Kobe-Brown Simulation Summer School 2015
Project: DPD Simulation of a Membrane

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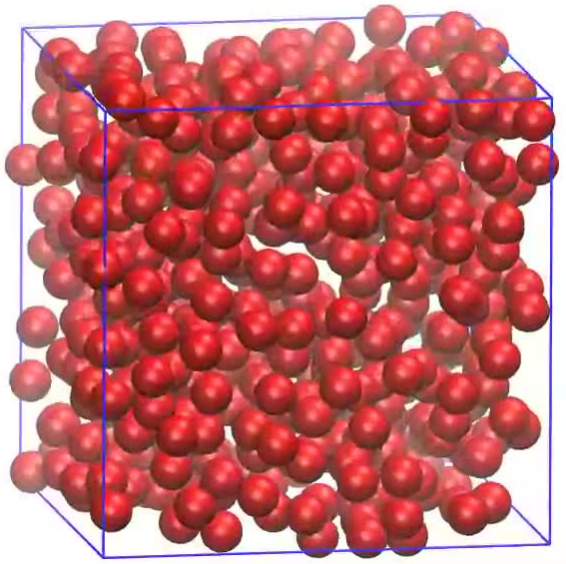
Week 1: Introduction to Molecular Dynamics (MD)

- Computer simulation of a large number of particles
- Trajectories of particles are determined by solving Newton's laws numerically
- Simulation proceeds in discrete time steps



Goal of Week 1

Write a two-dimensional MD simulation of liquid argon from scratch using C++!

- Forces calculated using Lennard-Jones (LJ) potential
- Velocity Verlet method used for numerical integration
- Experiment with different boundary conditions (periodic, reflecting, no-slip)

Lennard-Jones Potential

$$V_{i,j}(r_{i,j}) = 4\epsilon\left[\left(\frac{\sigma}{r_{i,j}}\right)^{12} - \left(\frac{\sigma}{r_{i,j}}\right)^{6}\right]$$

$$V_{i,j}(r_{i,j}) = \begin{cases} 4\epsilon\left[\left(\frac{\sigma}{r_{i,j}}\right)^{12} - \left(\frac{\sigma}{r_{i,j}}\right)^{6}\right] + \epsilon & \text{if } r_{i,j} \leq r_c \\ 0 & \text{otherwise} \end{cases}$$

