THE FERMI-PASTA-ULAM LATTICE

Background

The Fermi-Pasta-Ulam lattice is named after the experiments performed by Enrico Fermi, John Pasta, and Stanislaw Ulam in 1954-5 on the Los Alamos MANIAC computer, one of the first electronic computers. As reported in Ulam's autobiography [Uh], Fermi immediately suggested using the new machine for theoretical work, and it was decided to start by studying the vibrations of a string under the influence of nonlinear internal forces. Nonlinearity makes the computations very difficult and the problem could not be attacked by standard mathematical methods. However, physical intuition suggested that the motion of such a string would eventually "thermalize". The purpose of the experiment was to investigate the rate of thermalization.

For the computer calculations, the string was approximated by a finite sequence of point particles with nearest-neighbour interactions — a lattice model.

As explained in the ATC for the Lattice Models category, the motion of the lattice is governed by a system of ordinary differential equations, and it is these equations that the computer solves, numerically.

The results more than justified the trouble of carefully formulating the experiment and programming it on a very primitive machine, for they went completely against all expectations. In fact the motion did not seem to to thermalize at all. The previously accepted beliefs thus had to be re-examined, and this re-examination led eventually to the discovery of soliton theory, one of the main themes of 20th century mathematics.

How to view the demonstration

The Fermi-Pasta-Ulam string is the black curve. Although it appears continuous, it is in fact made up of the motion of individual points (the blue curve represents the velocities of these points). The number of points (i.e. the number of particles in the lattice) can be changed by choosing Lattice Parameters in the Action menu, and various other adjustments are possible, as explained in the Lattice Models ATC. Fermi-Pasta-Ulam actually used a lattice with (at most) 64 particles.

The energies of the normal modes (see the Lattice Models ATC) are the red/green bars in the left hand corner. Thermalization means, roughly speaking, that the heights of the red/green bars equalize after a sufficiently long period of time. More precisely, it is the time averages of their heights which equalize, and these are represented by the blue bars.

The fact that this does not happen is the surprising feature of the Fermi-Pasta-Ulam experiment. What happens, and what Fermi-Pasta-Ulam observed, is first of all that only the first few normal modes are excited, and in addition that the motion is almost periodic. This can be detected by watching the motion of the red/green bars; after some time they return (apparently) to the original configuration.

Various initial shapes can be chosen from the Lattice Parameters menu, but the almost periodicity seems to occur regardless of the initial shape of the string (or the initial configuration of the red/green bars).

Further aspects

To put this observation into context, it is necessary to consider the effects of different internal forces in the string. As explained in the Lattice Models

ATC the internal force is specified by a function $T(y)$. By choosing the User Lattice Model from the Lattice Models menu, the function $T(y)$ can be specified (as well as the usual Lattice Parameters). To switch on the energies of the normal modes, select Show Normal Mode Display from the Action menu.

For example, $T(y) = ky$ (where k is a positive number) gives the motion of a "standard" string, which is exactly periodic. The red/green bars behave even more simply — they remain constant.

The Fermi-Pasta-Ulam case is $T(y) = y + \alpha y^2$; the default value of α in 3D-XplorMath is 0.3. (Fermi-Pasta-Ulam also considered $y + \alpha y^3$ and a piecewise linear function, with similar results.) The effect of the small nonlinear term αy^2 is to "disturb" the periodic behaviour of the linear case, and the red/green bars no longer remain constant. But, as we have observed, some vestiges of periodicity remain.

This is surprising because a "randomly chosen" nonlinear internal force $T(y)$ generally leads to the thermalization that Fermi-Pasta-Ulam expected. For physical reasons, $T(y)$ should be of the form $ky+N(y)$ where $N(y)$ is a nonlinear term which remains small during the motion. For example, $T(y) = y + 100y^3 +$

$5y^4 + 5y^5$.

Why is the Fermi-Pasta-Ulam lattice so special? This question took some time to answer, because the necessary mathematical tools were insufficiently developed at that time. In addition there were various sources of distraction: the mathematical string is only an idealized model of a "real" physical situation, the discrete lattice is in turn only a model of that string, and furthermore any computer calculations are subject to numerical and rounding errors. In fact the philosophical questions surrounding such "simulation" experiments, and the subject of "experimental mathematics" in general, are still being debated (see [We]).

However, it is by now generally agreed that the Fermi-Pasta-Ulam lattice is a genuine phenomenon and that it can be explained by a combination of powerful theories: the Kolmogorov-Arnold-Moser (KAM) theory, the theory of completely integrable Hamiltonian systems, and soliton theory.

The KAM theory explains, very roughly speaking, that a system which is close enough to a completely integrable Hamiltonian system retains some of the predictable behaviour of such a system. The Fermi-

Pasta-Ulam lattice happens to be close to the Toda lattice, which (some 20 years after the FPU experiments) was discovered to be a completely integrable Hamiltonian system. The Toda lattice is discussed further in the ATO for the Toda lattice (select Toda from the Lattice Models menu).

Soliton theory refers to the study of special solutions (solitons) of certain nonlinear wave equations such as the Korteweg-de Vries (KdV) equation. These solutions have unexpectedly persistent behaviour (in contrast to "randomly chosen" nonlinear waves, which either disperse or break after a sufficiently long time). It turns out that the differential equations of the FPU lattice can be considered as a discrete approximation to the KdV equation; hence it is plausible that the FPU lattice admits soliton-like solutions as well.

References

[Pa] R.S. Palais, *The symmetries of solitons*, Bull. A.M.S. **34** (1997 (see pages 355–359 for a discussion of the FPU experiments)), 339–403.

[To1] M. Toda, *Nonlinear Waves and Solitons.*, Mathematics and its Applications, 5, Kluwer, 1989 (an advanced mathematical treatment of lattices and solitons).

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[Ul] S.M. Ulam, *Adventures of a Mathematician*, Univ. of California Press, 1991 (see chapter 12).

[We] T.P. Weissert, *The Genesis of Simulation in Dynamics. Pursuing the Fermi-Pasta-Ulam Problem*, Springer, 1997 (a historical account of the FPU lattice and the ensuing mathematical — and philosophical — turmoil).