Tasks labeled by the sign are optional and are worth extra credits.

General information

Contact: zsolt.lazar@ubbcluj.ro
Course website: MS Teams
Assignment: Submitted assignment should be archived folder with its name containing the assignment number and title of the assignment, e.g., `02_Random_walk_part_1`. The folder should be uploaded as a compressed archive containing the student's name, e.g., `Smith_John_02_Random_walk_part_1.zip`.

Requirements

Reports should include:

1. Students name
2. Title
3. Statement of the problem
4. Hypotheses
5. Strategy/method
6. Conclusions
7. Complete compilation/installation/execution instructions. Specifying dependencies are appreciated.
8. Results from demo runs including screen captures of charts, etc. - where it applies - should be included.
9. Detail the parameters used for the demonstrated runs (on the Figures)
10. Describe the environment(s) where the testing was successful (compilers, libraries, environments,...)
11. Have a list of source files attached.

Source code should be readable:

12. properly segmented, consistently indented
13. generously commented (including the description of the approach)
14. self-explanatory naming of variables

All programing tasks have to be implemented in C/C++. Some of the tasks are to be implemented ALSO in a language with vector/matrix operation capabilities like Python or Matlab. These are marked with a P/M sign.
In these cases emphasis is on employing builtin functions of the language and avoiding loops. The algorithms do not have to be fully equivalent to their C variant but rather focusing on simplicity as primary goal.
Difference between the two approaches (C vs. Python/Matlab), if any, together with benefits, drawbacks and limitations should be discussed.
Submission beyond deadline is possible but penalized.

Week 05 - Equilibration of a Brownian-particle

Deadline: 15.05

Consider the one dimensional model of Brownian-particle in a heat bath with a Langevin-type equation of motion

$$m\frac{dv}{dt} = -\mu v + R$$

where μ is the dissipation coefficient, R is a random force acting on the particle. This has a Gaussian distribution with zero mean and $\langle R^2 \rangle = \mu kT/\Delta t$ variance. (Δt is the time resolution)

1. simulate the motion of the particle starting from $x(0) = 0$ with a certain velocity $v(0) = v_0$.

   Hint: m, μ and v_0 can be taken as unity. Use a simple Eulerian method for solving the differential equation

2. show that the equilibrium distribution of the particle's velocity is of Maxwell-Boltzmann type

3. show that it is of Maxwell-Boltzmann type even for non-Gaussian random force, e.g., uniform distribution.

4. find by analytical tools the limits (min&max) of the uniform force distribution that reproduces the same equilibrium Maxwell-Boltzmann distribution as the one obtained from a normally distributed random force.

5. prove the above result by simulation

6. compare the time evolution of the velocity distribution function in the two cases (normal vs. uniform distribution of random force)

7. add a harmonic external force and study the dependence of the energy on the temperature (+10%)

8. use a double-well type of external potential ($U(x) = ax^4 - bx^2$) and study the behaviour of the dynamics at different temperatures (+10%)