$$r_c \approx 2^{\frac{1}{6}}\sigma$$

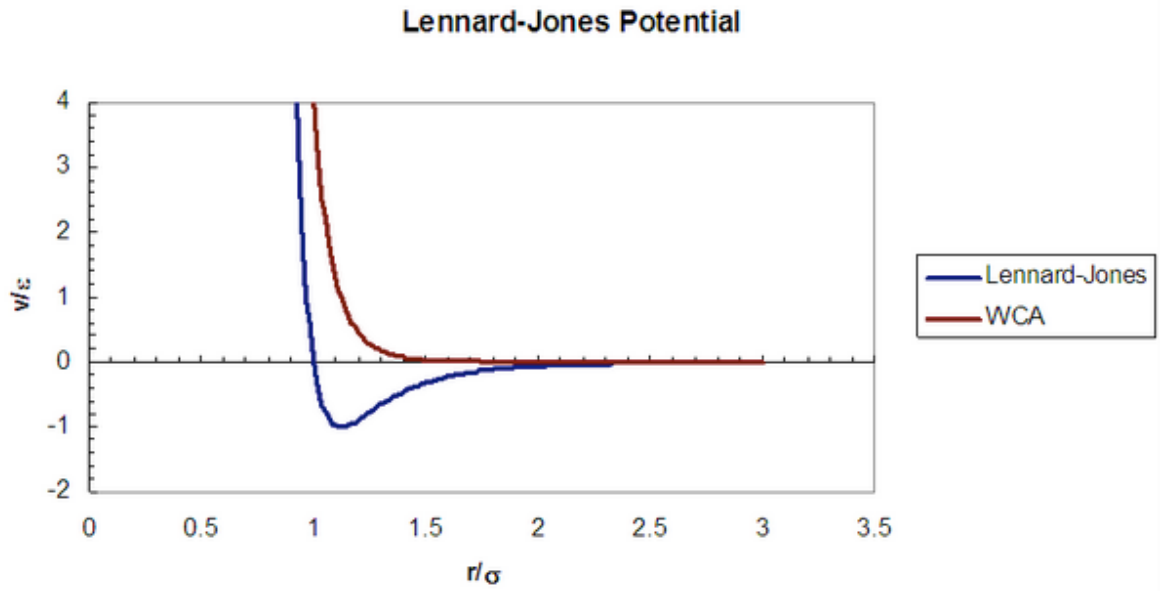
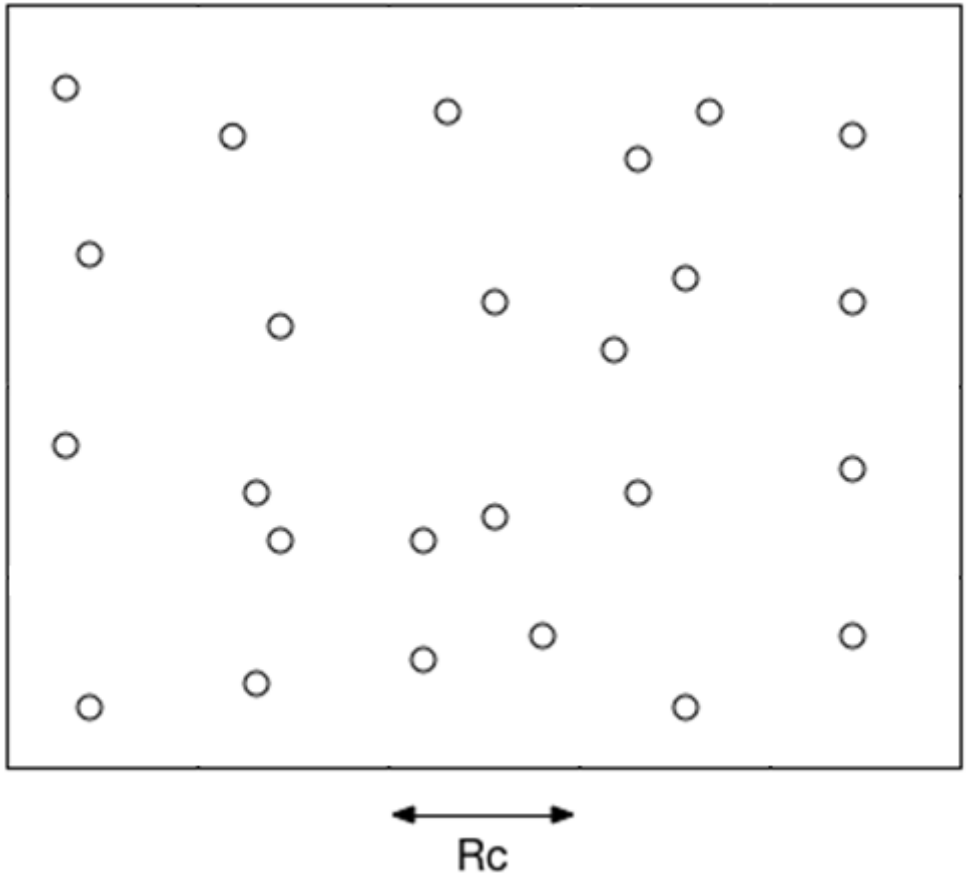
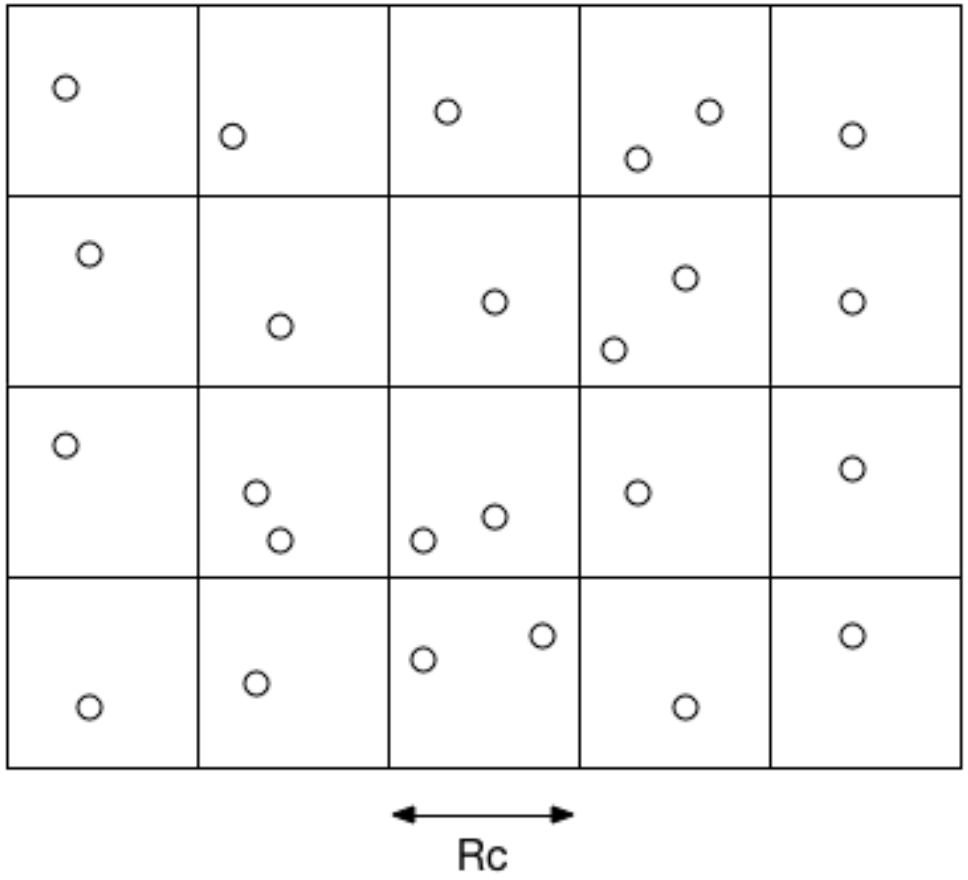


