The investigation of the Fermi-Pasta-Ulam problem using a symplectic integration method Project report

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1 Motivation

I have implemented a 4th and 10th order symplectic integration composition method, and a "regular" 4th order Runge-Kutta method in Python 3 in order to investigate the Fermi-Pasta-Ulam problem. My first motivation was to get to know geometrical integrators better, because these methods are widely used in celestial dynamics and N-body dynamics (e.g. molecular dynamics) [1]. I chose to investigate the FPU-problem because I wanted to reproduce the famous super-recurrence phenomenon observed in this system [2].

2 The FPU-problem

As the first computers appeared in the 1940s, they were used for investigating physical systems numerically. In the early 1950s Fermi and Ulam chose to integrate the weakly nonlinear, fixed-end, one dimensional chain of N-1 moving mass points having the Hamiltonian [3]:

$$H = \frac{1}{2} \sum_{k=1}^{N-1} p_k^2 + \frac{1}{2} \sum_{k=0}^{N-1} (q_{k+1} - q_k)^2 + \frac{\lambda}{3} \sum_{k=0}^{N-1} (q_{k+1} - q_k)^3,$$
(1)

where p_k, q_k is the momentum/displacement from equilibrium position of the kth particle, and λ is a small number. This type of Hamiltonian is also called α -mode [4]. In my simulations I used N = 32.



Figure 1: Schematic figure showing a linear chain of N particles. We denote the displacements from the equilibrium positions by q_k instead of x_k for the sake of transparency

The simulation was to serve as an assertion of ergodicity and equipartition of energy, because it was believed that the small anharmonicity in the system would lead to equipartition between the degrees of freedom. That is why it was straightforward to introduce normal mode coordinates the following way [2]:

$$A_l = \sqrt{\frac{2}{N}} \sum_{k=0}^{N-1} q_k \sin\left(\frac{kl\pi}{N}\right).$$
⁽²⁾

With the above transformation we get for the transformed Hamiltonian the following[4]

$$H_{transformed} = \frac{1}{2} \sum (\dot{A}_k^2 + \omega_k^2 A_k^2) + \lambda \sum C_{klm} A_k A_l A_m, \qquad (3)$$

where $\omega_k = 2 \sin\left(\frac{k\pi}{2N}\right)$ is the frequency of the *k*th mode and the dot denotes time derivative. The constants C_{klm} will not be used, therefore we do not need them. During the historical simulation the energy of the first few modes were investigated, given by:

$$E_k = \frac{1}{2} \left(\dot{A}_k^2 + \omega_k^2 A_k^2 \right). \tag{4}$$

The initial conditions were given by (k = 1...31):

$$q_k^0 = \sin\left(\frac{k\pi}{N}\right), \qquad (5)$$
$$p_k^0 = 0.$$

In other words, only the first mode was excited. (I used the same initial conditions). The results were a surprise: After a certain amount of time the energy began to return to the first mode only, contradicting the equipartition of energy. This phenomenon, also called 'super-recurrence phenomenon' is the subject of this project. For the transformation into normal coordinates, Fast Fourier Transform (FFT) was applied.

3 Theoretical background of the applied numerical method

Let us denote the coordinates of phase space by $\mathbf{p} := (p_1, p_2 \cdots, p_N)^T$, the particle momenta and $\mathbf{q} := (q_1, q_2 \cdots, q_N)^T$, the particle coordinates. Given a Hamiltonian, H, the equations of motion are the following:

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathbf{q} = \nabla_{\mathbf{p}}H\tag{6}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p} = -\nabla_{\mathbf{q}}H.\tag{7}$$

For a numerical integrator, let us define a so-called flow map, Ψ , which is a $\mathbb{R}^{2N} \to \mathbb{R}^{2N}$ mapping, where N is the number of particles. If, after a timestep *Deltat*, the new coordinates are \mathbf{q}' and \mathbf{p}' , the effect of Ψ can be shown as follows:

$$\begin{pmatrix} \mathbf{p}' \\ \mathbf{q}' \end{pmatrix} = \Psi_{\Delta t} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}.$$
(8)

We call such a flow map symplectic, if it preserves the following 2-form:

$$\Omega = \mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p},\tag{9}$$

where \wedge denotes the usual wedge-product in differential geometry [5]. The above two-form can be thought of as the volume form in phase space, so in other words symplecticness means – after Liouville's theorem [6] – the conservation of the Hamiltonian. It is extremely useful to construct such integrators, as in physics conservation of energy is crucial.

