Computational Science 1

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Seminar
Exercises

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Exercise 9 (10.1.2013):

Normal modes and waves

from ***An Introduction to Computer Simulation Methods***,
Chapter 9, Problems 9.2-4,6,7

a) Modify the `Oscillators` class to solve the dynamical equations of motion by implementing the `ODE` interface. Choose units such that the ratio $k/m = 1$. Use an algorithm that is well suited to oscillatory problems. Compare the numerical and the analytical solution for $N = 10$.

b) Use the initial values of u_j so that the system is in one of its normal modes. Consider the normal modes with $n = 3$ and $n = 8$. Set the initial velocities equal to zero. Describe the displacement of the particles. Is the motion of each particle periodic in time? What is the period? Does the system remain in a normal mode indefinitely? Finally, choose the initial particle displacements equal to random values between -0.5 and $+0.5$. Is the motion of each particle periodic in this case?

c) Modify your program so that periodic boundary conditions (BC) are used. Choose the initial condition corresponding to the normal mode $n = 2$. Does this initial condition yield a normal mode solution for periodic BC? For fixed BC there are $N + 1$ springs, but for periodic BC there are N springs. Why? Choose the initial condition corresponding to the $n = 2$ normal mode, but replace q_n adequately. Does this initial condition correspond to a normal mode? Now try $n = 3$, and other values of n. Which values of n give normal modes?

   Modify your program so that free BC are used, which means that the masses at the end points are connected to only one nearest neighbor. A simple way to implement these BC is to set $u_0 = u_1$ and $u_N = u_{N+1}$. Use the initial condition corresponding to the $n = 3$ normal mode found using fixed BC. Does this condition correspond to a normal mode for free BC? Is $n = 2$ a normal mode for free BC? Are the normal modes purely sinusoidal?

   Choose free BC. Let the initial condition be a pulse of the form, $u_1 = 0.2$, $u_2 = 0.6$, $u_3 = 1.0$, $u_4 = 0.6$, $u_5 = 0.2$, and all other $u_j = 0$. After the pulse reaches the right end, what is the phase of the reflected pulse, that is, are the displacements in the reflected pulse in the same direction as the incoming pulse (a phase shift of zero degrees) or in the opposite direction (a phase shift of 180 degrees)? What happens for fixed BC?