Particle Fluctuations in Ion Channels

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Particles undergo Brownian motion and pass-through Ion channels, with multiple particles being in the channel at once.

Particles – Ions such as potassium, sodium, calcium, etc.

Ion channels - proteins arranged to allow passage from one side of a cell membrane to another.

Brownian motion - random fluctuations in a particle’s position in a fluid.

**Problem:** Difficult to make statistical measurements at a cellular level, and look at the particles inside in the ion channel.

**Goal:** Starting from standard Brownian motion understand how particles are transported through ion channels, specifically how they behave inside the channel.
Simulation Set up

- Simulate long particle trajectories in periodic bounded region
- In region there is a box to represent ion channel
- Number of particles in box counted at each time step
- Calculate Mean Squared Displacement (MSD) of number of particles in the box
MSD for Brownian Motion

$$MSD(\tau) = \langle \Delta r(\tau)^2 \rangle = \langle [r(t + \tau) - r(t)]^2 \rangle$$

- \(r(t)\)- Particle position at time \(t\)

• MSD describes particle movement

• Useful because mean displacement is 0

• Standard Brownian motion has a linear MSD

$$\langle \Delta r(\tau)^2 \rangle = \frac{2kTd}{\zeta} \tau$$, Where \( \frac{2kT}{\zeta} \) is a constant, \( d \) is dimension

• MSD of number of particles in a box is not linear

Theoretical MSD

For Number of Particles in the Box

\[
\langle (N(t + t_0) - N(t_0))^2 \rangle = 2N_0 \left[ \left( 1 - e^{-\frac{W^2}{4Dt}} \right) \sqrt{\frac{4Dt}{\pi W^2}} + 1 - \text{erf}\left( \frac{W}{\sqrt{4Dt}} \right) \right]
\]

Notation:
- \(N_0\) - avg. number of particles
- \(W\) - Width of box
- \(D\) – Diffusion Coefficient
- \(N(t)\) - Number of particles within the box
Adjusting Theoretical

• MSD, $\langle N^2(t) \rangle$, fitted to $b \times t^a$ for **early times**
• In both theoretical and simulated $a \approx 0.5$
• $b$ has various values
• In theoretical $b = \sqrt{\frac{4D}{\pi W^2}} \approx 0.1$
Adjusting Theoretical

Values of $b$ fitted to $c \times \left(\frac{H}{W}\right)^d + g$

$d \approx -1$

$\text{Theoretical}(b_\infty) = c = g = 2 \sqrt{\frac{4D}{\pi W^2}}$

Value of $b$ can be now written as

$b_\infty \times \left(\frac{W}{H} + 1\right) = \frac{H \times W}{W + H}$
\[
\langle (N_c(t + t_0) - N_c(t_0))^2 \rangle = 2N_0 \left[ \left(1 - e^{-\frac{W^2}{4Dt}}\right) \sqrt{\frac{4Dt}{\pi W^2}} + 1 - \text{erf}\left(\frac{W}{\sqrt{4Dt}}\right) \right]
\]

\[
\langle (N_c(t + t_0) - N_c(t_0))^2 \rangle = 2N_0 \left[ \left(1 - e^{-\frac{B^2}{8Dt}}\right) \sqrt{\frac{8Dt}{2\pi B^2}} + 1 - \text{erf}\left(\frac{B}{\sqrt{8Dt}}\right) \right]
\]

\[B = \frac{H \times W}{W + H}\]

Accounts for added dimension

Only for early times
Future Work

- Look at long times
- Statistical errors
- When particles have finite size
- Limited number of particles in the box
Thank You!

Questions?