

Project 3 Requirements

April 14, 2008

1. Implement the Velocity Verlet integration algorithm to simulate dynamic movement of a system of particles. An RK4 integration method should also be provided for comparison purposes, with an option in the View to select either algorithm for the simulation.
2. Implement the Pair List algorithm for increased efficiency of calculating steric forces between particles. The View should also provide a checkbox option to enable/disable the Pair List optimization during a simulation.
3. Define a force function to simulate the expansion of a closed ring of cell membrane units under pressure, resulting in eventual rupture (breaking of a spring link between elements). The pressure function should cease to be applied after rupture occurs. The ring should contain a minimum of 32 particles.
4. Provide performance and accuracy metrics (displayed in the view):
 - Performance metric: $\frac{(NumParticles)(SimTime)}{WallTime}$
 - Accuracy metric: plot of total kinetic energy of all particles vs. simulation time