Intensive Computation – Homework 4

15th May 2019

Molecular Dynamics

Exercise 1 – Hard sphere model 1D

Write a script that:

- Considers a one-dimensional system with at least 5 particles (mass m=1 and given diameter)
- Simulates the evolution of the system according to the Hard Sphere model, assigning the position and velocity to each particle, and assuming that the motion line is limited by a barrier both on the left and on the right side
- Produces a film of the particles' motion.

Exercise 2 – Hooke model 1D

Write a script that:

- Considers a one-dimensional system with at least 4 particles (mass m=1 and same fixed diameter for all particles, fixed spring length *d*, fixed elastic constant *k*)
- Simulates the evolution of the system according to the Hooke's Law model, using
  1) the solution with Euler method for differential equation
  2) the exact solution obtained by using eigenvalues and eigenvectors
- Produces the graph of the motion of each particle with time on the horizontal axes and particle position on the vertical axis, for both the approximated solution and the exact solution (an example of graph for four particles is shown in Figure 6 page 15 on *Molecular Dynamics* - L. Fosdick)
- Produces a film of the particles' motion.

Exercise 3 – Lennard-Jones model 2D

Write a script that:

- Considers a two-dimensional system consisting of particles (mass m=1 and given diameter)
- Simulates the evolution of the system where the force acting on particles is computed according to the Lennard-Jones model using
  1) Euler method
  2) Verlet method
- Produces a film of the particles' motion for each method, for a comparison.

Exercise 4 (Optional) – Hooke model 2D

Write a script that:

- Considers a two-dimensional system with several particles (mass m=1 and given diameter)
- Simulates the evolution of the system where the force acting on particles is computed according to the Hooke's Law model, by using either the Euler or Verlet method
- Produces a film of the particles motion.

Remark on Hooke Law: interaction among particles is modeled by defining which pairs of particles are connected by a spring, the length *d* of the spring, and the elastic constant *k.*