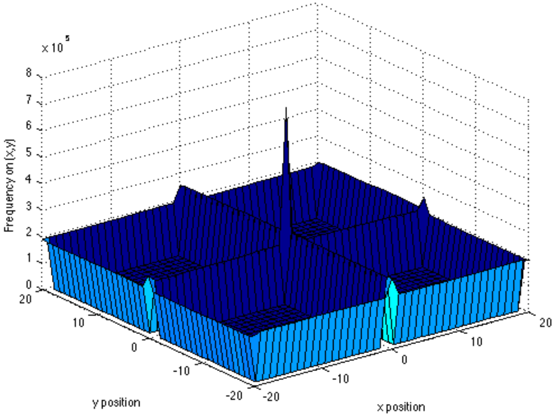
Extra dimension

- Walk in $\mathbb{Z}^2$ with a negligible wall: persistency 0.9, $t = 100$, $r = 1000$, and $n = 20$.



Extra dimension

- Walk in $\mathbb{Z}^2$ with a negligible wall: persistency 0.999, $t = 100$, $r = 1000$, and $n = 20$.



Super-Gaussian

- Gaussian curve: $f(x) = \exp\left(-\left|\frac{x}{a}\right|^2\right)$

Super-Gaussian

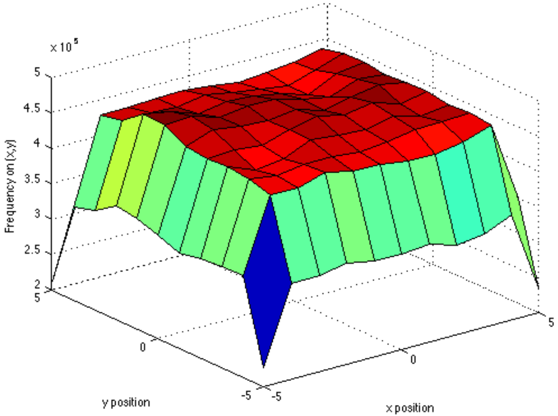
- Gaussian curve: $f(x) = \exp\left(-\left|\frac{x}{a}\right|^2\right)$
- Super-gaussian curve: $f(x) = \exp\left(-\left|\frac{x}{a}\right|^n\right)$, for $n < 2$

Extra dimension

- Walk in $\mathbb{Z}^2$ with wall

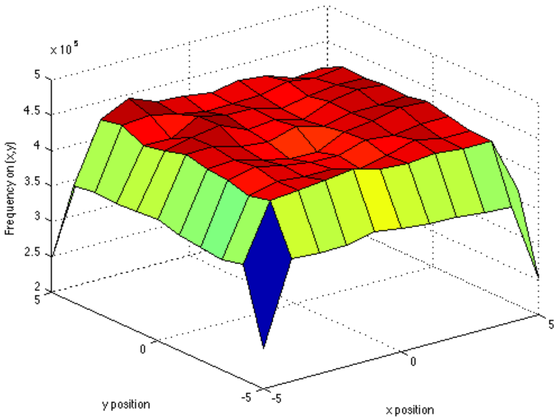
Extra dimension

- Walk in $\mathbb{Z}^2$ with wall: persistency 0, $n = 5$, $t = 10^4$, $r = 100$.



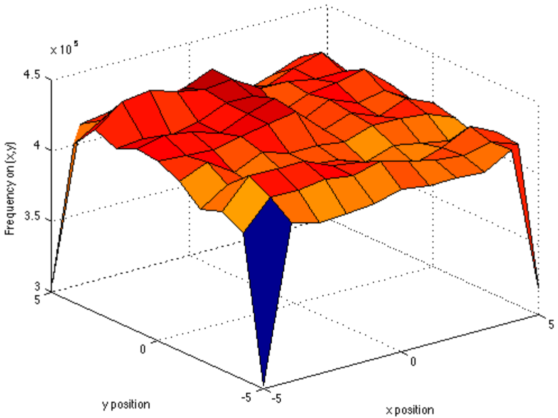
Extra dimension

- Walk in $\mathbb{Z}^2$ with wall: persistency 0.2, $n = 5$, $t = 10^4$, $r = 100$.