Let us suppose, that the Hamiltonian of the system can be decomposed the following way:

$$H = H_1 + H_2 + \dots + H_k, (10)$$

for which the following statement holds:

$$\{H_i, H_j\} = 0, (11)$$

where $\{A, B\}$ means the Poisson bracket of A and B [6]. Let us assume moreover, that the Hamiltonian can be decomposed the following way:

$$H(\mathbf{p}, \mathbf{q}) = T(\mathbf{p}) + V(\mathbf{q}), \tag{12}$$

as it is certainly satisfied in our case. It can be shown ([1]) that with these requirements a symmetric symplectic integrator can be obtained the following way:

$$\Psi_{\Delta t} = \Phi_{c_s \Delta t, V} \circ \Phi_{d_s \Delta t, T} \cdots \circ \Phi_{c_1 \Delta t, V} \circ \Phi_{d_1 \Delta t, T} \circ \Phi_{c_0 \Delta t, V}, \tag{13}$$

where Φ is the numerical integrator of T or V (they are integrable due to the decomposition defined above), $c_k, d_l, k = 0, 1 \cdots s; l = 1, 2 \cdots s$ are optimally defined constants with the constraint of $\sum_k c_k = \sum_k d_k = 1$, whereas s is the order of the integrator. I used two different integrators, one of order 4, and another of order 10. The corresponding constants can be found in [7, 8], respectively. Function composition is denoted by \circ , hence the name composition method for this kind of symplectic integration. For an excessive description see e.g. [1].

4 Results

4.1 The phenomenon of "super recurrence"

My primer aim was to reproduce the famous super recurrence phenomenon. For this I have made three different simulations, using different numerical methods: 4th order Runge-Kutta, a 4th order and a 10th order simplectic integration composition method. I simulated the first three harmonic modes for 160 periods. One period lasts for an amount of time obtained from the following equation [2]

$$T = \frac{2\pi}{\omega_1},\tag{14}$$

where

$$\omega_1 = 2\sin\left(\frac{\pi}{2N}\right).\tag{15}$$

The task was to reproduce the following figure (taken from [2]):



Figure 2: Harmonic energy modes in the FPU problem, taken from literature.

The energy units were multiplied by a factor for transparency. I did not take this way, that is ehy on the following figures the energy values may differ. Nevertheless, a quantitative comparison is totally possible. The time units were the same. The method whose results was the closest to the figure above was the RK4.

As it can be seen, we have almost perfect agreement regarding the first three harmonic modes.



(a) Harmonic energy modes from literature (b) Harmonic energy modes obtained by RK4

Figure 3: Comparison of RK4-results with literature data



(a) Harmonic energy modes obtained by SI4 (b) Harmonic energy modes obtained by SI10

Figure 4: Comparison of simplectic integration methods of different order

In the case of symplectic integration we can see that although the same results are obtained, yet with a greater variance. This is the price of symplecticness: In order for the numerical method to be symplectic, i.e. preserving the Hamiltonian, it must have a bigger "error", although decreasing with higher order.

4.2 Investigating the role of λ

I have investigated how the harmonic energy (E_{har}) depends on the λ coupling parameter. Heuristically, one would argue that the smaller value λ has, the more closer E_{har} gets to a constant value (although it will not be exactly constant). However by increasing λ , the harmonic energy will be more and more 'fragmented' in a sense that it may show bigger differences in time. For this I have made simulations investigating four different values for λ . The results can be seen on figure 5.



Figure 5: The harmonic energy in case of different λ -parameters

We can draw the conclusion, that at small values of λ the perturbation can be neglected and the harmonic energy hardly changes (on the scale of the $\lambda = 3$ case). By increasing the coupling parameter, the harmonic energy becomes more and more "chaotic". For a deeper insight see e.g. [4].

4.3 Comparison of numerical accuracy of the used numerical methods

I have investigated the numerical accuracy of the symplectic integration method I implemented for the solution of the above described problem, and I have also made a comparison between this and the fourth-order Runge-Kutta method. The basis of comparison was the numerical accuracy which was estimated by the Hamiltonian of the problem. As H does not explicitly depend on time itself, its value ought to remain constant hence the well-known relation from analytical mechanics [6]:

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \{H, H\} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t},\tag{16}$$

which is zero in our case. In spite of this, due to numerical inaccuracy the Hamiltonian is not constant which gives an approximation for the error of the given numerical method. I defined the error as follows:

$$\operatorname{Error} = \frac{(H_{max} - H_{min})}{H_{max}}\%.$$
(17)

With this definition I have made simulations with different time steps (Δt) both for the symplectic integrator (SI-CM) and the Runge-Kutta (RK4). The results can be seen on the following figure:



Figure 6: Comparison of numerical errors in case of different timesteps

We can conclude that the symplectic integration method is more precise in most cases (in case of $\Delta t=10^{-3}$ s it is approximately the same). In case of smaller timesteps no huge difference is observed although it would be indicated by the higher order of the SI-method. This is due to the fact that these simulations runned for a relatively short time ($\approx 20T$). In this region the RK4-method is still acceptable as far as energy conservation is concerned. Had the simulations runned longer, a more noticeable difference would have been observed because of the non-symplecticness of RK4.

5 Discussion

A simplectic integration method and the famous RK4-method was implemented in Python 3 and compared in terms of numerical accuracy and efficiency by investigating the FPU-problem. The super-recurrence phenomenon has been observed, and the role of the coupling parameter has been investigated. We can conclude that although the RK4 is not symplectic, for this particular problem, most probably due to the short period of simulated time, it is more efficient than the symplectic integration method. It should be noted however, that had we simulated for a much longer period of time, the advantages of the symplectic method would have clearly been shown, i.e. it conserves the Hamiltonian, whereas in the case of "regular" RK4 for longer times energy begins to "slip out" from the system [1].

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