Computational Physics II 5640 Spring 2018

Project Assignment 3

Due: Wednesday April 11

Fermi-Pasta-Ulam-Tsingou nonlinear lattice. Use velocity-verlet integration to study the famous Fermi-Pasta-Ulam-Tsingou (FPUT) nonlinear chain problem. Consider $N+2$ particles with a mass m arranged in a one-dimensional lattice shown in Fig. 1. The particles can move in one dimension and are coupled by nonlinear springs. At equilibrium, the spacing between neighboring particles is a (lattice constant), and we use u_n to denote the relative displacement of the n-th particle with respect to the equilibrium position; the instantaneous position is then $X_n(t) = na + u_n(t)$. In this assignment, we consider a chain with fixed ends, i.e. $u_0 = u_{N+1} = 0$ for all t; only the N particles in the middle are movable. Their dynamics is governed by the following nonlinear equation:

$$m\,\ddot{u}_n = k(u_{n+1} + u_{n-1} - 2u_n) + \alpha\left[(u_{n+1} - u_n)^2 - (u_n - u_{n-1})^2\right], \tag{1}$$

where dot means time derivative, k is the linear spring constant, and α is a parameter characterizing the strength of nonlinearity. The chain with the above quadratic nonlinear interaction is called the PFU-α model. A similar model with cubic nonlinear interaction is called FPU-β model.

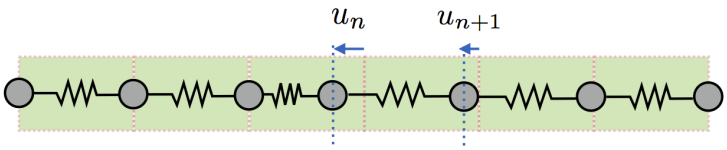

Figure 1: Schematic diagram of the FPU model.

(1) First consider the linear chain problem with $\alpha = 0$. Show that the normal modes of the chain are standing waves with wavevector $q = m\pi/(N+1)$. Specifically, the normalized normal modes and the corresponding eigen-frequencies are

$$\xi_n^{(m)} = \sqrt{\frac{2}{N+1}}\sin\left(\frac{mn\pi}{N+1}\right), \qquad \omega^{(m)} = 2\sqrt{\frac{k}{m}}\sin\left(\frac{m\pi}{2(N+1)}\right). \tag{2}$$

(2) Implement the Velocity-Verlet algorithm to solve the FPU chain. As a test of the code, first simulate the dynamical evolution of the linear chain ($\alpha = 0$) by exciting only the fundamental mode $m = 1$. More specifically, use the following as the initial conditions: $u_n(t=0) = \mathcal{A}\,\xi_n^{(1)}$, and $\dot{u}_n(t=0) = 0$; here $\mathcal{A}$ is some constant characterizing the strength of the initial perturbation. Plot the kinetic energy and potential energy as a function of time; see Fig. (2). The two energies are defined as follows for linear FPU chain:

$$E_K = \sum_{n=1}^{N}\frac{m\,\dot{u}_n^2}{2}, \qquad E_P = \sum_{n=0}^{N}\frac{k}{2}(u_{n+1} - u_n)^2, \tag{3}$$

These two energies oscillate with a period $\pi/\omega^{(1)}$. On larger scales, the total energy $E_{\rm tot} = E_K + E_P$ should remain constant if the Verlet algorithm is correctly implemented. At small scales; see Fig. 2 (right), the energy is not exactly conserved. The error $|E_0 - E|/E_0$ is of order 10^{-6}, where $E_0 = E(t = 0)$. The error oscillates with the same period as E_K, E_P. Verify the δt^2 scaling of the errors by plotting the error at $t = \pi/(2\omega^{(1)})$ (where the maximum error occurs) versus the discrete time step δt used in the Verlet algorithm; see Fig. 3.

