Computational synergetics

As a heuristic tool, used to explore complex dynamical behavior, computers allow us to discover unexpected linkages and new concepts in nonlinear systems.

Norman J. Zabusky

Computers, used in what I shall call the "heuristic mode," can greatly enhance our understanding of the mathematics of nonlinear dynamical processes—a field that is taking on increasing importance as we explore the complex behavior that even simple systems often exhibit. As I shall try to show, computers allow us to penetrate into unexplored regions of mathematics and to discover unforeseen linkages among ideas.

Almost everyone who has used a computer has experienced instances where computational results have sparked new insights: uncovering mistakes in derivations or calculations; suggesting when to try a new *ansatz* or analytic approach; or, occasionally, shining the light of inspiration into areas that had been thought devoid of new concepts or fundamental truths. It is this last use that I call heuristic, where the computer is being used to increase awareness of essential phenomena and thereby lead to a discovery.

Instead of attempting a philosophical discussion of these general ideas, I will try in this article to show with concrete examples how numerical solutions of complex nonlinear problems—often displayed most naturally by graphs or cinemas—may liberate us from the prejudices of our conservative and sometimes misguided intuitions. My examples will be drawn from work on nonlinear partial differential equations, particularly from my own work on the Fermi–Pasta–Ulam problem and solitons. I will also illustrate the state of progress in two frontier areas: vortex dynamics of two-dimensional incompressible wakes and jets, and axisymmetric supersonic jets (figure 1).

Nonlinear problems are almost always difficult, often with solutions that are unexpected and thus hard to obtain *a priori*. A computer can in such situations serve as a probe, to force an opening into an obscure or resistant region. Numerical answers to a problem can lead a prepared investigator to a solution by conventional analysis—occasionally an exact solution but more often an asymptotic form. In attempting to understand the details of the computer solution one may uncover a new group of problems or a new aspect of the given equations that give rise to a deeper understanding. An example of this synergism took place at Los Alamos in the 1940s. Enrico Fermi noticed that a set of computational results was insensitive to changes in a parameter. When he set it to zero, he was left with equations that were analytically tractable, obviating the need for much further calculation and giving a much clearer insight into the physics.[1]

Historical perspective

Lewis Richardson in his remarkable book, *Weather Prediction by Numerical Processes* (written, in part, at the front in World War I, and published in 1922), foresaw how computers could revolutionize our understanding and prediction of meterological processes through numerical solution of partial differential equations. However, he seemed unaware of the complexity of the physical problem, and he was not aware of the stability conditions required for a numerical solution for the coupled partial differential equations. (Richard Courant, Kurt O. Friedrichs and Hans Lewy were the first to investigate such conditions, in 1928.)

John von Neumann, who had been intimately involved with numerical analyses of fluid-dynamics problems during World War II, foresaw all the fundamental points I am trying to make. In a famous lecture[2] in 1946 he asked "To what extent can human reasoning in the sciences be more efficiently replaced by mechanisms?" and "What phases of pure and applied mathematics can be furthered by the use of large-scale, automatic computing instruments?" He continued:

> Our present analytical methods seem unsuitable for the solution of the important problems arising in connection with nonlinear partial differential equations and, in fact, with virtually all types of nonlinear problems in pure mathematics. The truth of this statement is particularly striking in the field of fluid dynamics. Only the most elementary problems have been solved analytically in this field. . . .
>
> The advance of analysis is, at

