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The Fermi–Pasta–Ulam 'numerical experiment': history and pedagogical perspectives

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Abstract

The pioneering Fermi–Pasta–Ulam (FPU) numerical experiment played a major role in the history of computer simulation because it introduced this concept for the first time. Moreover, it raised a puzzling question which was answered more than 10 years later. After an introduction to this problem, we briefly review its history and then suggest some simple numerical experiments, with the Matlab© code provided, to study various aspects of the 'FPU' problem.

1. The physical question

The 'FPU problem', as it is known presently, bears the name of the three scientists[3] who wanted to study the thermalization process of a solid [1]. As revealed by Ulam later [2], these authors were looking for a theoretical physics problem suitable for an investigation with one of the very first computers, the MANIAC (Mathematical Analyzer, Numerical Integrator and Computer). Their work, published in 1955 in a classified Los Alamos National Laboratory report, had been completed shortly before the death of Enrico Fermi in 1954. Ulam told later that Fermi did not suspect the importance of this discovery and considered this work as 'minor'. He nevertheless intended to talk about it at the conference of the American Mathematical Society where he had been invited just before he became seriously ill.

Fermi, Pasta and Ulam decided to study how a crystal evolves towards thermal equilibrium by simulating a chain of particles of unitary mass, linked by a quadratic interaction potential,

[3] Ms Mary Tsingou, who took part in the numerical study with Fermi, Pasta and Ulam is not an author of the report, however, her contribution is recognized in two lines of the acknowledgment section of the FPU report.

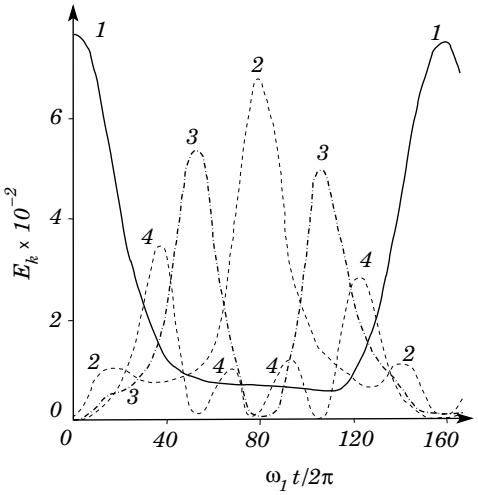

Figure 1. FPU recurrence: the plot shows the time evolution of the kinetic and potential energy $E_k = \frac{1}{2}(\dot{A}_k^2 + \omega_k^2 A_k^2)$ of each of the four lowest modes. Initially, only mode 1 was excited (from [1]).

but also by a weak nonlinear interaction. One of the one-dimensional systems they considered is described by the Hamiltonian

$$H = \sum_{i=0}^{N} \frac{1}{2} p_i^2 + \sum_{i=0}^{N} \frac{1}{2}(u_{i+1} - u_i)^2 + \frac{\alpha}{3} \sum_{i=0}^{N} (u_{i+1} - u_i)^3, \tag{1}$$

where u_i is the displacement of atom i, along the chain, with respect to its equilibrium position, and p_i is its momentum. The stiffness of the harmonic spring and the lattice spacing have been set to 1, without loss of generality. The coefficient $\alpha \ll 1$ measures the strength of the nonlinear contribution to the interaction potential. The two ends of the chain were assumed to be fixed, i.e., $u_0 = u_{N+1} = 0$.

The common approach in physics is to think in terms of 'normal modes', related to the displacements through $A_k = \sqrt{2/(N+1)} \sum_{i=1}^{N} u_i \sin(ik\pi/N + 1)$ with the frequencies $\omega_k^2 = 4\sin^2(k\pi/2(N+1))$. They provide a basis to rewrite Hamiltonian (1) as

$$H = \frac{1}{2} \sum_{k=1}^{N} \left(\dot{A}_k^2 + \omega_k^2 A_k^2\right) + \frac{\alpha}{3} \sum_{k,\ell,m=1}^{N} c_{k\ell m} A_k A_\ell A_m \omega_k \omega_\ell \omega_m, \tag{2}$$

where the coefficients $c_{k\ell m}$ are given, for example, in [3]. The last term, generated by the nonlinear contribution to the potential, leads to a coupling between the modes, and scales as $N^{3/2}$.

