Department of Applied Physics, Chalmers, Göteborg
Göran Wahnström, Joakim Nyman, Anders Lindman 2014-11-04

E2 Fermi-Pasta-Ulam problem

You will here consider the Fermi-Pasta-Ulam problem, a simple model for non-linear dynamics. This exercise will also serve as an introduction to `C`.

The Fermi-Pasta-Ulam model consists of a one-dimensional chain of masses connected with non-linear springs. The so called α-model is defined by the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=0}^{N} \left[\frac{\kappa}{2}(u_{i+1} - u_i)^2 + \frac{\alpha}{3}(u_{i+1} - u_i)^3 \right]$$

where m is the mass of the particles, u_i the displacement of particle i from its equilibrium position, and $p_i \equiv mv_i$ the corresponding momentum. The harmonic force constant is denoted by κ and α is a measure of the anharmonic coupling strength. The boundary conditions are $u_0 = u_{N+1} = 0$. In the harmonic case, with linear springs only ($\alpha = 0$), the solution can be written in terms of normal modes Q_k and P_k, according to

$$Q_k = \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} \sqrt{m} u_i \sin\left(\frac{ik\pi}{N+1}\right), \quad k = 1, \ldots, N$$

$$P_k = \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} \sqrt{m} v_i \sin\left(\frac{ik\pi}{N+1}\right), \quad k = 1, \ldots, N$$

and the total energy is the sum of the energies in the different modes

$$E_{tot} = \sum_{k=1}^{N} E_k = \frac{1}{2} \sum_{k=1}^{N} \left[P_k^2 + \omega_k^2 Q_k^2 \right]$$

where

$$\omega_k = 2\sqrt{\frac{\kappa}{m}} \sin \frac{k\pi}{2(N+1)}$$

The inverse transforms are

$$u_i = \sqrt{\frac{2}{N+1}} \sum_{k=1}^{N} \frac{Q_k}{\sqrt{m}} \sin\left(\frac{ik\pi}{N+1}\right), \quad i = 1, \ldots, N$$

$$v_i = \sqrt{\frac{2}{N+1}} \sum_{k=1}^{N} \frac{P_k}{\sqrt{m}} \sin\left(\frac{ik\pi}{N+1}\right), \quad i = 1, \ldots, N$$

In the non-linear case, with $\alpha \neq 0$, the solution is not known and the use of computer simulations becomes indispensable, as realized by Fermi *et al*[1]. The total energy is no longer exactly given by the sum of the energies in the different modes.

[1] A link to a PDF containing the original research article can be found on the FPU page on Wikipedia: `http://en.wikipedia.org/wiki/Fermi-Pasta-Ulam_problem`

Fermi *et al.* argued that for weak anharmonicity one expect to get equipartition of the energy among the various modes.

For the present system it is customary to use the units m=a=τ=1, where a is the equilibrium length of the springs and $\tau^{-1} = \sqrt{\kappa/m}$.

Task

1. Write a C program that solves harmonic FPU problem, with $\alpha = 0$. This problem is similar to the one studied in the fourth task of E1. Assume that all energy is initially localized in mode $k = 1$, i.e. $E_k(t = 0) = E_0\ \delta_{1k}$, and only kinetic, i.e. $P_k = \sqrt{2E_0}\ \delta_{1k}$ and $Q_k = 0\ \forall k$. Consider the case $N = 32$ and assume $E_0 = N$. On the homepage you find a C program (`E2.c`) that gives some hints regarding the transformation between u and Q as well as v and P.

   Perform a simulation with the time-step $\Delta t = 0.1$ for the time-span $t_{max} = 25000$. Plot $E_k(t),\ k = 1, 2, ..., 5$. Verify that $E_k(t) = E_k(0)$, i.e. no energy exchange takes place among the modes. (1p)

2. You should now consider the anharmonic FPU problem. Introduce the non-linear spring coupling and study the two cases $\alpha = 0.01$ and $\alpha = 0.1$. Use the same setup as in the previous task and present your results in the same way. In this case you should obtain energy exchange between the different modes. (2p)

3. Consider again the non-linear case with $\alpha = 0.01$ and $\alpha = 0.1$, but now consider a considerably longer time-span, $t_{max} = 10^6$. In this case it becomes time-consuming to evaluate and save the energy in the various modes at each time-step and the output file becomes very large. Therefore, modify the C program so that the energy is calculated and saved to file only once for each 1000 time-steps. Determine the mode energies $E_k(t)$ at the corresponding times, i.e. at

   $$t_n = 1000 n \Delta t, \quad n = 1, 2, \dots$$

   Compute the time-average of the mode energies

   $$\bar{E}_k(t) = \frac{1}{t} \int_0^t dt'\ E_k(t')$$

   Plot your results for $\bar{E}_k(t)$ for all 32 modes with logarithmic scale for both axis. Do you obtain equipartition of the energy? (1p)