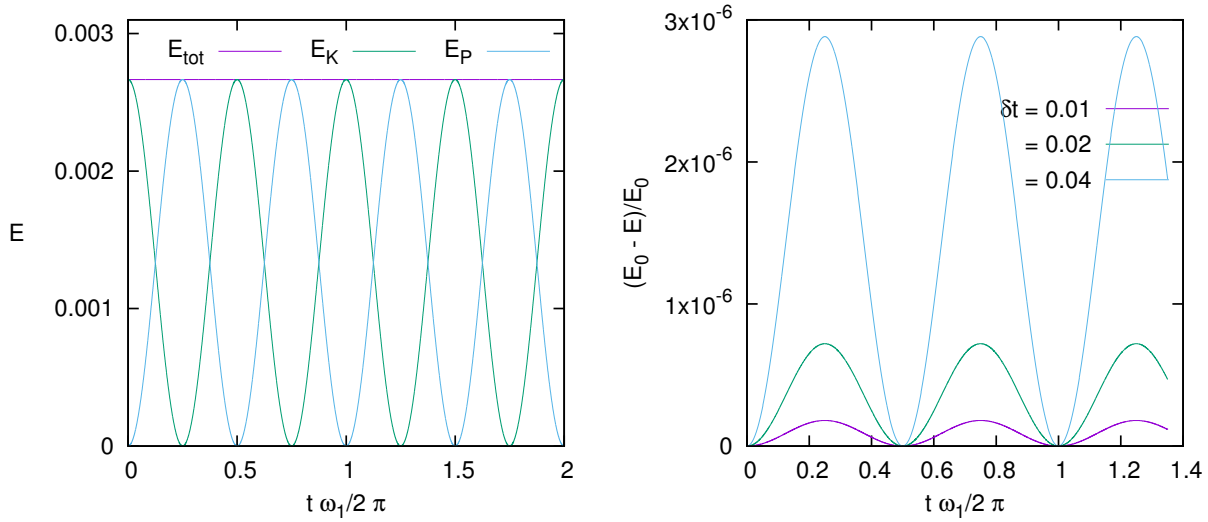

Figure 2: (Left) The total energy, as well as kinetic and potential energy vs time. (Right) The error of the total energy $(E_0 - E)/E_0$ vs time for different size of time step δt. In these simulations, $m = k = 1$, $\alpha = 0$, $N = 36$, and the initial perturbation $\mathcal{A} = 0.2$.

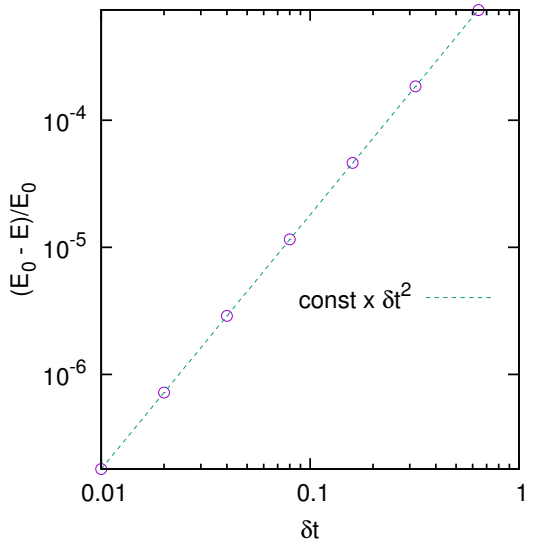

Figure 3: Scaling of the error (energy) with the time step δt for velocity Verlet algorithm.

(3) Next we excite the linear chain with some localized perturbations. Specifically, we use the following initial conditions: $u_n(t=0) = 0$, and $\dot{u}_n(t=0) = \mathcal{B}\exp\left[\frac{-(n-L/2)^2}{\sigma_0^2}\right]$, where $\mathcal{B}$ is a constant and σ_0 characterizes the width of the local perturbation. To investigate how the energy spreads over the system, we first define a local energy:

$$E(n) = \frac{m\dot{u}_n^2}{2} + \frac{k}{4}\left[(u_{n+1}-u_n)^2 + (u_n - u_{n-1})^2\right]. \tag{4}$$

This is basically the kinetic energy of n-th particle and sum of half the potential energy of the two springs connected to this particle. Run the simulation and plot the $E(n)$ vs n at different simulation time t; see Fig. 4 for an example. The initial perturbation splits into two fronts propagating in opposite directions with a velocity $v \sim \sqrt{k/m}$. You are encouraged to investigate how the energy spreads in a nonlinear FPU chain ($\alpha \neq 0$) (extra credit).

