Computational Physics II 5640, Spring 2017

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1 Fermi-Pasta-Ulam nonlinear lattice

1.1 Introduction

The Fermi-Pasta-Ulam (FPU) lattice is a non-linear system of a string of $N+2$ masses connected by springs, with the masses on either end fixed. This system gives dynamics governed by the force 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 k is the spring constant and α is the strength of the non-linearity. The set $\{u_i\}$ is the displacement vector, i.e. the distance a mass is displaced from its own minimum potential. Where as the set $\{\dot{u}_i\}$ is the velocity vector of the system. This is the so-called FPU-α model, as it only has a quadratic term. We will solve the behavior of the FPU-α system using the Velocity-Verlet Method.

The VV method is simple. Starting with an initial $\{u_i\}$, and $\{\dot{u}_i\}$, we can simulate the time evolution of a system by updating these vectors in systematic fixed time steps. The first step is to update $\{u_i\}$ by:

$$u_n^{t+1} = u_n^t + \dot{u}_n^t\delta t + \frac{1}{2}\ddot{u}_n^t\delta t^2 \tag{2}$$

where t is the time step index and δt is the length of the time step. We do this for all n before we update $\{\dot{u}_i\}$ by:

$$\dot{u}_n^{t+1} = \dot{u}_n^t + \frac{1}{2}(\ddot{u}_n^t + \ddot{u}_n^{t+1})\delta t \tag{3}$$

by repeating these steps for many time steps the system vectors will evolve in time. This is how we simulate the FPU lattice.

1.2 Energy Conservation

The first thing we need to do is test our code for the linear case. We expect a harmonic oscillator to support standing wave solutions as:

$$\ddot{u}(n) = \frac{k}{m}u(n) \tag{4}$$

supports the solution

$$u(n) = A\sin\left(\sqrt{\frac{k}{m}}n\right) + B\cos\left(\sqrt{\frac{k}{m}}n\right), \tag{5}$$

but as the lattice is fixed at both ends we know B must be equal to 0. We follow from here to the traditional solution that the FPU linear lattice must have normal eigen modes and frequencies:

$$\xi^m = \sqrt{\frac{2}{N+1}}\sin\left(\frac{mn\pi}{N+1}\right), \quad \omega_n^m = 2\sqrt{\frac{k}{m}}\sin\left(\frac{m\pi}{2(N+1)}\right). \tag{6}$$

We have everything we need to test that our method conserves energy. We will start with initial conditions:

$$u_n^{t=0} = \mathcal{A}\xi_n^1, \quad \dot{u}_n^{t=0} = 0, \tag{7}$$

where we have exited the first mode with amplitude $\mathcal{A}$. We then use our VV algorithm to evolve the system in time, plotting the kinetic and potential energy, as well as their sum as a function of time, where the kinetic energy and potential energy are equal to

$$E_K = \sum_{n=1}^{N}\frac{m\dot{u}_n^2}{2}, \quad E_p = \sum_{n=0}^{N}\frac{k}{2}(u_{n+1} - u_n)^2. \tag{8}$$

We can see from figure 1(a) that energy is nicely conserved, but there is some error, given by $|E_0 - E|/E_0$, where $E_0 = E(t=0)$. The error oscillates with the same period as the energies and after doing our simulation for several values of δt we find it has a scaling like δt^2 which can be seen in figure 2.

