MSDM 5003 Homework 2 Hints

1. For the purpose of this homework, it suffices to use first order numerical schemes, such as Euler's method, for solving the differential equations. A brief overview on Euler's method is given in Appendix A. Other numerical schemes are equally acceptable for the purpose of this homework. You are reminded that Prof Qian discussed during lecture how to obtain the value of ζ at each time instance from a normally distributed random variable depending on the time discretisation.

   (a) You are free to choose the initial condition, that is the value of $x(0)$, for your simulation as the problem displays translational symmetry. However, with the foresight that the mean square displacement ensemble average $\langle [x(t) - x(0)]^2 \rangle$ is sought, it is clearly advantageous to choose $x(0) = 0$.

   (b) You are reminded that the long-term behaviour of the particle is sought and so you have to dedicate a certain time interval at the beginning of your simulation as a transient run. Moreover, since the PDF sought is stationary, instead of repeating the simulation for an ensemble of particles, it suffices to follow the trajectory of a single particle, so long as the trajectory is monitored at uniform time intervals. This view point is advisable because for the simulation of every different particle, a separate transient run is required.

Appendix A Euler's method

In this homework, you are required to solve ordinary differential equations (ODEs) numerically. In case you have not come across numerical methods for solving ODEs, a brief overview on Euler's method is given here for your reference. Error analysis is included for completeness only and is **NOT** required for the purpose of this homework.

The general form of a first order ODE is

$$\frac{dx}{dt} = f(x,t). \tag{1}$$

The goal is to obtain the solution $x(t)$ as a function of t for a certain function $f(x,t)$ of x and t. Consider the Taylor expansion of the solution $x(t)$ about t:

$$x(t+h) = x(t) + h\left.\frac{dx}{dt}\right|_{t=t} + \frac{1}{2}h^2\left.\frac{d^2x}{dt^2}\right|_{t=t} + O\left(h^3\right). \tag{2}$$

For a small step h, it is justified to keep the Taylor series up to first order in h only. Ignoring terms of degree greater than 1 in h in Eq. (2) and bringing in Eq. (1), we have

$$x(t+h) \approx x(t) + hf(x,t). \tag{3}$$

If the value $x(t_o)$ for x at a particular $t = t_o$ is known, Eq. (3) can be applied iteratively to obtain the values $x(t_o+h)$, $x(t_o+2h)$, $x(t_o+3h)$, *ad infinitum*, one after another. Clearly, by using Eq. (3), the error up to leading order incurred from a *single step* is

$$\frac{1}{2}h^2\left.\frac{d^2x}{dt^2}\right|_{t=t_o} = \frac{1}{2}h^2\left.\frac{df}{dt}\right|_{t=t_o}. \tag{4}$$

If x is evolved from $t = a$ to $t = a + Nh = b$ in N steps, with step size $h = (b-a)/N$, the error accumulated up to leading order is

$$\sum_{k=0}^{N-1}\frac{1}{2}h^2\left.\frac{df}{dt}\right|_{t=a+kh} = \frac{h}{2}\left(\sum_{k=0}^{N-1}\left.\frac{df}{dt}\right|_{t=a+kh}h\right) \approx \frac{h}{2}\left(\int_a^b\frac{df}{dt}\,dt\right) = \frac{h}{2}\left\{f[x(b),b] - f[x(a),a]\right\}. \tag{5}$$

In conclusion, Euler's method leads to an error of order h^2 for a *single step* but a *total* error of order h.