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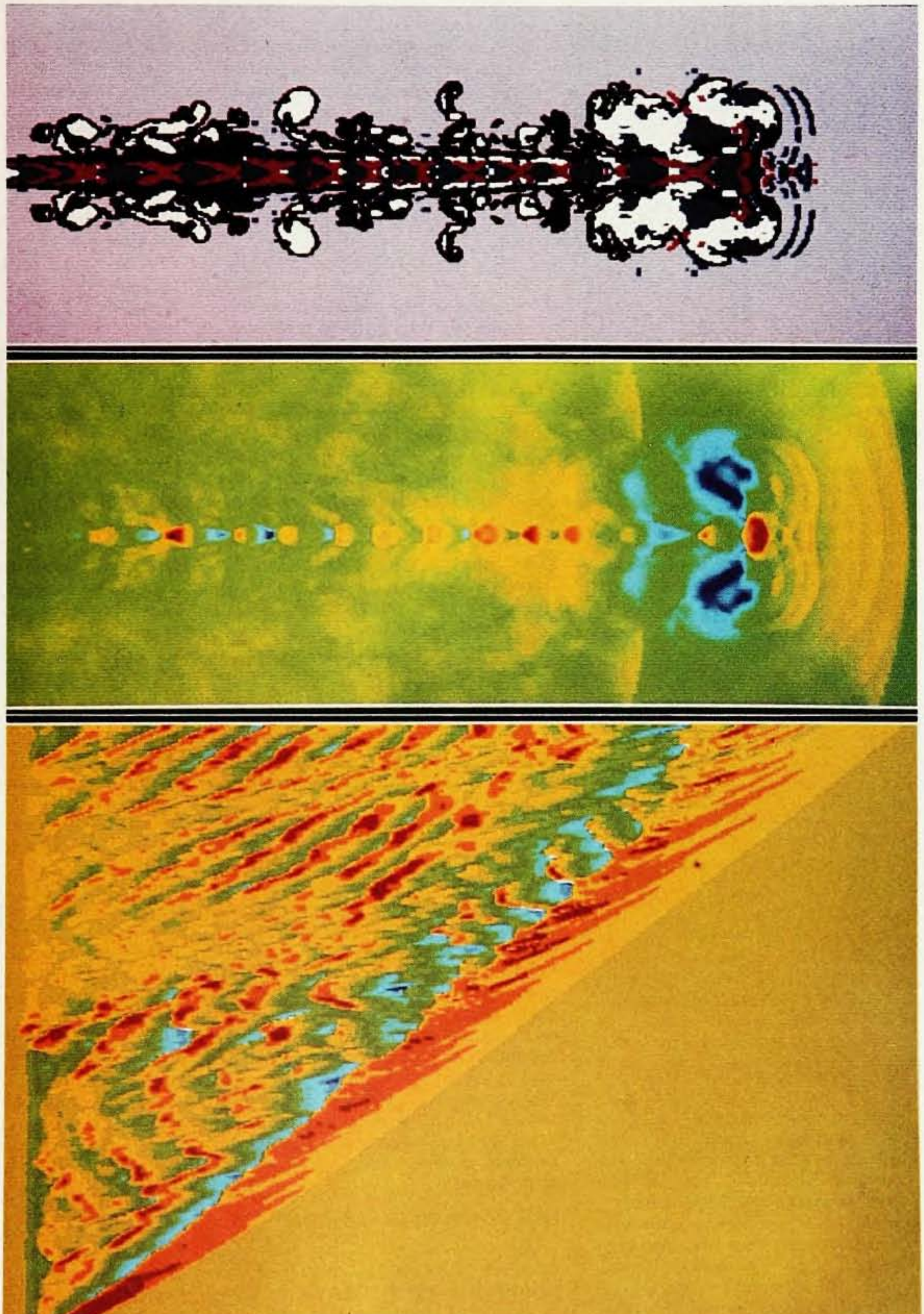
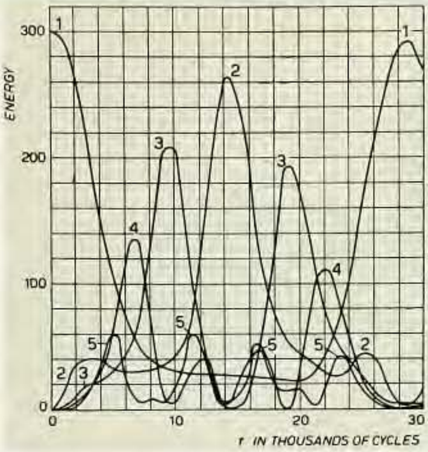
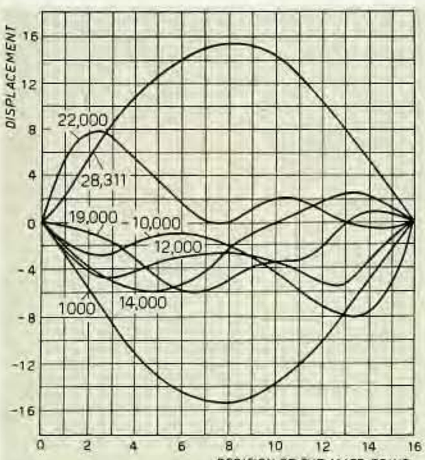


Supersonic jet. The jet, moving with a speed of Mach number 3.0 and having an initial density 0.1 times that of ambient gas, enters continuously at left (at $z = 0$, $r < 1$). Figures **a** and **b** show the state of affairs at $t = 60$ units. **a** Outline of the beam and cocoon; regions of divergence (or expansion) (that is, for which $\rho^{-1}\mathrm{d}\rho/\mathrm{d}t = \nabla\cdot\mathbf{u} \gtrsim 0$) are shown in blue, convergence ($\nabla\cdot\mathbf{u} \lesssim 0$) are red, neutral regions ($\nabla\cdot\mathbf{u} \sim 0$) are white. **b** Pressure in the volume: high-pressure regions are shown in red, low-pressure regions in blue, with intermediate pressures indicated in "rainbow" order. Note the shock wave at right. **c** Space-time diagram for the on-axis pressure; time increases up from $t = 0$ at bottom to $t = 60$ in units of (radius of jet)/(speed of sound in ambient medium). (Courtesy M. L. Norman, L. L. Smarr and K.-H. A. Winkler). Figure 1



Nonlinear lattice. These graphs, from the original paper[5] of Fermi, Pasta and Ulam, show (**a**) the total energy in each of the first five modes as a function of time, and (**b**) the displacement of the point masses at various times (in cycles). There are 32 masses, coupled by slightly nonlinear springs (linear plus quadratic potential), initially displaced into a single cosine wave. Note the almost perfect recurrence of the initial condition after about 30 000 cycles of oscillation. Figure 2



this moment, stagnant along the entire front of nonlinear problems.... This phenomenon is not of a transient nature, but ... we are up against an important conceptual difficulty ... yet no decisive progress has been made ... which could be rated as important by the criteria that are applied in other, more successful (linear!) parts of mathematical physics....

