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STOCHASTIC MODELS IN MOLECULAR BIOLOGY

Molecules in biological cells move by diffusion

Accurate but
not efficient

Molecular-based model

- ★ Molecules move as Brownian dynamics
- ★ Time driven algorithm

Efficient but
not accurate

Cube-based model

- ★ Molecules jump from one cube to another in discretized space
- ★ Continuous time discrete state Markov chain
- ★ Event driven algorithm

Convergence

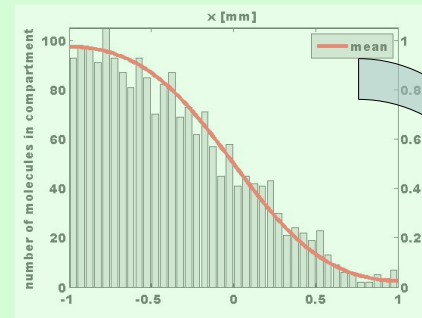


Figure 1

$$\begin{cases} \frac{\partial \varphi}{\partial t} = D \frac{\partial^2 \varphi}{\partial x^2} \\ \frac{\partial \varphi}{\partial x} = 0 \text{ on the boundaries} \end{cases}$$

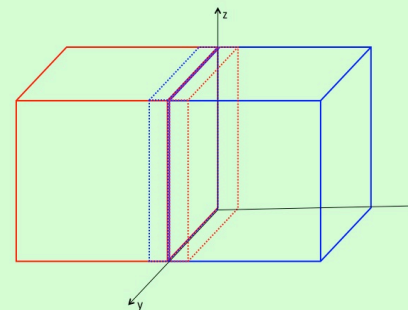


Figure 2

Accurate and
efficient

Multiscale model

- ★ Switching in time between cube based model (red) and molecular based model (blue) in Figure 2
- ★ Optimizing algorithms by introducing new coefficients
- ★ Sum up y and z directions at time $T=0.1s$ then see the distribution of x and comparison with the analytical solution in Figure 1