Image: http://s110.photobucket.com/user/ecfreema/media/LennardWCAPlot.gif.html

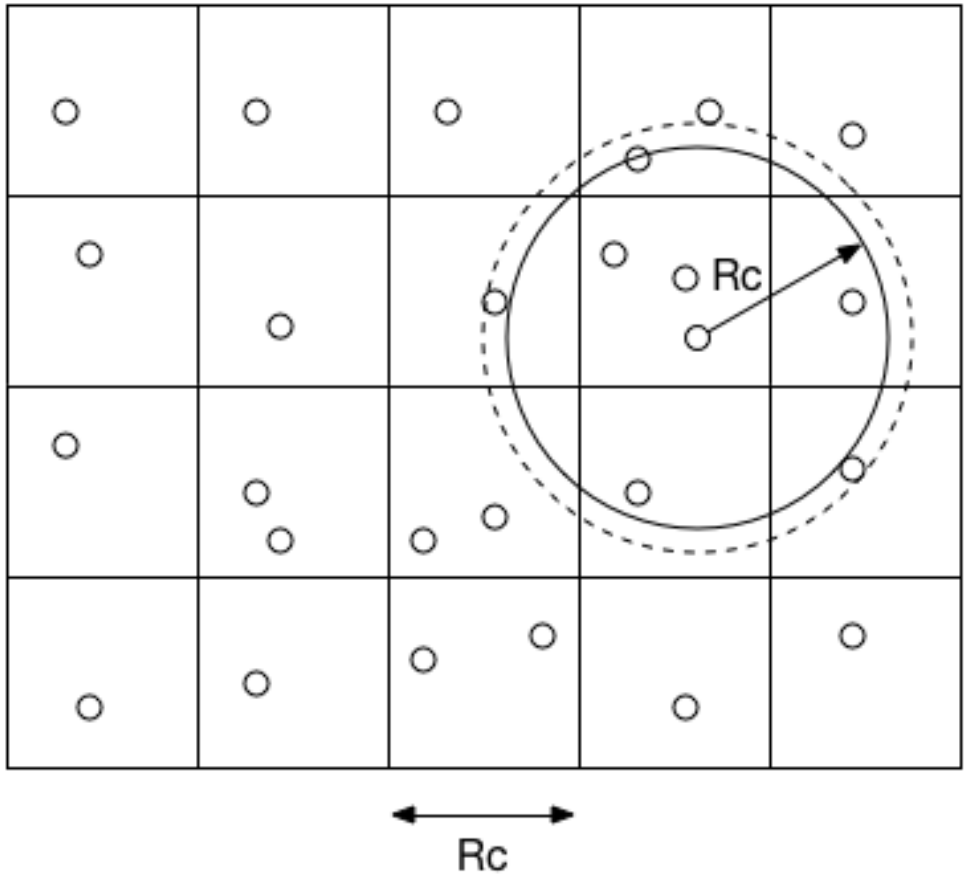
Force Calculation: Pairwise Forces



Force Calculation: Cell List Method

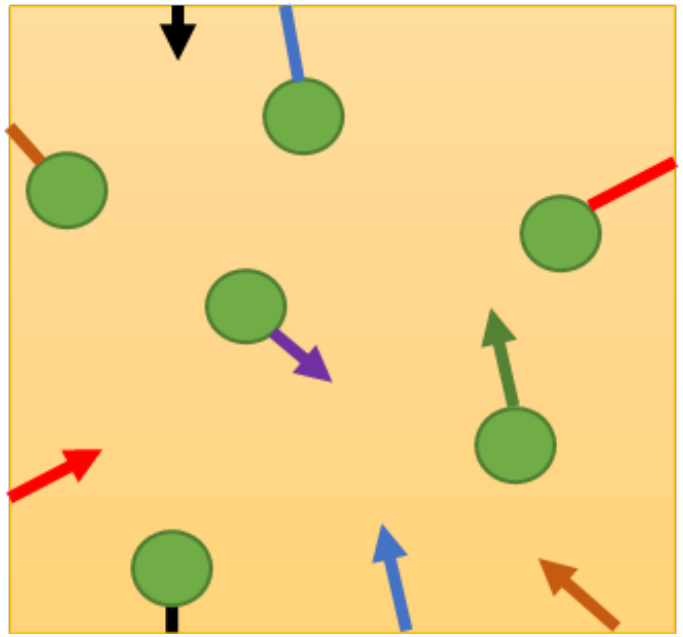


Force Calculation: Neighbor List Method

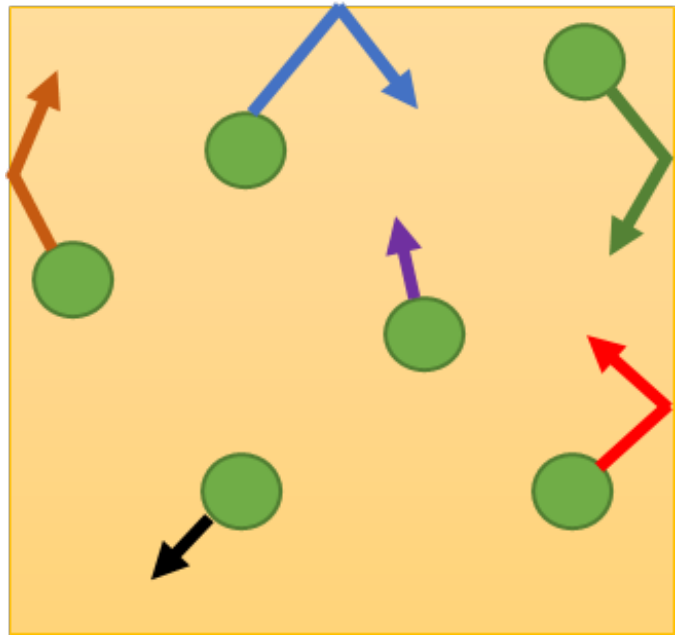


Boundary Conditions

