

Exercise 5 FYSA120 C++ numerical programming Winter 2015

PROJECT

Email the *commented* solution code (*.cpp, *hpp) as attachments to : fysy160(at)gmail.com Subject line: Project

1. Write a C++ program to simulate one-dimensional diffusion. The set of discrete points extends $-L < x < L$, so if there are M points, the lattice step is $h = 2L/M$. The constants are $L = 50$, $M = 100$, diffusion constant $D = 1$. The time step is $\tau = ch^2/(2D)$, where c is read from the console.

First, write the function `init()` that puts a gaussian (normal) distribution of particles around $x_0 = 0$, with width $\sigma = L/30$. The density in point i is initially

$$\rho_i = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-x_0)^2}{2\sigma^2}}; \quad (1)$$

Next, write a function `evolve()` that updates the density. Turning on diffusion, the density evolves to the next time step as

$$\rho_i(t + \tau) = \rho_i(t) + \frac{D\tau}{h^2}(\rho_{i+1}(t) - 2\rho_i(t) + \rho_{i-1}(t)) , \quad (2)$$

where the second derivative was discretized according to

$$\rho_i''(t) \approx \frac{1}{h^2}(\rho_{i+1}(t) - 2\rho_i(t) + \rho_{i-1}(t)) . \quad (3)$$

Using a sufficiently small but positive c , store the density at suitable times to file `density.dat` in format “time point density”. If you like, plot it using, say, `gnuplot` (start `gnuplot`, type `sp 'density.dat' w pm3d`). Don't write density to file at all times, it's too much.

I suggest you store the density profile in `std::vector<double> rho`. If you wish, try any initial density profile you like. Notice that eventually particles will diffuse out of your simulation box.