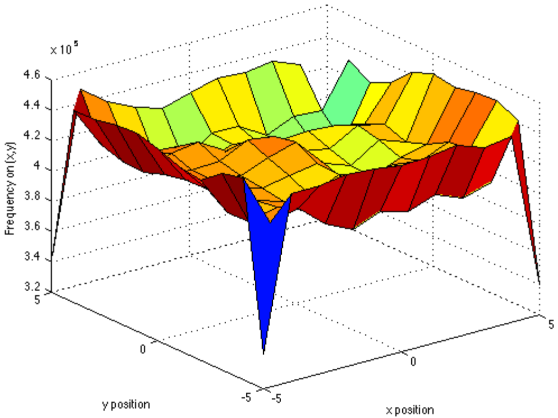
Extra dimension

- Walk in $\mathbb{Z}^2$ with wall: persistency 0.4, $n = 5$, $t = 10^4$, $r = 100$.



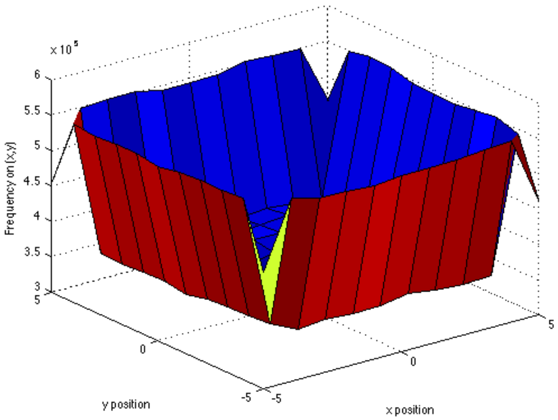
Extra dimension

- Walk in $\mathbb{Z}^2$ with wall: persistency 0.5, $n = 5$, $t = 10^4$, $r = 100$.



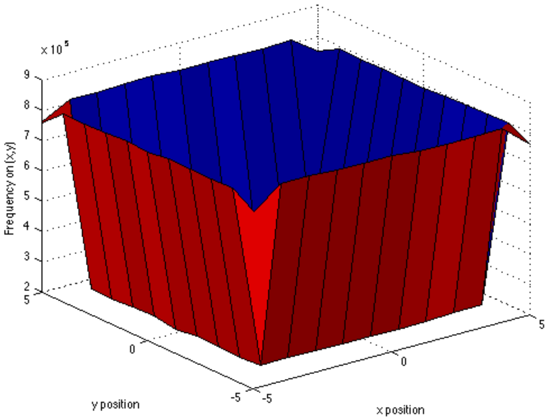
Extra dimension

- Walk in $\mathbb{Z}^2$ with wall: persistency 0.7, $n = 5$, $t = 10^4$, $r = 100$.



Extra dimension

- Walk in $\mathbb{Z}^2$ with wall: persistency 0.9, $n = 5$, $t = 10^4$, $r = 100$.



Observations

- Simulations match existing theories

Observations

- Simulations match existing theories
- Memory favors boundaries, asymptotically

Future work

Future work

- Generalized model

Future work

- Generalized model
- Finding a small set of determining parameters

Future work

- Generalized model
- Finding a small set of determining parameters
    - More study on boundaries

Future work

- Generalized model
- Finding a small set of determining parameters
  - More study on boundaries
- Match with experiment
  - Can we use Markov chains?
  - How do simulated mixing times compare with experiment?

Definition

The *mixing time* of a Markov chain $\mathcal{M}$ is the time until $\mathcal{M}$ tends to settle to a steady state.

Future work

- Generalized model
- Finding a small set of determining parameters
    - More study on boundaries
- Match with experiment
    - Can we use Markov chains?
    - How do simulated mixing times compare with experiment?

Definition

The *mixing time* of a Markov chain $\mathcal{M}$ is the time until $\mathcal{M}$ tends to settle to a steady state.

- Deriving diffusion coefficients (Fick)

Future work

- Generalized model
- Finding a small set of determining parameters
  - More study on boundaries
- Match with experiment
  - Can we use Markov chains?
  - How do simulated mixing times compare with experiment?

Definition

The *mixing time* of a Markov chain $\mathcal{M}$ is the time until $\mathcal{M}$ tends to settle to a steady state.

- Deriving diffusion coefficients (Fick)
- Lazy random walks

Acknowledgements

A huge thanks to:

- Prof. Jörn Dunkel
- Mentor Andrew Rzeznik
- MIT-PRIMES
- My parents