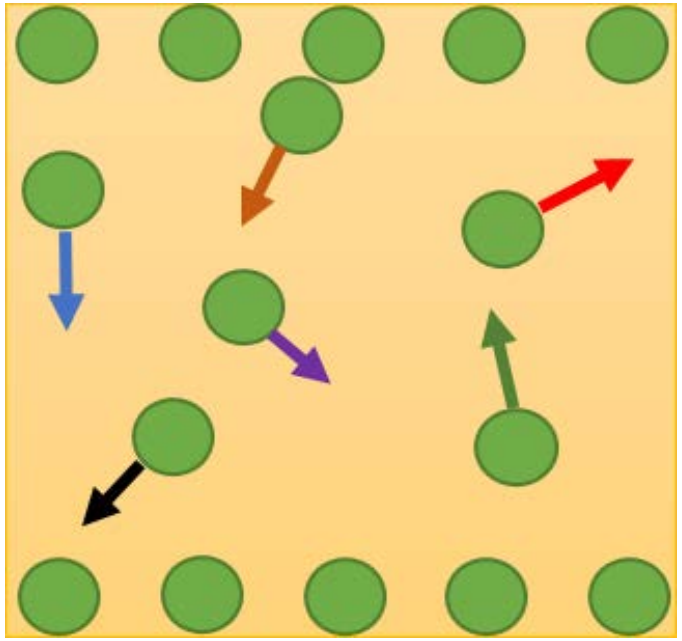
Periodic



Reflecting



No-slip



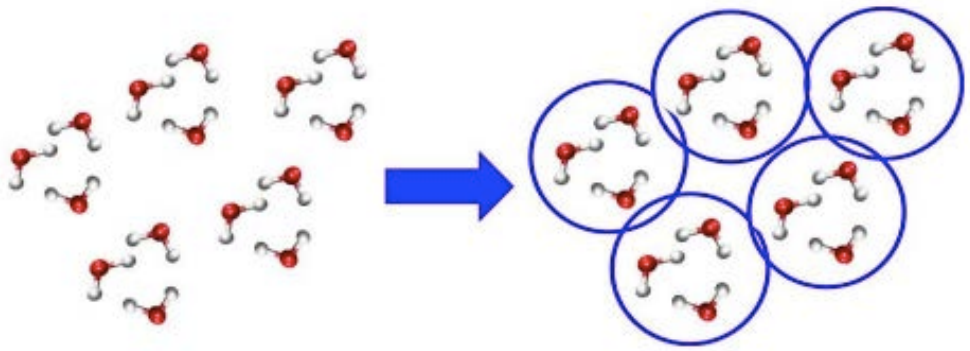
Testing the Code: Flow in a Pipe

- 3D rectangular channel with no-slip walls
- Channel filled with LJ fluid
- Uniform force along channel due to pressure gradient (Poiseuille flow)

→ Parabolic velocity profile?

