

LATTICE MODELS

Background

A “lattice model” is a system of differential equations which represents the motion of a network or “lattice” of particles, where the motion is produced by forces acting between adjacent particles. Physical examples could be the vibrations of atoms or molecules in a substance, or the oscillations of an arrangement of masses connected by springs. Mathematically, the motion is governed by a system of ordinary differential equations (Newton’s equations). As well as being natural examples, lattice models can exhibit a wide spectrum of behaviours, providing insight into the theory of differential equations.

One such example, the Fermi-Pasta-Ulam lattice, was a starting point for research into “soliton equations”, a major theme which today spans several areas of pure and applied mathematics as well as physics. It was one of the first “mathematical experiments” made possible by the advent of electronic computers.

Although it can be reproduced easily and quickly on modern machines, it is still impressive and truly represents a mathematical phenomenon that cannot be observed using only traditional pencil and paper calculations. Further information about this experiment is given below, and in the ATO for the FPU Lattice.

The examples considered here are all one-dimensional lattices. This means a linearly arranged sequence of particles with each particle connected to the next one by a spring. An alternative (but mathematically equivalent) description of such a system can be helpful: if the displacement of each particle from its equilibrium position on the horizontal axis is vertical instead of horizontal, the particles move in a wave-like fashion. The analogy with wave motion — that a lattice can be considered as a discrete approximation to a wave — is a useful aid to visualization, and in fact there are deep mathematical connections between lattice models and wave equations.

Some mathematical terminology and assumptions

The basic mathematical ingredient is the differential equation $y'' = -ky$, where k is a positive constant

and y is the extension of a (stretched or compressed) spring. This is Newton's equation for the motion of a particle of unit mass at the end of an ideal spring, the spring being fixed at the other end. We assume that the only force acting on the particle is the tension in the spring, which is proportional to y by Hooke's law. For a lattice model this example is generalized in two ways: there will be several particles (and springs), and the tension will be a function $T(y)$ which is not necessarily linear.

To be precise, we consider a one-dimensional lattice, where N particles of unit mass lie on a straight line, and we denote their positions by

$$Y_1(t), Y_2(t), \dots, Y_N(t)$$

at time t . We assume that the force in the spring connecting Y_i to Y_{i+1} depends upon the extension of the spring from an equilibrium position of the whole lattice in which $Y_i = e_i$, and that $e_1 < \dots < e_N$. Let $y_i = Y_i - e_i$ be the displacement of Y_i from its equilibrium position e_i . Then the extension of the spring at time t is $y_{i+1}(t) - y_i(t)$, and our assumption can be written

force on Y_i from the spring connecting Y_i to $Y_{i+1} =$

$$T(y_{i+1} - y_i)$$

for some function T (we assume the same function T applies to all springs). The force on Y_{i+1} from the same spring will be $-T(y_{i+1} - y_i)$.

When $1 < i < N$, Newton's equation for Y_i is

$$(Y_i'' =) y_i'' = T(y_{i+1} - y_i) - T(y_i - y_{i-1}),$$

and in the special case when Hooke's law holds, so that $T(y) = ky$ for some positive constant k , it is

$$y_i'' = ky_{i-1} - 2ky_i + ky_{i+1}.$$

For the cases $i = 1$ and $i = N$, the equations are similar, but with appropriate "boundary conditions". For simplicity we consider only two cases: periodic boundary conditions, i.e. $y_1 = y_N$, or zero boundary conditions, i.e. $y_0 = y_{N+1} = 0$ (this means that we extend the lattice by adding an immovable particle at each end). For the initial positions we take $y_i(0) = a_i$, with $e_1 + a_1 < e_2 + a_2 < \dots < e_N + a_N$. For the initial velocities we take $Y_i'(0) = y_i'(0) = 0$. In addition, we assume that the equilibrium positions are equally spaced, i.e. the natural length of each spring is the same.

How to view the demonstration

Choose a lattice model from the Lattice Models menu. After clicking on the default demonstration to stop it, choose Set Lattice Parameters from the Action menu. Then select boundary conditions, initial shape (the values of a_1, \dots, a_N), and display style. Longitudinal Display shows the “actual lattice”. To see a wave-like representation of the lattice motion, choose Transverse Display, which plots the values of the function $y_i(t)$ vertically above the equilibrium position of the i -th particle and joins the resulting dots by successive black lines. The blue lines have the same meaning for the functions $y'_i(t)$.

Several numerical values can be entered or modified at the same time:

Lattice Length

Density: average mass per unit length

Vertical Scale Factor: this re-scales the Transverse Display

Number of Nodes in Lattice: for a larger number of nodes, i.e. particles, the motion of the lattice will appear more “wave-like”

Width of Initial Pulse: applies when “sinusoidal” ini-

tial shape is selected.

Time step-size: used for numerical solution of the system of o.d.e. (for a larger step-size, numerical errors are more likely to be significant)

Click OK to start the demonstration, which shows the lattice moving in real time.