FPU thought that, due to this term, the energy introduced into a single mode, mode $k = 1$ in their simulation, should slowly drift to the other modes, until the equipartition of energy predicted by statistical physics is reached. The beginning of the calculation indeed suggested that this would be the case. Modes 2, 3, ..., were successively excited. However, by accident [4], one day they let the program run long after the steady state had been reached. When they realized their oversight and came back to the room, they noticed that the system, after remaining in a steady state for a while, had then departed from it. To their great surprise, after 157 periods of the mode $k = 1$, almost all the energy (all but 3%) was back to the lowest frequency mode, as shown in figure 1.

The initial state seems to be almost perfectly recovered after this recurrence period. Further calculations, performed later with faster computers, showed that the same phenomenon repeats many times, and that a 'super-recurrence' period exists, after which the initial state is recovered with a much higher accuracy. Thus, contrary to the expectations of the authors, the drift of the energy of the initially excited mode 1 towards the modes with a higher wave number does not occur. This highly remarkable result, known as the FPU paradox, shows that nonlinearity is not enough to guarantee the equipartition of energy.

2. Fermi, Pasta and Ulam: the characters

Born in Rome, Enrico Fermi (1901–1954) was one of the brightest physicists of the twentieth century, and made major experimental and theoretical discoveries. His name is famous for his contributions to statistical physics, elementary particle physics, and the control of nuclear energy. Thanks to his trip to receive the Nobel prize in Sweden in 1938, he left fascist Italy and emigrated to the United States where he studied atomic fission and set up the first controlled chain reaction in Chicago in 1942. He was naturally called to be one of the leaders of the Manhattan project for the development of nuclear energy and the atomic bomb. We are less familiar with his work on various nonlinear problems at the end of his life, before his premature death from stomach cancer.

John R Pasta (1918–1981) did not have such a bright career. In spite of his interest in physics he had to leave the New York City College during the great depression. He was first a real estate agent and then a police officer in New York from 1941 to 1942. Then he was recruited as a radar and cryptography specialist by the American army during the second world war. His earnings as a GI allowed him to return to the University, where he got a PhD in theoretical physics in 1951. He immediately started to work in Los Alamos, on the MANIAC computer which was under construction and testing. His career developed as a computer expert for the Atomic Energy Commission, where he extensively developed the Mathematics and Computer Division. Then Pasta became a physics professor and, in 1964, the dean of the computer science department of the University of Illinois, where he focused on the use of computers to solve applied problems in physics and mathematics.

Born in Poland, Stanislaw M Ulam (1909–1984) quickly became interested in mathematics and obtained a PhD in 1933 under the supervision of Stefan Banach (1892–1945). Following a first invitation by Von Neumann to the prestigious Princeton Institute for Advanced Study in 1935, he visited the Unites States several times before leaving Poland finally before the start of the second world war. He became an American citizen in 1943, and was invited by von Neumann himself to join the Los Alamos team to prepare the atomic bomb. Among other things he solved the problem of the initiation of fusion in the hydrogen bomb. In collaboration with N C Metropolis he invented the Monte Carlo method to solve problems requiring a statistical sampling. He stayed in New Mexico until 1965 before his appointment as a mathematics professor at Colorado University.

The FPU numerical experiment was performed on the MANIAC (Mathematical Analyzer, Numerical Integrator and Computer) built in 1952 for the Manhattan project, which was used in the development of 'Mike', the first hydrogen bomb. Richard Feynman (1918–1987) and Nicholas C Metropolis (1915–1999), exasperated by the slow and noisy mechanical calculators which were nevertheless necessary to the design of the bombs, promoted its construction. The name of the computer, MANIAC, was chosen by the project director, N C Metropolis, who hoped that it would stop the rising fashion of naming computers by acronyms. The effect was exactly the opposite although, according to Metropolis [4], George Gamow (1904–1968) was instrumental in rendering this and other computer names ridiculous when he dubbed the

MANIAC 'Metropolis And von Neumann Install Awful Computer'. The MANIAC was able to perform about 10^4 operations per second, which must be compared to the 10^8 operations per second of any personal computer today. It is Fermi who had the genius to propose that computers could be used to study a problem or test a physical idea by simulation, instead of simply performing standard calculus. He proposed to check the prediction of statistical physics on this system, now called FPU.