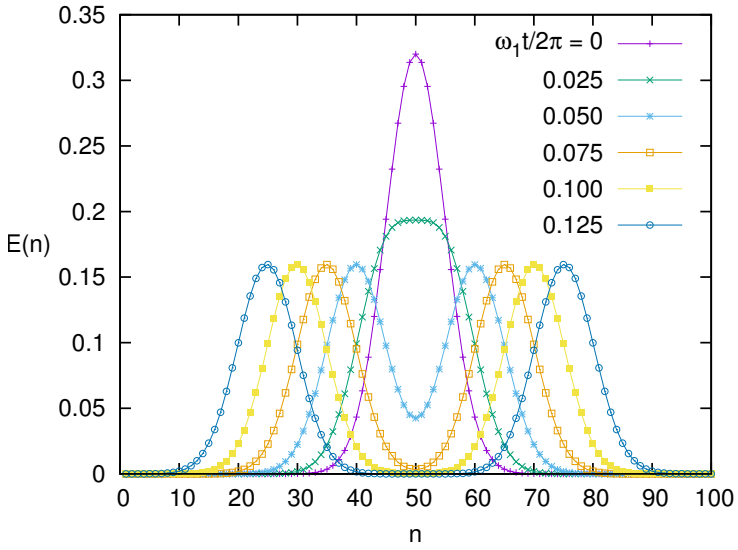

Figure 4: Distribution of local energy $E(n)$ at different simulation times. Parameters used in the simulations are: $m = k = 1$, $\delta t = 0.04$, $\mathcal{B} = 0.8$, $\sigma_0 = 10$, and $N = 100$.

(4) We now consider the energy distribution in nonlinear FPU chain. We again excite only the fundamental $m = 1$ mode of the chain at $t = 0$. Run the simulations and plot the energy of the first few normal modes as a function of simulation time t; see Fig. 5. To compute the mode energy, first we decompose the displacement $\{u_n\}$ into the normal modes $u_n(t) = \sum_{m=1}^{N} Q_m(t)\xi_n^{(m)}$. The mode amplitude can be computed as

$$Q_m(t) = \sum_{n=1}^{N} u_n(t)\,\xi_n^{(m)} = \sqrt{\frac{2}{N+1}}\sum_{n=1}^{N} u_n(t)\sin\left(\frac{mn\pi}{N+1}\right). \tag{5}$$

The energy stored in m-th mode is then

$$E_m(t) = \frac{m}{2}\left[\dot{Q}_m^2 + (\omega^{(m)})^2\, Q_m^2\right]. \tag{6}$$

At $t = 0$, all energy is contained in the fundamental mode $m = 1$, consistent with our initial condition. We then expect the energy will slowly drifted to other modes, until the equipartition of energy, a consequence of ergodicity, would have been reached. This is indeed the case at the initial stage of the time evolution, as $Q_1(t)$ decays while other higher-energy modes gain energy. However, after some longer time $t_{\rm return} \sim 120(2\pi/\omega_1)$, most of the energy returns to the initial $m = 1$ mode. Verify this behavior in your simulations. You are also encouraged to study how the returning time depends on the nonlinear parameter.

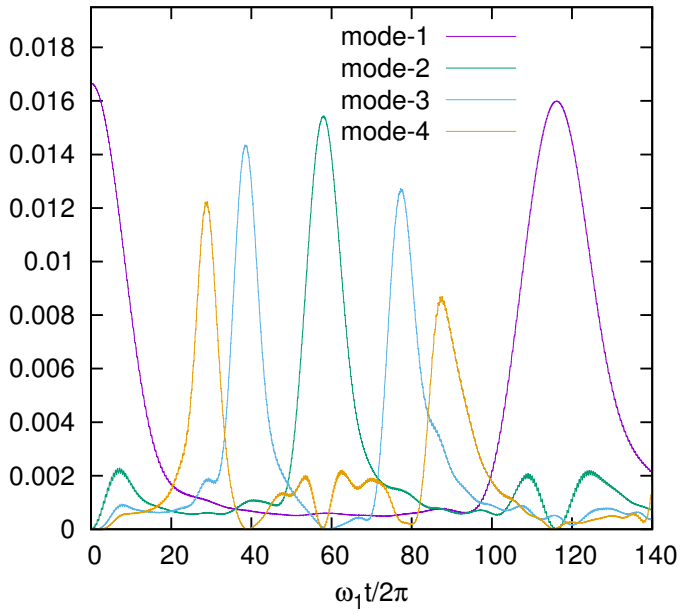

Figure 5: Mode energy E_m as a function of time showing the recurrence behavior. Parameters used are $m = k = 1$, $\alpha = 1.25$, $\delta t = 0.02$, $\mathcal{A} = 0.5$, $N = 36$.