Further aspects: the energies of the normal modes

To understand the different kinds of behaviour of lattice models it is necessary to introduce some practical criteria. The red, green and blue displays in the left hand corner of the Transverse Display provide one such, the energies of the normal modes. (These displays can be turned on by choosing Show Normal Mode Display from the Action menu.) If the Transverse Display is regarded as an approximation to a wave, the normal modes would be the Fourier components of that wave. The precise meaning of these displays will be explained next (see also the ATOs for the Fermi-Pasta-Ulam lattice and the Toda lattice).

First consider the linear case: take $T(y) = y$ in the User Lattice Model¹ (or $T(y) = ky$ for any positive

¹The internal force is $-T(d)$ in 3D-XplorMath, so $-d$ should

number k). The system

$$y_i'' = T(y_{i+1} - y_i) - T(y_i - y_{i-1}) = y_{i+1} - 2y_i + y_{i-1}$$

can be transformed by a change of variable to a “diagonal” system

$$z_l'' = \lambda_l z_l$$

(because the matrix of coefficients is a symmetric matrix). Thus, although the oscillations of the particles of the lattice are “coupled”, they become uncoupled when viewed in terms of the new variables z_l . In other words, the motion of this lattice is mathematically equivalent to the motion of N independent ideal springs. The total energy $\frac{1}{2}z_l'^2 - \lambda_l z_l^2$ (kinetic energy plus potential energy) of each spring is a constant, independent of time, which depends only on the initial position and velocity. It is called the energy of the l -th normal mode.

The red, green and blue display in the left hand corner shows the values of the kinetic energy (red bar) and the potential energy (green bar) of each normal mode, at each moment in time. Although these vary,

be entered in the internal force box.

their sum remains constant, for each normal mode. Note that the l -th normal mode does not refer to the l -th particle; it refers to motion of the lattice in which z_l varies but $z_1, \dots, z_{l-1}, z_{l+1}, \dots, z_N$ are constant. For example, if the initial shape of the transverse display is sinusoidal, only one normal mode is “excited”, but to produce this kind of motion almost all particles of the lattice have to move.

Now consider the nonlinear case. Although the differential equations make sense for any nonlinear function $T(y)$, it is natural to consider first the situation where the particles are disturbed only slightly from their equilibrium positions, and where $T(y)$ is approximately ky when y is small. (In fact the theory of lattice models has been developed primarily with this situation in mind, and we shall focus on this.) For example, take $T(y) = y + 0.5y^2$ or $T(y) = y + 0.5 \sin y$ in the User Lattice Model². The effect of the nonlinearity is noticeable: the energies of the normal modes are no longer constant. Mathematically, this is not surprising, as there is no reason to expect them to be constant in the nonlinear case. All that can be said is that the sum of all the normal mode energies — the

²Enter $-d - 0.5d^2$ or $-d - 0.5 \sin d$ in the internal force box.

total area of the red and green bars — is constant, because this is the total energy of the whole lattice (a conservative system).

(There is a subtlety concerning the definition of the energies of the normal modes, as the definition given earlier only applies in the linear case. If we only consider small displacements of the lattice, however, it suffices to use the energies of the normal modes of the linearization, and this is what the demonstration is showing. For motion with large displacements, therefore, the Normal Mode Display has no relevance.)

The behaviour of the energies of the normal modes is a criterion for studying lattice models. A subsidiary criterion is the time average of the total energy of each normal mode, which is measured by the blue bars in the display. Initially the height of each blue bar is equal to the sum of the heights of the corresponding red and green bars, but as time passes the blue bars indicate the relative “importance” of the various normal modes. For a lattice with many particles, the “typical” behaviour of the blue bars is that, after a sufficiently long period of time, they all settle down to approximately the same value. A mathematical analysis of this phenomenon is quite difficult

(see [Pa]), but there is a compelling physical reason. Namely, in the absence of any special features (such as linearity), a nonlinear system with many degrees of freedom should behave increasingly randomly, like the molecules in a gas: a particle with greater than average energy will tend to lose energy through its interactions with its neighbours, and conversely for a particle with less than average energy. In physics, this behaviour is called thermalization.

By trying various nonlinear forces in the User Lattice Model this hypothesis — and many other hypotheses about the energies of the normal modes — can be tested. On the other hand, certain choices of forces give surprisingly different results — see the ATOs for the Fermi-Pasta-Ulam lattice and the Toda lattice.

REFERENCES

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- [To1] M. Toda, *Nonlinear Waves and Solitons.*, Mathematics and its Applications, 5, Kluwer, 1989 (an advanced mathematical treatment of lattices and solitons).
- [To2] M. Toda, *Theory of Nonlinear Lattices*, Springer Series in Solid-State Sciences, 20, Springer-Verlag, 1989 (an advanced mathematical treatment of lattices and solitons).
- [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).