Week 2: Dissipative Particle Dynamics (DPD)

- Particle simulator like Molecular Dynamics
- Coarse-graining: model groups of atoms as single “beads”

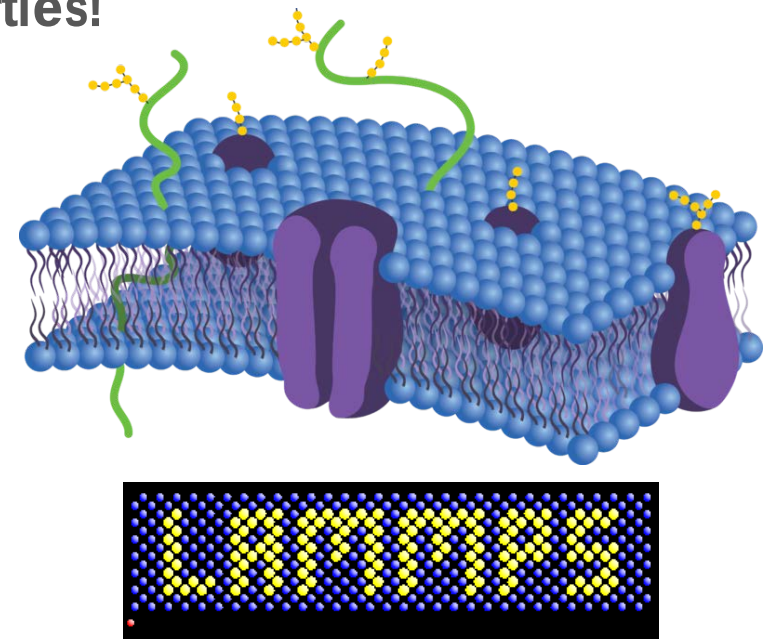


- Reduced complexity allows simulating **larger** systems while still modeling flows

Image: http://arxiv.org/pdf/1506.06202.pdf

Goal of Week 2

Simulate a 3D bilipid membrane with DPD and study its properties!



- Method: LAMMPS particle simulator

  → same algorithms as Week 1, but parallel/optimized

- Means: Brown CCV Computing Cluster “Oscar”

  → 657.8 Teraflops across 7,632 Intel Xeon E5 cores

Images: http://www.ck12.org/biology/Phospholipid-Bilayers/lesson/Phospholipid-Bilayers, lammps.sandia.gov

DPD Force Equation

- In MD, only force was due to LJ pairwise interactions
- DPD has **three** forces:

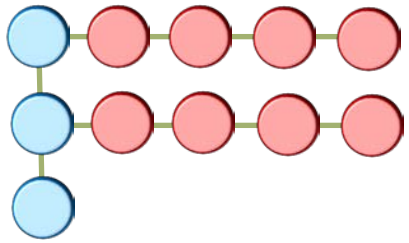
$$F_i = \sum_{j \neq i} \vec{F}_{ij}^{C} + \sum_{j \neq i} \vec{F}_{ij}^{D} + \sum_{j \neq i} \vec{F}_{ij}^{R}$$

Conservative force (soft repulsion), **Dissipative** force (viscous resistance), **Random** force (thermostat)

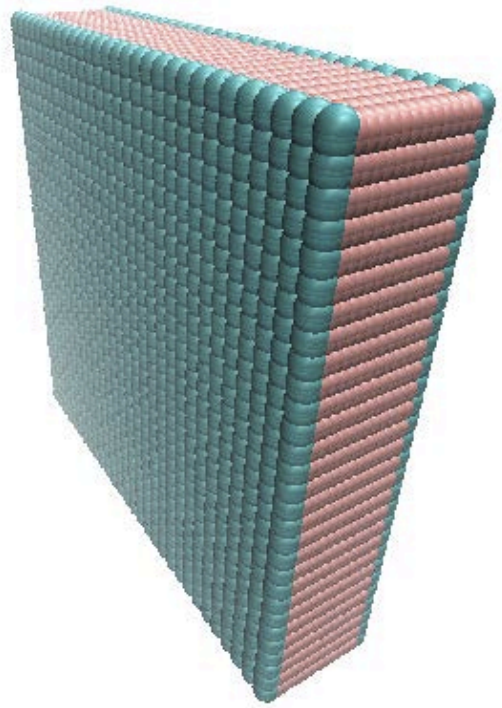
- New forces compensate for coarse-graining to yield similar mechanics

Creating a DPD Bilipid Membrane

- Built out of **lipids**:



- **Blue** = hydrophilic head particles
- **Red** = hydrophobic tail particles
- Harmonic (spring) bonds
- Initialize on cubic lattice

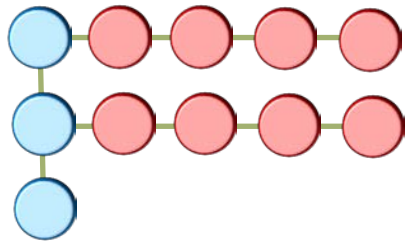


Tunable Parameters to Achieve Stability

- Structure of lipids (e.g., number of tail beads)
- Dimensions of lattice for initialization (e.g., space between lipids)
- Spacing between two halves of membrane
- **Conservative** coefficient a_{ij} and **dissipative** coefficient γ for different types of beads (water, heads, tails)

Exploring DPD Parameters

- For **water**, a_{ij} = 25.0 and γ = 4.5 (Groot, Warren 1997)
- For lipid **heads** and **tails**: ???



