

MCSC6280: Particle Based Modeling and Simulation

Assignment 2

September 29, 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. Langevin Dynamics: Calculating D

- Write a program to perform Langevin dynamics of a single particle in infinite space in **three dimensions**.
- Write a program to calculate the MSD as a function of time. Plot the MSD versus Δt in x , y , and z all on the same plot. Include the exact solution as derived in class. Calculate D in each dimension. Comment on the results. Do this for both i) the overlapping windows method and ii) the no-correlation, no overlapping windows conditions.
- Calculate the total D . Compare to the expected result and comment.
- Run the simulations for at least three different values of the thermal energy kT . Plot D versus kT . Compare to the expected result and comment. From here on out, you can use the no-correlation, no overlapping windows condition to save time.
- Run the simulations for at least three different values of the friction coefficient ζ . Plot D versus ζ . Compare to the expected result and comment.
- Run the simulations for at least three different values of the particle mass m . Plot D versus m . Compare to the expected result and comment.

To be handed in:

- your simulation program
- your program to calculate D
- all D values and plots outlined above
- Your comments on all results.

Notes:

- you can base your program off the program used in class, but note that in that program we assumed a mass of 1!
- it takes a lot of data to get good values for D . Going up to a maximum time of about 1 million integration steps is typical.
- in Langevin Dynamics, diffusion corresponds to the long time limit. Be careful when extracting D from the data!