The discovery that resulted from this study has not only been at the origin of the soliton concept and of many features of chaotic phenomena, as discussed in the following section, but it also introduced the concept of a *numerical experiment*. This had far reaching consequences, leading to a complete revolution in the investigation of physical phenomena. The computer was no longer used only to perform a calculation that could not be done using a pencil and napkin, but to check a theoretical conjecture that could not be proven analytically, or even to provide the theorist with 'experimental' results that wait for a mathematical proof: a source of problems, as in a 'true laboratory experiment'. Of course, the *numerical experiment* does not possess all the complexity of a true physical experiment, because the reality which is represented is highly virtual. However today, in numerical simulations of condensed matter systems, one reaches such a level of confidence that sometimes it has happened that a laboratory experiment has been questioned because a numerical experiment had given contrary indications [5]. Today, *computational physics* is an established discipline and it is considered as sort of separated from both theoretical and experimental physics. Students are currently trained in computational physics as in other disciplines, and specialized journals publish the results of the research in this field. This big epistemological and sociological change began with the FPU experiment.

3. Epilogue: the solution of the FPU problem

Pursuing the solution of the FPU paradox, two main lines of thought were followed. On the one side, people like J Ford [6] focused on the Fourier mode dynamics, looking for non-resonance conditions that could explain the inefficient energy transfer. No convincing explanation was found before the news spread of a theorem announced by Kolmogorov [7], and then proven by Moser [8] and Arnold [9] (KAM theorem), which states that most orbits of slightly perturbed integrable Hamiltonian systems remain quasi-periodic. Although *qualitative* explanations of the FPU recurrence were obtained following this path no *quantitative* explanation has to our knowledge been obtained so far. In contrast, a remarkable result was obtained by Izrailev and Chirikov [10], following KAM theory. If the perturbation is so strong that nonlinear resonances 'superpose', the FPU recurrence is destroyed and one obtains a fast convergence to thermal equilibrium. This prediction was tested numerically and is nowadays the basis of the phenomenon called the 'strong stochasticity threshold' [11].

The other line of thought, which went towards the so-called *continuum limit*, led to the solution of the FPU paradox by Zabusky and Kruskal [12] in terms of the dynamics of *solitons* [13]. Starting from the FPU equations of motion, derived from Hamiltonian (1),

$$\ddot{u}_i = (u_{i+1} + u_{i-1} - 2u_i) + \alpha[(u_{i+1} - u_i)^2 - (u_i - u_{i-1})^2], \tag{3}$$

and restricting the investigation to long wavelength modes, they could derive the Korteweg–de Vries equation [14],

$$w_\tau + \tfrac{1}{24} w_{\xi\xi\xi} + \alpha w w_\xi = 0, \tag{4}$$

where the field w is a conveniently rescaled spatial derivative of the displacement field u_i, τ is a rescaled time and $w_x = \partial w/\partial x$.

The sinusoidal initial condition develops sharp fronts and then breaks into a series of pulses, which are solitons. They preserve their shapes and velocities and, during their motion

in the finite system with periodic boundary conditions[4], from time to time, they come back to the positions that they had initially, restoring the initial condition. This is why the FPU recurrence is observed.

It is important to emphasize that the FPU paradox would probably not have been a mystery for more than 10 years if, before Zabusky and Kruskal, somebody had had the idea of looking carefully at the dynamics of the nonlinear lattice as a function of the space coordinates (see the suggested numerical experiment in section 5). But physicists were so used to analysing linearized problems, which naturally lead to a description in Fourier space, and only adding nonlinearity afterwards as a coupling between the modes, that the observation of the solitons emerging from the sinusoidal initial condition had not been done.