It is important to avoid a misunderstanding at this point. One may be tempted to qualify these [shock wave and turbulence] problems as problems in physics, rather than in applied mathematics, or even pure mathematics. We wish to emphasize that it is our conviction that such an interpretation is wholly erroneous....

They give us the first indication regarding the conditions that we must expect to find in the field of nonlinear partial differential equations, when a mathematical penetration into this area, that is so difficult of access, will at least succeed. Without understanding them and assimilating them to one's thinking even from the strictly mathematical point of view, it seems futile to attempt that penetration....

That the first, and occasionally the most important, heuristic pointers for new mathematical advances should originate in physics, is not a new or a surprising occurrence. The calculus itself originated in physics....

We conclude by remarking the really efficient high-speed computing devices may, in the field of nonlinear partial differential equations as well as in many other fields which are now difficult or entirely denied of access, provide us with those heuristic hints which are needed in all parts of mathematics for genuine progress. .... This should ultimately lead to important analytical advances.

Stanislaw Ulam emphasized the role of good graphics in his discussion[3] of computing machines as a heuristic aid in 1960—a discussion he also headed "synergesis." The visualization of mathematics will also be a focus of this article. I will try to demonstrate how signatures that show up in graphical displays can serve as nuclei around which a well-prepared investigator can form ideas and concepts: One good graph that highlights the evolution of a coherent pattern can be worth more than a thousand equations. Appropriate graphical displays (and I will show some below), especially ones that are constructed and compared on a screen as the investigator interacts with the computer, will improve our ability to choose wisely among promising paths. This mode of investigation couples naturally with the usual approaches of experiment, theoretical formulation, theorem proving, and asymptotic approximation.[4]

Heat conduction in a lattice

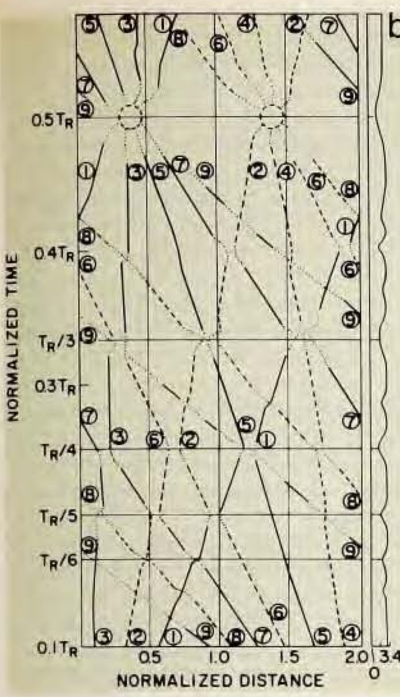
One of these intractable nonlinear problems is the conduction of heat in a nonmetallic lattice. Already in 1914, Peter Debye suggested that the finite thermal conductivity of these lattices arises from the nonlinear interactions among lattice vibrations (what we now call phonon–phonon scattering). The problem of deducing a finite thermal conductivity for an anharmonic lattice has challenged theoretical physicists for the last fifty years, and has produced a great many false starts and a great many theories that overlook some essential fact. No one doubts that the connection exists, but the derivation had proved elusive.

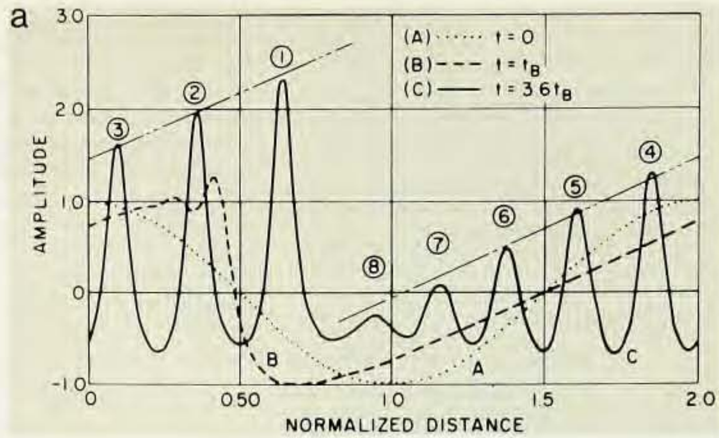
To illuminate the problem, Fermi, John Pasta and Ulam set out in 1955 to investigate how long it takes a long-wavelength oscillation to equilibrate in a nonlinear one-dimensional continuous string. Such a system was generally considered to obey the usual "ergodic" behavior, in which an initial energy distribution relaxes, to be shared equally among all the degrees of freedom of the system. The specific case considered[5] by Fermi, Pasta and Ulam is a discrete version of the string: a set of N identical masses in a line between fixed walls, coupled to each other (and the walls) by identical springs, each with a small power-law nonlinearity.