Exploring DPD Parameters (End Result)

For heads: $a_{ij} = 14$ and $\gamma = 4.5$
For tails: $a_{ij} = 14$ and $\gamma = 4.5$
Between water and head particles: $a_{ij} = 13$ and $\gamma = 4.5$
Between water and tail particles: $a_{ij} = 90$ and $\gamma = 4.5$
Between tail and head particles: $a_{ij} = 42$ and $\gamma = 4.5$

Simulation 1: Pinned Membrane

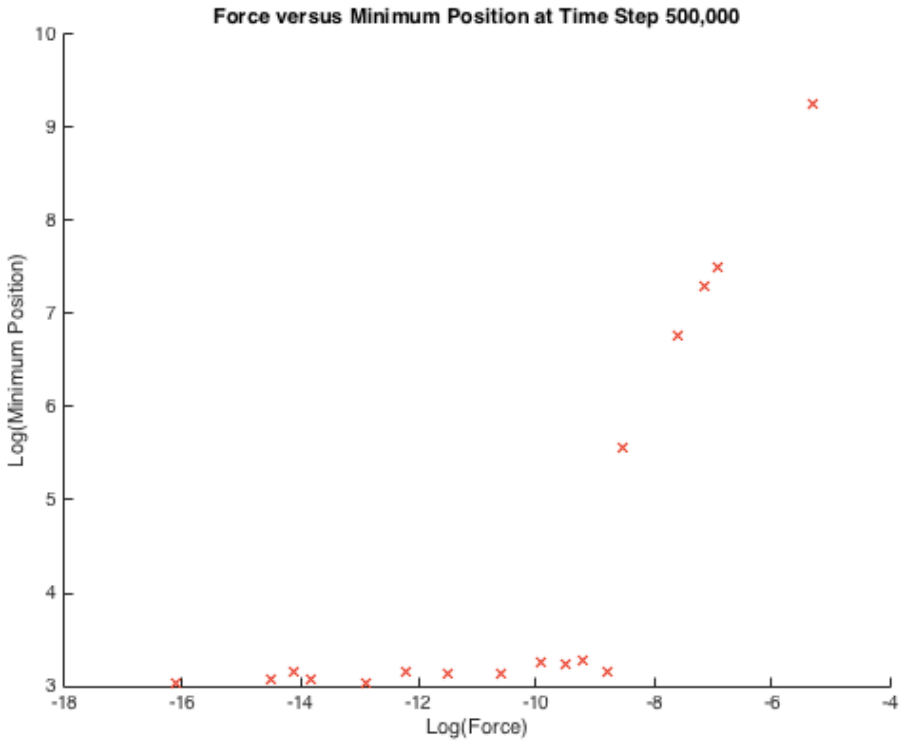
- Pin (fix in place) corners of membrane
- Subject membrane to uniform orthogonal force

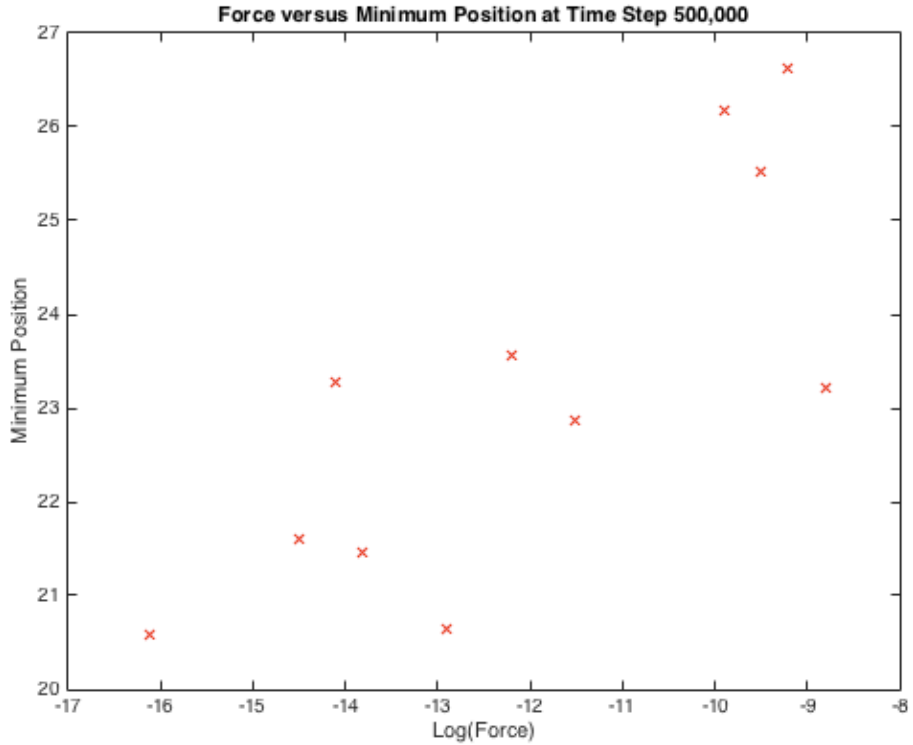
→ What shape is formed?