4. The remake: FPU and the Japanese school

The history of the FPU problem is quite rich, as documented in the report by Ford [15] and in the recent book by Weissert [16]. We will not discuss it in this paper but we will just recall that some of the contributions to *Chaos* [17], printed this year to celebrate the anniversary of the FPU experiment, are devoted to a brief historical reconstruction.

Because of its relevance to the determination of a quantitative formula for the recurrence time, we will discuss briefly the contribution of the Japanese school, which has been very active in this field since the 1960s.

The original FPU report [1], not published, was known by very few people, most of them within America. This is why, in Japan, Nobuhiko Saito (born in 1919) together with his PhD student Hajime Hirooka (born in 1939) were developing closely related research works in complete ignorance of what had been done in Los Alamos ten years earlier.

As explained by the title of Hirooka's PhD thesis, 'The approach to thermal equilibrium in a nonlinear lattice', the motivation was to explore the mechanism of ergodicity. As the mechanics of collisions in a gas was too complicated, they thought that an anharmonic lattice would be a more appropriate system; it appeared finally that its dynamics was difficult to solve. This is why in 1964 they started to perform numerical simulations on a small computer provided by NEC: it took all night to compute the evolution for only five lattice sites during several periods of the lowest mode! In 1965 they switched to the new supercomputer provided by Hitachi Co., installed at Tokyo University under a national plan for all Japanese universities and research institutes.

Saito and Hirooka considered a one-dimensional anharmonic lattice with quadratic and quartic potentials between neighbouring particles, and with both ends fixed. The initial excitation was slightly different since all particles were at rest, whereas a constant force was applied to the first particle. They also prepared a similar system, with only harmonic potentials, and analytically calculated several quantities of interest, in particular the long-time averages of the squares of the velocities of the particles $\langle \dot{u}_i^2 \rangle$ and the correlations $\langle \dot{u}_i \dot{u}_{i+1} \rangle$ of the velocities of neighbouring particles. The long-time averages of $\langle \dot{u}_i^2 \rangle$ were the same for all particles, but the correlation functions did not vanish in the long term, and the Maxwellian distribution of velocities was not observed, contrary to their expectations.

It is interesting to emphasize that they hesitated to publish these results because they were not familiar with the computer calculation and were afraid of having introduced some errors. However, they found numerical experiments similar to the FPU original one in several papers on nonlinear oscillation, in particular, those of Ford [6]. These papers also convinced

[4] The calculation performed by Zabusky and Kruskal used periodic boundary conditions, while the FPU calculation used fixed boundaries. This does not change the analysis because the solitons either pass through the boundaries and enter on the opposite side or they are totally reflected.

Morikazu Toda to study solitons and to introduce the lattice with exponential interactions, nowadays called the Toda lattice [18].

Soon after, they also learned that the original FPU report was reproduced in the *Collected Papers of Enrico Fermi* [1]. Very excited, Saito and Toda read the paper at the library of Tokyo University of Education (now Tsukuba University). As they had found results similar to those of Fermi, Pasta and Ulam, Saito and Hirooka finally decided to publish their calculations [19]. Afterwards, they considered the simpler FPU initial condition and found the induction phenomenon and the occurrence of the random character of lattice vibrations.

Finally, they discovered the Zabusky–Kruskal seminal paper [12] soon after the publication of their papers in 1967. Norman Zabusky went to Kyoto in 1968 for the International Conference of Statistical Mechanics, where he showed his movies and in particular the KdV cinema, which 'has the power to communicate unbiased information in a credible manner, much beyond the power of words, graphs and equations'.

At that time, Toda gave the first analytical estimate of the recurrence time, based on the exact solutions of the exponential lattice, nowadays called the Toda lattice. Introducing the period $T_1 = 2N$ of the first mode and the amplitude a of the initial sine wave, he got

$$T_R = \frac{3}{\pi^{3/2}\sqrt{2}} \frac{N^{3/2}}{\sqrt{a\alpha}} T_1 \simeq 0.38 \frac{N^{5/2}}{\sqrt{a\alpha}}, \tag{5}$$

which compares well with the first empirical estimate due to Zabusky. Toda's result was a little larger than Zabusky's formula: the pre-factor is 0.31 instead of 0.38 in equation (5). The discrepancy is due to the fact that, when solitons pass through each other, they accelerate because of the compression of the lattice. See [20] for a more complete discussion and [21] for a recent check of formula (5).