Much to their surprise, when Fermi, Pasta and Ulam performed the calculations on the MANIAC computer at Los Alamos, they found that the oscillations of the system showed "very little, if any, tendency toward equipartition of energy among the degrees of freedom." The most striking aspect of the behavior was a near-recurrence of the initial condition after a large number of oscillations: after 158 of the linear system's periods $2\pi(m/\kappa)^{1/2}$ more than 97% of the energy was restored to the fundamental mode. Varying the strength of the nonlinearity and the number N of particles (from 16 to 64) produced no qualitative differences in the behavior. Figure 2 shows results for one of the cases. The returns are clearly not numerical artifacts.

One could now take two different approaches: either to worry about the lack of equilibration and look for it elsewhere or to wonder if the character of these solutions is an aspect of something more general. The first (and, I suspect, more common) approach would lead one to other models to try to find some that did exhibit the equipartion one is looking for—by changing masses or spring constants, for example; or it could lead one to appeal to intuition to argue that in real, three-dimensional systems there are so many degrees of freedom and so many trajectories in phase space that the expected ergodic behavior is much more likely than in the one-dimensional system Fermi, Pasta and Ulam considered. The other (which I would call the heuristic) approach would lead one to ask, is there something essentially new and interesting in these near recurrences that the computer has found—do they result from the manner in which we made a discrete problem for the computer from the original, continuous one? It turns out that is does.

If we look at the graphs for the Fermi–Pasta–Ulam calculations we can see that, contrary to expectations,





Solutions of the Korteweg–de Vries equation. These graphs, from N. J. Zabusky, M. D. Kruskal, *Phys. Rev. Lett.* **15**, 240 (1965), show (**a**) the solutions of the KdV equation at three different times, and (**b**) trajectories of the maxima on a space–time diagram from $t = 3.6$ $t_B = 0.1t_R$ to $t > 0.5t_R$ (t_R is the near-recurrence time). The peaks into which the solution breaks up are numbered in **a**; the same numbers are used for the trajectories in **b**. The parameter δ of equation 3 is 0.022; the initial waveform is $u(x,0) = \cos\pi x$, and the boundary conditions are periodic. Compare this figure with figure 2 for usefulness in elucidating the soliton concept. Figure 3

only a small number of modes participate in the dynamics. Recognizing this, Martin D. Kruskal suggested that one should be able to see similar behavior in a continuum model as well, that is in a model described by a nonlinear partial differential equation. Kruskal's stimulating presentation of this problem at a seminar at Princeton in 1960 led me to join him in trying to unravel the problem posed by the Fermi–Pasta-Ulam results.

A typical textbook derivation of the wave equation will start with Newton's second law for coupled masses in one dimension and proceed to the limit as the masses become a continuum, for example by letting the distance h between them approach zero while keeping the mass per unit length and the spring stiffness constant. For a nonlinear (cubic) potential, the discrete version is of the form

$$m\partial_t^{\,2} y_n = \kappa(y_{n+1} - 2y_n + y_{n-1}) \times [1 + \alpha(y_{n+1} - y_{n-1})]$$

The term in α arises from the cubic part of the potential energy. (One can choose the time step for solving the differential equations on the computer to be sufficiently small that it does not affect the results.) To produce the continuum version, we let

$$h \to 0$$
$$Nh \to 1$$
$$h^2\kappa/m \to c^2$$
$$2\alpha h \to \epsilon$$

To lowest order in h, then, the discrete equation becomes

$$\partial_t^{\,2} y = c^2(\partial_x y)[1 + \epsilon\partial_x y] \qquad (1)$$

The fixed boundaries of the string require $y(0,t) = y(1,t) = 0$. Here we use the shorthand $\partial_x \equiv \partial/\partial_x$ and $\partial_t \equiv \partial/\partial_t$. (Note that for a linear string ϵ is 0, and the equation simply reduces to the ordinary wave equation for waves propagating with a speed c.) To analyze the continuum equation, Kruskal assumed periodic boundary conditions, that is $y(0,t) = y(1,t)$, and was able to reduce the nonlinear wave equations via an asymptotic heuristic argument and several changes of variables to the first-order equation

$$\partial_t u + u\partial_x u = 0 \qquad (2)$$

(the dependent variable u here, which is roughly $\partial_x y + \partial_t y$, is related to what is called a Riemann invariant of the previous equation.) Solutions of this first-order equation are not well-behaved: With the initial and boundary conditions we have imposed, the derivatives of the solutions, u, become singular in a finite time t_B. There is no corresponding singularity apparent in the numerical calculations.

