

## Exercise 7 FYSY160 C++ numeerinen ohjelmointi Autumn 2011

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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  $\tau = ch^2/(2D)$ , where  $c$  is read from the console.

First, write function `init()`, that puts a Gaussian 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  $c \ll 1$ , 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 have the density profile stored as `vector<double> rho`. If you wish, try any initial density profile you like are welcome. Be ware, that eventually particles diffuse out of your simulation box.