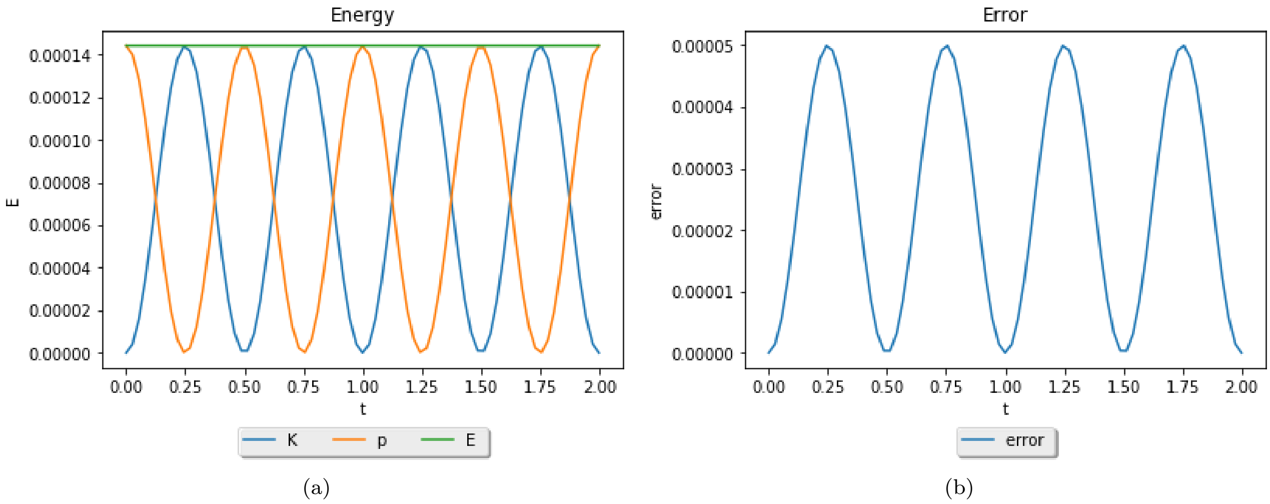


Figure 1: Note, Time axis in units of $\frac{\omega^1}{2\pi}$. $m = k = 1$, $\alpha = 0$, $N = 36$, and $\mathcal{A} = 0.2$.

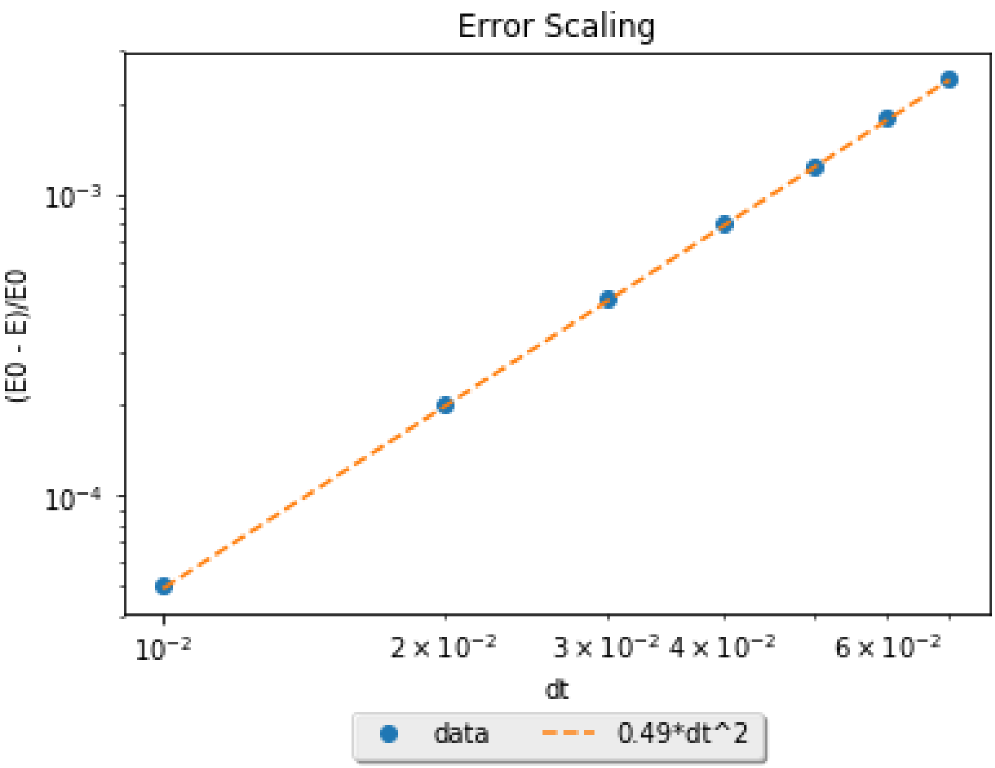


Figure 2: $m = k = 1$, $\alpha = 0$, $N = 36$, and $\mathcal{A} = 0.2$.