The question then arises, is the breakdown a result of the low-order approximation (which produced the first-order equation) or of the periodic boundary conditions (instead of the fixed boundaries)?

In 1962 I was able to show that equation 1 (the nonlinear wave equation) with fixed boundary conditions also exhibits the breakdown. Two years later Peter Lax was able to show that the same kind of breakdown occurs under a variety of conditions in the class of equations

$$\partial_t^{\,2} y + F(\partial_x y)\partial_x^{\,2} y = 0$$

Investigating the breakdown, or "blow-up," of solutions has now grown into a branch of analysis for systems of nonlinear partial differential equations.

Somewhat later in 1962, I did the calculations analogous to those of Fermi, Pasta and Ulam, but for periodic boundary conditions, and found the same near-recurrence of the initial condition. Like the results for fixed boundaries, the calculations show only a very small effect at the breakdown time t_B.

The Korteweg–de Vries equation

Given that the lattice solutions continue smoothly beyond the breakdown exhibited by the solutions of equations 1 and 2, how must we modify the continuum equations to model the lattice solution?

At a conference in 1963 on mathematical modeling,[6] we proposed keeping the next higher-order term in the spring length h to give a continuum equation that could avoid the breakdown and possibly model the near-recurrence phenomenon. We were thus led to explore the equation

$$\partial_t^{\,2} y = c^2(\partial_x^{\,2} y)(1 + \epsilon\partial_x y) + (c^2h^2/12)\partial_x^{\,4} y \qquad (3)$$

Essentially, by keeping the term with an explicit h in it, we are taking into account the graininess or dispersive effects of the medium. (Note that we are not taking into account the graininess of time that the computations also assume. Fermi, Pasta and Ulam had noticed that varying the time increment had some effect on their results; however, these effects are similar to those of the spatial graininess.)

At this point Kruskal applied some

The modified KdV equation

If the anharmonic part of the potential energy of the Fermi–Pasta–Ulam lattice described in the text is changed from cubic to quartic, the asymptotic limit yields a modified Korteweg–de Vries equation:

$$\partial_t u + u^2 \partial_x u + \delta^2 \partial_x{}^3 u = 0$$

It has a localized solution

$$u = A\,\mathrm{sech}[(x - ct)/\Delta]$$

where $\Delta = 6^{1/2}\delta/A$ and $c = A^2/6$. Kruskal and I found several conservation laws. An incisive breakthrough came when Robert Miura, who was calculating conservation laws, realized an equivalence (the "Miura" transformation), namely:

If v is a solution of the modified KdV equation

$$\partial_\tau v - 6v^2 \partial_x v + \partial_x{}^3 v = 0$$

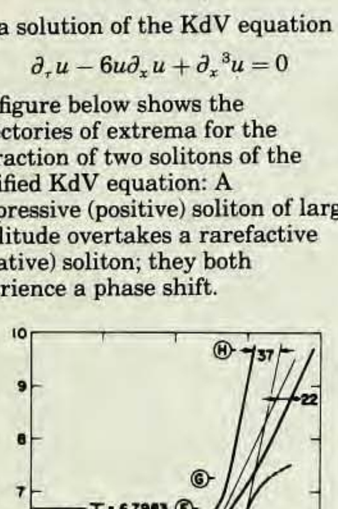
then

$$u = v^2 + \partial_x v$$

is a solution of the KdV equation

$$\partial_\tau u - 6u \partial_x u + \partial_x{}^3 u = 0$$

The figure below shows the trajectories of extrema for the interaction of two solitons of the modified KdV equation: A compressive (positive) soliton of larger amplitude overtakes a rarefactive (negative) soliton; they both experience a phase shift.



ideas from his work on an asymptotic theory for Hamiltonian systems having almost-periodic solutions and obtained the third-order equation[7]

$$\partial_t u + u \partial_x u + \delta^2 \partial_x{}^3 u = 0 \qquad (4)$$

Here the "slow time" t corresponds to $\epsilon ct/2$ in the earlier equation, and the parameter δ^2 is $h^2/12\epsilon$.

This equation was first obtained in 1895 by D. J. Korteweg and G. de Vries to describe the propagation of long-period waves in shallow water, of the sort observed by John Scott Russel in 1834 on the Union Canal near Edinburgh.[8] Since then it has cropped up in many other contexts as an asymptotic description of long-wave propagation. Korteweg and de Vries had already found a localized stationary solution:

$$u(x,t) = u_0 + A\,\mathrm{sech}^2[(x - ct)/\Delta] \qquad (5)$$

where $c = u_0 + A/3$ and $\Delta^2 = 12\delta^2/A$, that is, the propagation speed depends on the amplitude of the wave. They had also found periodic solutions, the so-called "cnoidal waves."