- Record extent of deflection for different forces

→ At what force does the membrane break?

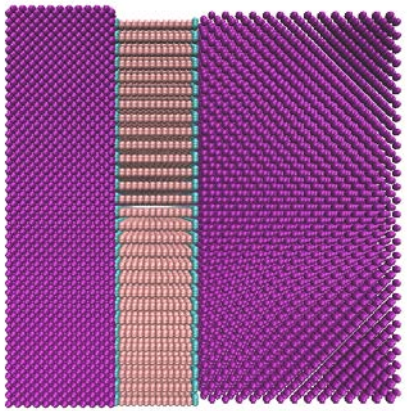
Forces and Membrane Breaking





Simulation 2: Density Difference

Numerical density:
10.0

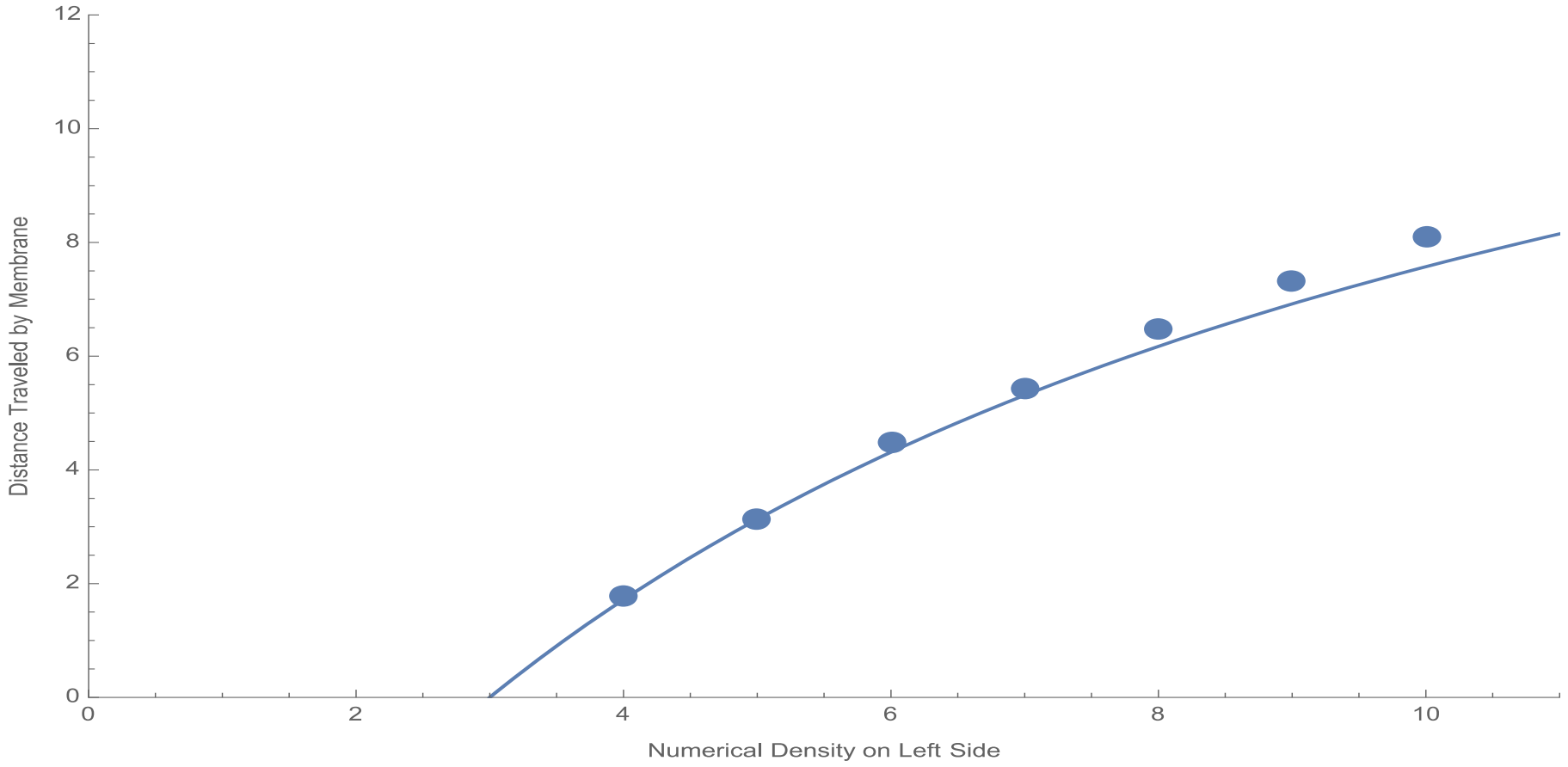


Numerical density:
3.0

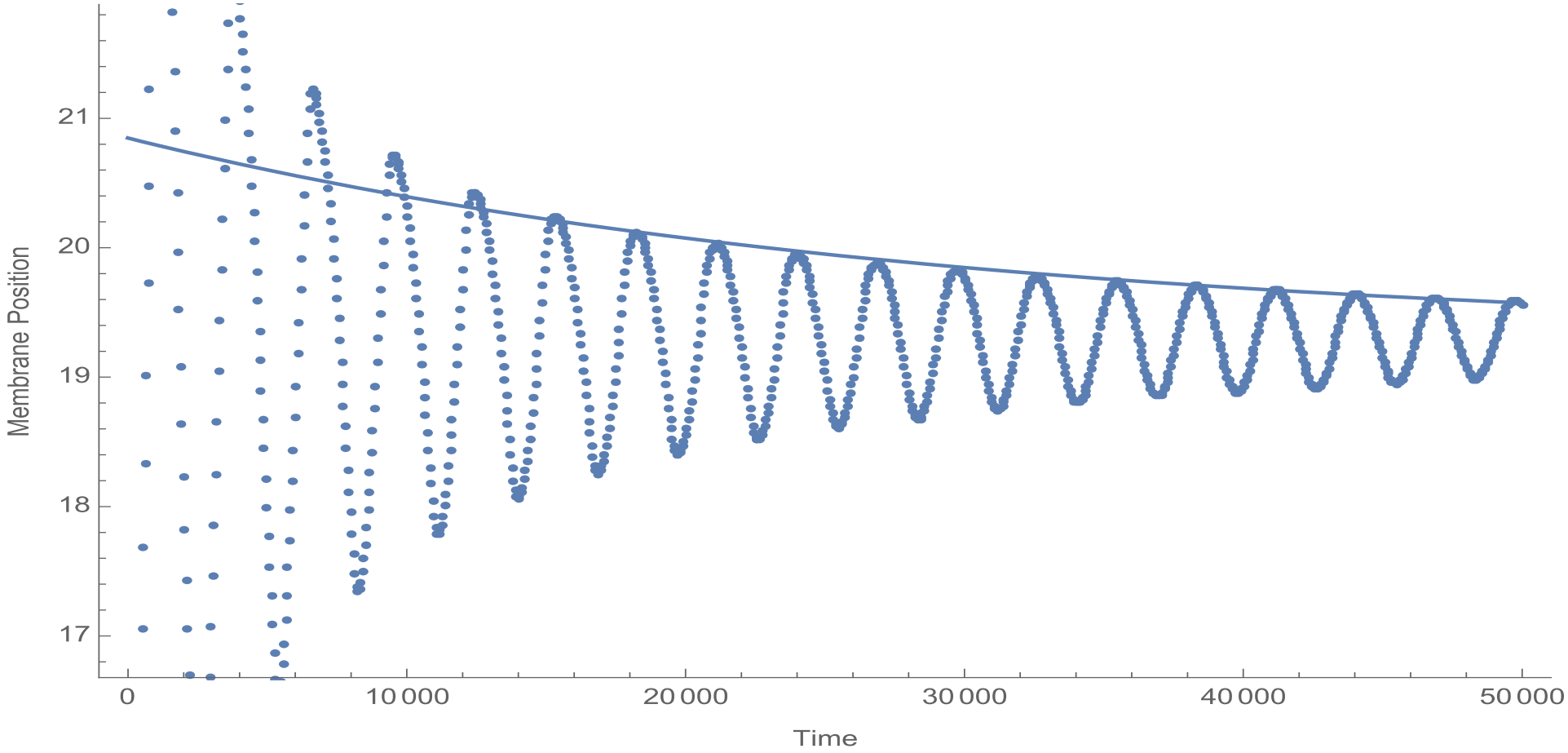
- Increase fluid density on one side of membrane
- Reflecting walls keep sides separate

→ How does the membrane move?

Final Distance Traveled by Membrane



Membrane Position Over Time



Project Recap

Week 1

- MD implemented from scratch in C++
- **Simulation**: Flow in a Pipe

Week 2

- DPD model of a membrane in LAMMPS (*project goal*)
- **Simulation**: Pinned Membrane
- **Simulation**: Density Difference

Thank you for your attention!