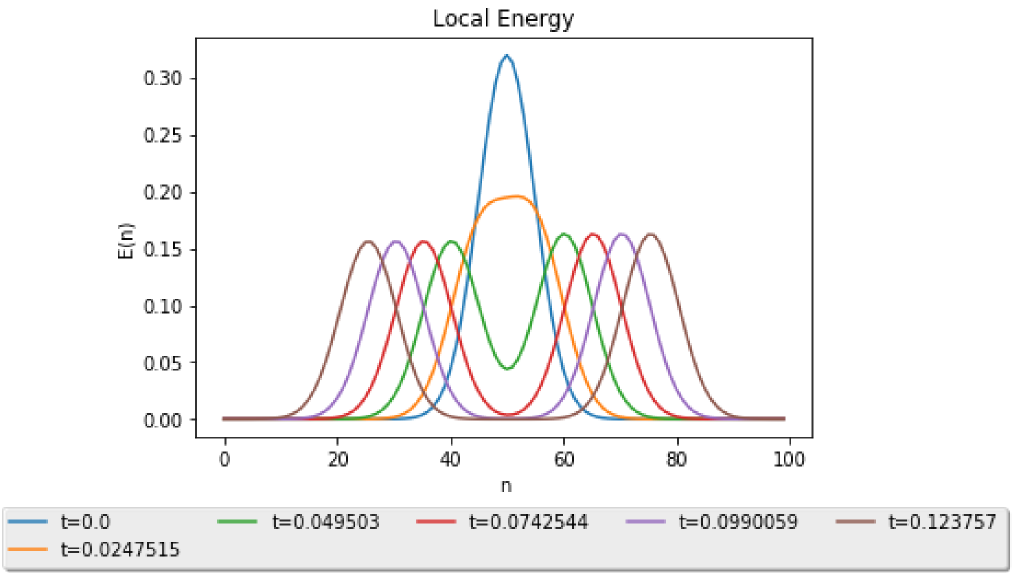


Figure 3: Note, Time axis in units of $\frac{\omega^1}{2\pi}$. $m = k = 1$, $\delta t = 0.04$, $\alpha = 0$, $N = 100$, $\mathcal{B} = 0.8$, and $\sigma_0 = 10$.

1.3 Energy Location

Next we want to see where the energy lives and goes within the lattice. To do so we define a local energy:

$$E_n = \frac{m\dot{u}_n^2}{2} + \frac{k}{4}\left[(u_{n+1} - u_n)^2 + (u_n - u_{n-1})^2\right]. \tag{9}$$

We start with an initial perturbation:

$$u_n^{t=0} = 0, \quad \dot{u}_n^{t=0} = \mathcal{B}exp\left[\frac{-(n - L/2)^2}{\sigma_0^2}\right], \tag{10}$$

where $\mathcal{B}$ is the amplitude and σ_0 the width of the initial perturbation. We expect from these initial conditions for the energy to start as a pulse that spreads to the edges with velocity $\approx \sqrt{k/m}$, which is what we see in figure 3.

From here we can study how α affects the evolution of the local energy. In figure 4 we can see how α affects the balance of the energy as it spreads, and if it gets too high, as seen in figure 4(c), we get a shockwave.

1.4 Mode Energy

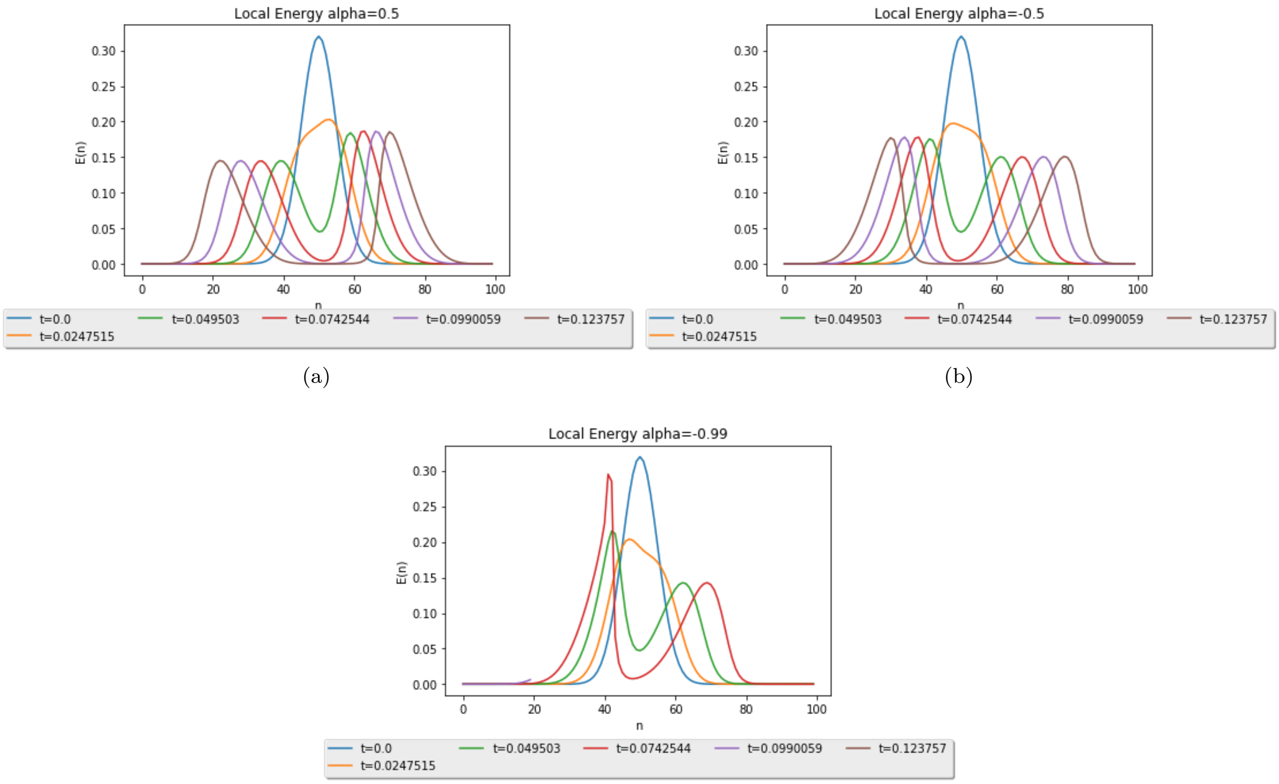
The last thing we want to check is how the energy is shared with the various eigenmodes. The first step is to note that the displacement can be written as a sum of the normal modes, $u_n^t = \sum_{m=1}^{N} Q_m^t \xi_n^m$. We can then do a flip and get:

$$Q_m^t = \sum_{n=1}^{N} u_n^t \xi_n^m = \sqrt{\frac{2}{N+1}} \sum_{n=1}^{N} u_n^t \sin\left(\frac{mn\pi}{N+1}\right). \tag{11}$$

Therefore the energy of the m-th mode is:

$$E_m^t = \frac{m}{2}\left[\dot{Q}_m^2 + (\omega^m)^2 Q_m^2\right]. \tag{12}$$

We then see how the energy, starting entirely in mode 1, is shared in time. We reuse the initial conditions from equation 7, and evolve the system in time keeping track of E_m for the first four modes. We can see from figure 5 that the energy leaves mode 1, but then around $t \approx 120(2\pi/\omega_1)$ we get a return to mode 1. This is to be expected and we can see from figure 6 that this behavior is entirely dependant on the value of α.



(a) (b) (c)

Figure 4: Note, Time axis in units of $\frac{\omega^1}{2\pi}$. $m = k = 1$, $\delta t = 0.04$, $N = 100$, $\mathcal{B} = 0.8$, and $\sigma_0 = 10$.

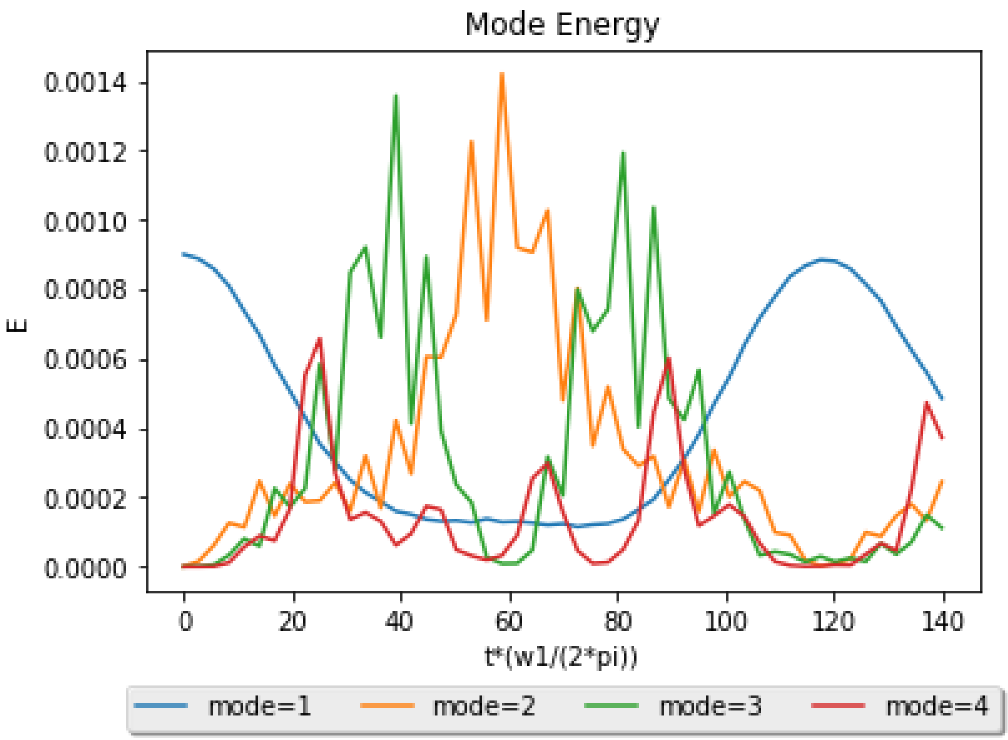
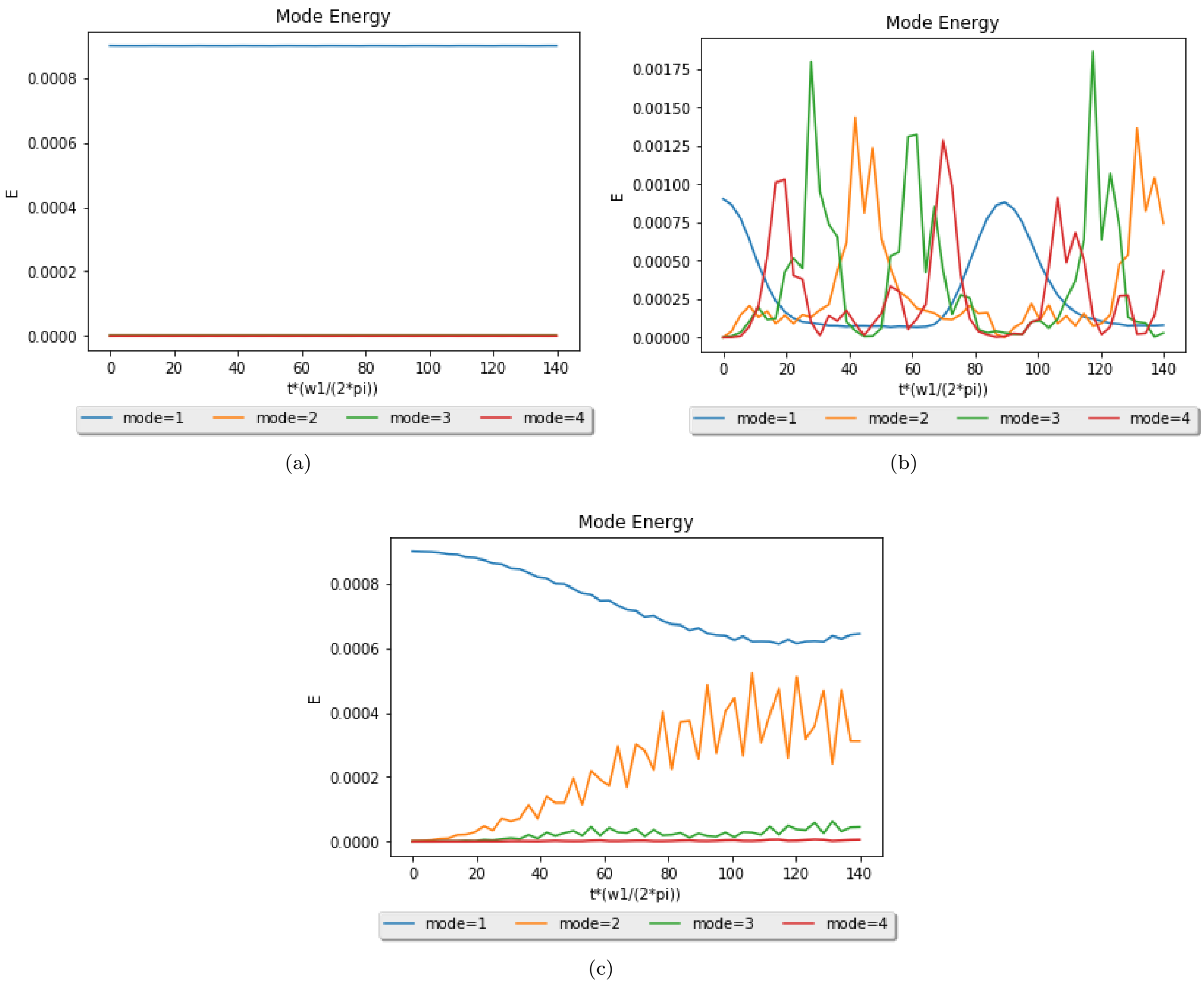


Figure 5: $\alpha = 1.25$, $m = k = 1$, $\delta t = 0.02$, $N = 36$, and $\mathcal{A} = 0.5$.



(a) (b) (c)

Figure 6: (a) $\alpha = 0.0$, (b) $\alpha = 2.25$, (c) $\alpha = 0.25$. $m = k = 1$, $\delta t = 0.02$, $N = 36$, and $\mathcal{A} = 0.5$.