Kruskal and I set out to find exact solutions by applying standard perturbation methods to find other solutions of the KdV equation, using equation 5 as a basis, but without much success. However, we found we could obtain two "conservation laws" of the form

$$\partial_t T^{(n)} + \partial_x X^{(n)} = 0 \qquad (6)$$

where $T^{(n)}$ and $X^{(n)}$ are functions of u and its spatial derivatives. Such relationships imply essentially that the integral of T over all x remains constant in time—that is T is a conserved quantity.

We then turned to a numerical simulation of the KdV equation with periodic boundary conditions, and with initial condition $u(x,0) = \cos\pi x$, corresponding to a long progressive wave on the lattice. We found the near-recurrence we expected, at a time I will call t_R, as well as other interesting results, but we did not understand the reasons for the recurrences any better than for the Fermi–Pasta–Ulam problem. Gary S. Deem had recently joined Bell Labs at Whippany and assisted us with the programming and graphics. Although we pored over numerous polar diagrams of modal energy vs. modal phase, and both energy and phase vs. time, they told us little of what was happening. So we began to look at the waveforms of $u(x,t)$ and quickly realized that the solitary-wave solution with the hyperbolic secant shape (equation 5) dominates the evolution of the waveform.[9] The "solitary" waves emerge from the initial waveform, propagate, and sometimes merge with other waves of different amplitudes to form smooth regions that soon decompose again to form the pulses that had merged.

Figure 3 shows the behavior of solutions of the Korteweg–de Vries equation for an initial cosine wave; the graphs show both the waveforms at various times and the trajectories of the maxima on a space–time diagram. After an initial period (corresponding approximately to $3.6t_B$), nine well-formed sech^2 pulses appear. When they interact with each other they "accelerate" or "decelerate," giving rise to a phase shift, but otherwise they are remarkably stable. To someone who regarded these sech^2 pulses as some kind of elementary particle it would appear as if they had briefly merged to form an excited state. The results were so dramatic that Deem and I summarized them in a computer-generated ciné film. This film also contains solutions to the modified KdV equation (see the box at left) and to the cubic lattice; it is in the Bell Labs film library, and I believe it has been an inspiration for research workers and students.

Somewhat later (in 1972) Fred Tappert produced contour plots of $u(x,t)$ on a space–time diagram. Figure 4, one of his plots, clearly shows five maxima emerging from the initial cosine wave, propagating with nearly uniform speeds, suffering phase shifts after interacting and temporarily "coalescing" at the near-recurrence time t_R. Note that although this information is in principle contained in plots of waveforms, such as those of figure 2, it is only in plots like this or in sequences that show the time evolution (as in a ciné film) that one could actually see the underlying regularity.

Solitons

The remarkable stability of these localized waveforms led us to call them "solitons." Other such localized, or periodic, stable waveforms have since appeared in many other physical contexts, and it is useful to define a soliton generally as

> a localized or solitary entity that propagates at a uniform speed and preserves its shape and speed in interactions with other such entities.

A more mathematically precise definition relates[10] the soliton amplitudes and speeds to the discrete eigenvalues of linear operators, but this will suffice for our purposes. The box at left shows another illustration of the phase shift resulting from the interaction of two solitons of the modified Korteweg–de Vries equation.

The existence of solitons clarifies the near-recurrences found by Fermi, Pasta and Ulam. Nearly any smooth initial condition leads to solitons arrayed according to size in a nearly linear fashion, as in figure 3a. They propagate through the system at various speeds and at some sufficient large time return to a similar, but ascending, nearly linear array; time reversibility then guarantees the near-recurrences. However, the question remains: Are these observations—for example, the persistence of solitons and the near-recurrences—mathematically exact?

At the time that we were doing these calculations at Bell Labs, Gerald B. Whitham found a third conservation law for the Korteweg–de Vries equation. Prompted by this discovery, we also began to look for more conserved quantities and soon found two more. Then Robert M. Miura found five more—there seemed to be no end. In fact, Clifford S. Gardner, who also joined our efforts at this time, was able to show, using an ingenious transformation, that the Korteweg–de Vries equation has an infinite number of conservation laws. This insight opened the way to an analytic understanding of the KdV equation. The Princeton group—Gardner, Greene, Kruskal and Miura—exactly linearized[11] the KdV equation in 1967 and were able to show that it is equivalent to what is called an isospectral eigenvalue problem; the constant eigenvalues are the invariant soliton amplitudes and the properly normalized eigenfunctions are related to the solitons that emerge from the initial waveform $u(x,0)$. There also exists an oscillatory solution of the KdV equation that corresponds to the continuous part of the eigenvalue spectrum.

