PHYS 511: Computational Modeling and Simulation - Fall 2018
Assignment #3, due Friday November 23, before class

Random walks and OpenMP

In the free atmosphere (far away from the ground surface, where the conditions of homogeneous and isotropic turbulence can be accepted) dispersion of aerosol particles in 2D can be described by the following equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} K \frac{\partial C}{\partial x} + \frac{\partial}{\partial y} K \frac{\partial C}{\partial y} \tag{1}$$

where $C(x, y)$ is the concentration of aerosol particles and $K(x, y)$ is dispersion coefficient.

Under certain conditions equation (1) is equivalent to a system of stochastic differential equations

$$\begin{cases} \frac{\partial X(t)}{\partial t} = \sqrt{2K}\, W_x(t) \\ \frac{\partial Y(t)}{\partial t} = \sqrt{2K}\, W_y(t) \end{cases} \tag{2}$$

where $X(t)$ and $Y(t)$ are the coordinates of an aerosol particle and $W_x(t)$ and $W_y(t)$ are independent δ-correlated Gaussian stochastic/random processes. The equivalence of (1) and (2) means that the probability distribution function of the stochastic/random vector process $\{X(t), Y(t)\}$ is described by means of (1). System (2) can be written in a mathematically more correct form

$$\begin{cases} X(t + \Delta t) = X(t) + \sqrt{2K\Delta t}\, \Omega_x \\ Y(t + \Delta t) = Y(t) + \sqrt{2K\Delta t}\, \Omega_y \end{cases} \tag{3}$$

where Ω_x and Ω_y are independent Gaussian random variables with mean value 0 and standard deviation 1.

Given initial condition, we can simulate the propagation of an aerosol particle through a random walk. When the number of particles is large we can then visualize the process of atmospheric dispersion.

It should be noted that if the number of steps is large and Δt is small enough then the normal distribution can be replaced with a uniform distribution in the interval $[-\sqrt{3}, \sqrt{3}]$, which has a standard deviation 1.

1. Write a Fortran program that simulates a random walk of $N = 10000$ particles. Initially, all particles are placed at the origin, i.e. $X_i(t = 0) = 0$ and $Y_i(t = 0) = 0$. You should perform $N_s = 5000$ steps with $\Delta t = 10$ sec. To make things a little more interesting let us use K value that is not constant, but a function of coordinates. Stricly speaking, when K is not constant, equations (3) must be modified, but under certain conditions they still remain accurate enough. Let us use the following expression for it: $K(x, y) = 10 \exp(-(x/100)^2 - (y/100)^2)$ [m^2/sec]

2. At the end of the simulation have your program store the coordinates of all particles in a file (each pair $\{X_i, Y_i\}$ in a separate line). Then using this data file, make a scatter plot of the resulting distribution. Make sure it looks meaningful. Briefly comment on the distribution in the report. Does it look as you expected?

3. Parallelize your code using OpenMP. Make sure it works as expected and compile it with the highest optimization level. Run calculations and measure the execution time using 1,2,4, and 8 threads. Is there any improvement? Include these timings in your report and comment on your findings.

4. Upload your files to subdirectory `as3` in your google drive directory shared with the instructor. Files to be submitted: `as3.f90` (program source), `report.txt`, and `positions.png` (scatter plot of final positions). You can also submit your gnuplot script if you wish (assuming that you used gnuplot for plotting).