

MCSC6280: Particle Based Modeling and Simulation

Assignment 2

October 11, 2015

Important Notes

- do your own work
- please submit your material as a single archive file (e.g. *.zip)
- the title of the archive file you submit must contain your last name and the assignment number
- for each question I indicate what material must be submitted; although not explicitly stated, **you must also include a discussion of the results!** (ie, does the result make sense? why or why not?)

1. Microscopic Plinko

Set up a Brownian dynamics simulation of the following system:

- 2D with $L = L_x = L_y = 50$
- 100 non-interacting particles starting at $x = L/2$ and $y = L + 5$
- fixed obstacles with a spacing of 2.5σ between them (σ is the size of the particle) filling space from (0,0) to (50,50). The obstacles should be offset by 1.25 in x and y so that they do not lie right at the borders.
- WCA potential between particles and obstacles
- periodic boundary conditions in x
- a force of -1 in the y direction applied to the particles
- all parameters set to one ($m, \zeta, \epsilon, \sigma$)
- the time step should be 0.005

For $kT = (0, 0.1, 0.2, 0.3, 0.4, 0.5)$, calculate the mean first passage time for the particles to go from the initial position to $y = 0$.

Repeat this for the case of no obstacles.

Plot the MFPT as a function of kT for both cases.

Discuss your results.

For the discussion, it may be very helpful to visualize your simulations via VMD.

Submit:

- your code for the obstacle case
- your plot with both lines
- your discussion of the results