In the early 1960s J. Perring and T. H. R. Skyrme nearly discovered solitons in a nonlinear field theory. In discussing field theories for models of mesons, Werner Heisenberg, Fermi, Wolfgang Pauli and others had suggested that field theories did not have to be linear. The model investigated by Perring and Skyrme is now called the sine-Gordon equation:

$$\partial_x{}^2\psi - c^2\partial_t{}^2\psi = \kappa^2\sin\psi \qquad (7)$$

(Its name arises as a punning variation on the Klein–Gordon linear model of a relativistic meson field.) The equation had, in fact, been known in differential geometry since the end of the last century and arose in the 1950s in studies of the motion of crystal dislocations. Perring and Skyrme found stationary solutions moving with a speed less than c, which have come to be known as particles, kinks or fluxons; there are also solutions of the opposite polarity—antiparticles, antikinks, or antifluxons. Perring and Skyrme investigated these solutions numerically. To their surprise, they found that kinks scattered elastically off a fixed boundary and they found waveforms that exhibited kink–kink scattering as well as kink–antikink scattering. Unfortunately, no further work developed out of these findings.

Why was this pioneering salient loss? One possibility is that a majority of particle physicists, at that time, believed in linear field theories. Furthermore, they felt that there was little insight to be gained from problems in one space dimension. Another, more probable, explanation is that the computational ambiance was neither broad nor detailed nor valued enough to sustain creative momentum to overcome the barriers of "establishment" intuition.

At about the same time that we were beginning to understand the near recurrences in the Fermi–Pasta–Ulam problem, Morikazu Toda in Japan found[12] a one-dimensional lattice system that supported solitary and periodic waves (see the box at right). For small-amplitude oscillations, the Toda lattice is consistent with the cubic lattice, which is where Fermi, Pasta and Ulam had started out.

In 1968, when I attended the International Conference on Statistical Mechanics in Kyoto, I was surprised to find that Toda had solved the two-soliton interaction for his lattice. It wasn't until 1974 that Maurice Henon and Hermann Flaschka showed the integrability of the Toda lattice and thus the persistence of multiply interacting solitons.

Most nonlinear problems do not fall into the class of integrable systems and they exhibit both coherent and "chaotic" behaviors. Leo Kadanoff discussed recent work on some ordinary differential equations and iterated maps in his article on paths to chaos (December, page 46). Particularly noteworthy examples of the synergetic use of the computer[4] are work by the meteorologist Edward N. Lorenz in the early 1960s and some discoveries by Mitchell Feigenbaum in the late 1970s. Lorenz, who is interested in weather predictability, explored the properties of a system of three ordinary differential equations that models a simple convective flow and found a "strange attractor," that is, chaotic behavior in a small region of phase space. Feigenbaum found universal properties of iterated maps, namely that there exist universal numbers that determine parameters at which simple systems change their evolutionary behavior (for example, double their recurrence period). The relevance of these results for realistic continuum systems is under active investigation.

The Toda lattice

Consider a lattice of point masses at positions r_n. Their potential energy is of the form

$$V(r) = (a/b)\mathrm{e}^{-br} + ar + \text{const}$$

In dimensionless form, the equations of motion are

$$\ddot{r}_n = \mathrm{e}^{-r_{n+1}} - 2\mathrm{e}^{-r_n} + \mathrm{e}^{-r_{n-1}}$$

Or, with

$$\dot{s}_n \equiv \mathrm{e}^{-r_{n-1}}$$

the equation of motion becomes

$$\ddot{s}_n/(1+\dot{s}_n) = s_{n+1} - 2s_n + s_{n-1}$$

which has soliton solutions of the form

$$s_n = \beta^2\,\mathrm{sech}^2(\alpha n \mp \beta t) \qquad \beta = \sinh\alpha$$

Vortex dynamics

Another problem, mentioned by von Neumann in his 1946 lecture, that leads to equations intractable by classical methods is the evolution of turbulent flows. The solution of such problems will elucidate such diverse fields as the evolution of jets and wakes and the predictability of atmospheric and oceanographic weather. Until very recently many of the analytical studies of turbulent flows employed wavenumber-dependent Fourier-transformed variables. Physical-space variables were not considered efficacious. That view is changing. In 1977, I wrote[13]

> In the last decade we have experienced a conceptual shift in our view of turbulence. For flows with strong velocity shear ... or other organizing characteristics, many now feel that the spectral or wavenumber-space description has inhibited fundamental progress. The next "El Dorado" lies in the mathematical understanding of coherent structures in weakly dissipative fluids: the formation, evolution and interaction of metastable vortex-like solutions of nonlinear partial differential equations....

This approach of examining things in physical space has recently been pursued by James McWilliams, of the National Center for Atmospheric Research.[14] He found that two-dimensional decaying flows with high Reynolds numbers did not exhibit Gaussian statistics because of the emergence (from an initial random-phase, power-law energy spectrum) of many isolated, "coherent" vortex states. In the discussion he notes, "Much of our present interpretation of atmospheric predictability limits is based upon (Fourier-space moment) closure theory solutions ... and the possibility of long-lived vortices may alter the interpretation." That is, an alternative approach to predictability may be emerging.