5. Pedagogical perspectives

It is quite easy with the contemporary computational tools to reproduce the original FPU experiment. An example is the simple MATLAB© code reported in the appendix, which solves the equations for the dynamics of the FPU model and computes the normal modes, A_k. We suggest students use it to reproduce different aspects of the FPU problem:

- Try to reproduce figure 1 using the original FPU initial condition given in the code. Be careful in the choice of amplitude a because the cubic lattice is unstable at large energies.
- By careful inspection of the difference field $(u_{i+1} - u_i)$, it is possible to detect the presence of propagating structures, which are indeed the solitons of the Zabusky–Kruskal analysis.
- Between $a = 1$ and $a = 10$, the FPU model with $N = 32$ undergoes relaxation to equilibrium [10]. Check the absence of FPU recurrences and the establishment of energy equipartition among the normal modes.
- Since the initial sine wave form solitons [12], it is quite natural to begin with a lattice soliton initial condition. The exact kink-like soliton solution for the Toda lattice [20] is

$$u_i(t) = \pm \frac{1}{2\alpha} \log \frac{1 + \exp[2k(i - 1 - i_0) \pm t \sinh k]}{1 + \exp[2k(i - i_0) \pm t \sinh k]}, \tag{6}$$

  where k is the inverse width. This solution is only approximate for the FPU lattice, and due to the fixed boundary conditions, one must put a kink (+) and an antikink (−) solution, centred around two different sites of the lattice. Our advice is to first choose a large lattice (e.g., $N = 128$). The time evolution of the derivative field $u_{i+1} - u_i$ shows the propagation of coherent structures, their mutual interactions and reflection from the boundaries.

- Try to reproduce the relevant scalings of formula (5), for instance, the $N^{2.5}$ dependence on the number of oscillators.
- Finally, try the Zabusky–Deem [22] initial condition $u_i = a \sin[i\pi N/(N+1)]$, which corresponds to the highest frequency mode. Similar oscillations of mode energies as those of long wavelengths are observed. Try to characterize these recurrences.

The scaling of formula (5) is quite different from that of the Poincaré recurrence time [23], which can be shown to increase exponentially with N in the harmonic limit [24]. No striking change of this scaling should occur for a small nonlinearity, e.g. in the FPU recurrence region, although nothing is rigorously known for this case. The interested student can find the statement of Poincaré recurrence theorem in most books on statistical mechanics. However, in simple words, the theorem states that whenever a dynamical system preserves phase-space volume in its time evolution (and this is the case of Hamiltonian systems, including the FPU oscillator chain), 'almost all' trajectories return arbitrarily close to their initial position, and they do this an infinite number of times. The exponential scaling with N of the Poincaré recurrence time with respect to the algebraic one of Toda's formula proves that the FPU recurrence is not a manifestation of this phenomenon. It is remarkable that although certainly Fermi and Ulam did know the Poincaré theorem, they did not quote it at all in their paper as a possible explanation of the observed recurrence[5].

Another pedagogical aspect, which is worth discussing in connection with the FPU experiment, is the relation between a *continuum* and *discreteness*. Analytical 'human' approaches to the problem consider continuous variables, while with computers it was natural and necessary to use discretized variables; the human and the computer ways of dealing with physical problems were therefore for the first time in confrontation. The only discreteness appearing in the FPU model is the spatial one: the oscillators are put on a lattice. Time flows continuously and the displacement field variable u_i is also continuous. Models of spacetime evolution have been considered where time is discrete, while the lattice variable is still continuous: the so-called *coupled map lattices* [25]. The Hamiltonian versions of these types of models exist in the sense that phase-space volume is conserved by the dynamical evolution, although the total energy is not. The extreme case of discreteness is that of *cellular automata* [26], for which also the lattice variable takes a discrete set of values. Depending on the physical system at hand, one model or another has been considered as appropriate, and several examples exist where even the extreme discrete case of cellular automata provides a good representation of the physical process under analysis.

