Computational Science 1

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Seminar
Exercises

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Exercise 10 (17.1.2013):

Localization due to defects

from ***An Introduction to Computer Simulation Methods***,
Chapter 9, Problems 9.22

a) Modify your program developed in Exercise 9 so that the mass of **one** oscillator is equal to one fourth that of the others. Set $N = 20$ and use fixed boundary conditions. Compute the power spectrum over a time $T = 51.2$ using random initial displacements between -0.5 and $+0.5$ and zero initial velocities. Sample the data at intervals of $\Delta = 0.1$ which corresponds to a Nyquist frequency of $\omega_Q = \pi/\Delta \approx 31.4$. The normal mode frequencies correspond to the well-defined peaks in $P(\omega)$. Consider at least three different sets of random initial displacements to insure that you find all the normal mode frequencies.

b) Apply an external force $F_e = 0.3 \sin \omega t$ to each particle. (The steady state behavior occurs sooner if we apply an external force to each particle instead of just one particle.) Because the external force pumps energy into the system, it is necessary to add a damping force to prevent the oscillator displacements from becoming too large. Add a damping force equal to $-\gamma v_i$ to all the oscillators with $\gamma = 0.1$. Choose random initial displacements and zero initial velocities and use the frequencies found in part (a) as the driving frequencies ω. Describe the motion of the particles. Is the system driven to a normal mode? Take a "snapshot" of the particle displacements after the system has run for a sufficiently long time so that the patterns repeat themselves. Are the particle displacements simple sinusoidal functions? Sketch the approximate normal mode patterns for each normal mode frequency. Which of the modes appear localized and which modes appear to be extended? What is the approximate cutoff frequency that separates the localized from the extended modes?