In this respect, quite advanced still open questions related to the FPU recurrence are as follows. Is the recurrence also observed in the 'Hamiltonian' coupled map lattices and in cellular automata? Is it related to the propagation of coherent structures which have some resemblance to solitons? How does the recurrence time scale with the system size? These are open research issues on which a curious PhD student might want to challenge his own computational skills, taking the opportunity to make his own first 'numerical experiment', a privilege once reserved only to a few people isolated in a deserted region of New Mexico.

Acknowledgments

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[5] This fallacious possibility has been considered by others (who perhaps did not know the theorem as well as Fermi and Ulam) when the news about the FPU experiment spread around.

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Appendix. MATLAB© code

Codes are available at the website http : //perso.ens-lyon.fr/Thierry.Dauxois/fpu.html

Main program

```
N=32;                          % Number of particles must be a power of 2
alpha = 0.25;                                        % Nonlinear parameter
TMAX = 10000; DT = 20;                               % tmax and Delta t
tspan=[0:DT:TMAX];
options=odeset('Reltol',1e-4,'OutputFcn','odeplot','OutputSel',[1,2,N]);
% Test different tolerances, changing Reltol
for I=1:N,
a=1; b(I)=a*sin(pi*I/(N+1));  b(I+N)=0;       % FPU initial condition
%a=1; b(I)=a*sin(pi*N*I/(N+1)); b(I+N)=0;     % Zabusky-Deem init. cond.
%k=0.8;  sk=(sinh(k))^2;  ek=exp(-k);  i1=I-N/4;  i2=i1-N/2;  % Solitons
%b(I)=-0.5/alpha*log((1+exp(2*k*(i1-1)))/(1+exp(2*k*i1)));
%b(I)=b(I)+0.5/alpha*log((1+exp(2*k*(i2-1)))/(1+exp(2*k*i2)));
%b(I+N)= sk*ek/alpha/cosh(k*i1)/(exp(-k*i1)+exp(k*i1)*exp(-2*k));
%b(I+N)=b(I+N)-sk*ek/alpha/cosh(k*i2)/(exp(-k*i2)+exp(k*i2)*exp(-2*k));
omegak2(I)=4*(sin(pi*I/2/N))^2;                      % Mode Frequencies
end
[T,Y]=ode45('fpu1',tspan,b',options,N);            % Time integration
for IT=1:(TMAX/DT),
TIME(IT)=IT*DT*sqrt(omegak2(1))/2/pi;            % Time iteration loop
YX(IT,1:N+1)=[0 Y(IT,1:N )];  YV(IT,1:N+1)=[0 Y(IT,N+1:2*N )];
sXF(IT,:)=imag(fft([YX(IT,1:N+1)  0 -YX(IT,N+1:-1:2)]))/sqrt(2*(N+1));
sVF(IT,:)=imag(fft([YV(IT,1:N+1)  0 -YV(IT,N+1:-1:2)]))/sqrt(2*(N+1));
Energ(IT,1:N)=(omegak2(1:N).*(sXF(IT,2:N+1).^2)+sVF(IT,2:N+1).^2)/2;
for J=2:N-1,                                          % Space loop
DifY(IT,J)=Y(IT,J+1)-Y(IT,J);
end
end
plot(TIME, Energ(:, 1), TIME, Energ(:, 2), TIME, Energ(:, 3), TIME, Energ(:, 4));
surf(DifY);   % Space derivative field to show the soliton dynamics
```

fpu1 function

```
function dy=fpu1(t,y);
N=32;alpha=0.25;
D(N+1)=y(2)-2*y(1)+alpha*((y(2)-y(1))^2-y(1)^2);D(1)=y(N+1);
D(2*N)=y(N-1)-2*y(N)+alpha*(y(N)^2-(y(N)-y(N-1))^2);D(N)=y(2*N);
for I=2:N-1,
D(N+I)=y(I+1)+y(I-1)-2*y(I)+alpha*((y(I+1)-y(I))^2-(y(I)-y(I-1))^2);
D(I)=y(N+I);
end
dy=D';
```

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