One of the classic problems of inhomogeneous turbulence is the flow of a viscous fluid past a bluff obstacle or over a thin flat plate, such as an airplane wing, bridge span or even mountain range. The flow is stable for low velocities (low Reynolds numbers). As the velocity is increased, the laminar flow becomes unstable on the downstream side and localized vortical regions grow and are shed into the flow. These form (often very pretty) double

Contour plot of solutions of the KdV equation. This is essentially a more detailed plot than figure 3b, but of analogous information. In this case, the initial waveform is again $\cos\pi x$; the boundary conditions are periodic, and the parameter δ is somewhat larger than 0.022. (The number of solitons under these conditions is about $0.2/\delta$.) This—previously unpublished figure—was produced by F. D. Tappert in 1972. Figure 4

rows of vortex regions, called "vortex streets." At still higher Reynolds numbers, experimenters have observed a sudden breakdown of the slowly changing pattern, which usually results in more chaotic and turbulent regions. These qualitative features have been known for a long time. In the 1960s experiments by Hiroshio Sato and his colleagues and by S. Taneda indicated the possible development of vortices in the wake of a flat plate, and Taneda found evidence of wavelength growth (approximately doubling) in the far wake.[13] Gary Deem and I were the first to try to understand aspects of this wake behavior computationally.[15]

In describing the flow of an incompressible fluid one starts with the Navier–Stokes equations. These are essentially Newton's second law for the fluid and the equation of continuity

$$\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} = -(1/\rho_0)\nabla p + \nu\nabla^2\mathbf{u} \quad (8)$$
$$\nabla\cdot u = 0$$

Here $\mathbf{u}$ is the velocity of fluid and ρ_0 is a constant density; p is the pressure and ν is the kinematic viscosity. Although nature is three-dimensional, one can gain a great deal of insight from well-chosen two-dimensional problems where there are only two coordinates and the velocity vector has only two components, $\mathbf{u} = (u,v)$, which greatly reduces the computational burden. In our computer simulations we used a finite-difference algorithm on a periodic domain.

Let us consider a flat plate that extends along the negative x-axis, with a lip somewhat to the left of $x = 0$. The fluid flows to the right. Experiments have shown that a little downstream from the lip of the plate, the laminar velocity profile can be approximated by a Gaussian function of the cross-stream position y; we shall take this position as $x = 0$. Because the memory and speed of computers are inadequate to model the complete physical domain, we considered a periodic region, namely $\mathbf{u}(x + L, y) = \mathbf{u}(x, y)$, which can be thought of as a window "panning" a piece of the fluid as it translates downstream. To start things off we introduced a perturbation: the lowest sinusoidal harmonic mode (proportional to $\sin 2\pi x/L$), which has the largest growth rate. Figure 5 shows a sequence of contour plots of the vorticity

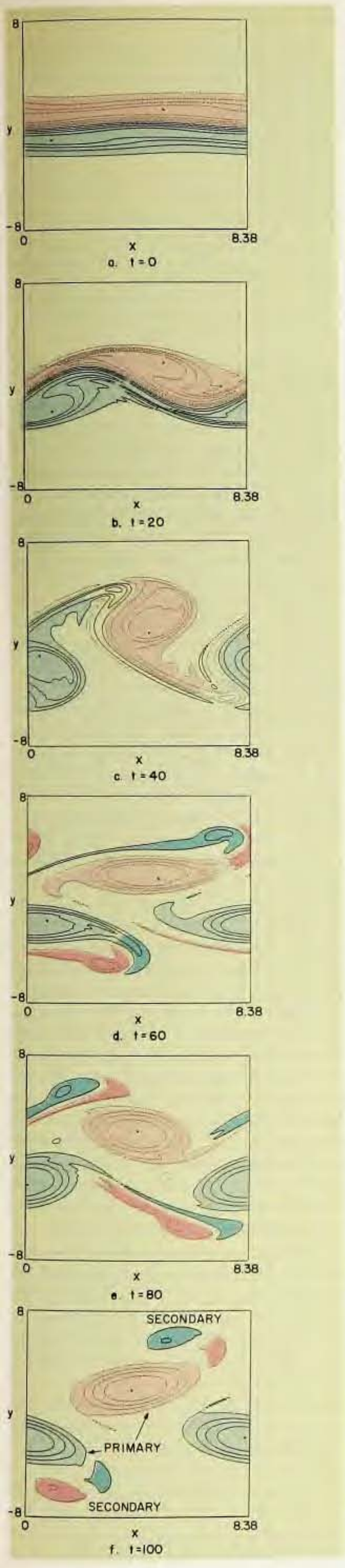
$$\omega = \hat{z}\cdot\nabla\times\mathbf{u} = \partial_x v - \partial_y u \quad (9)$$

obtained from the solution that has evolved from this linearly unstable profile. We see the growth of large primary and smaller secondary vortex regions. The secondary regions are a manifestation of opposite-sign vortex entrainment and are first clearly seen in figure 5d. We made a careful comparison of the flow at different times and found that the primary vortices, which are elliptical in shape, are slowly "nutating"; this is due to the interaction of the mean flow with the elliptical vortex regions and has been calculated quantitatively. This effect was observed, but not recognized, by Sato, and provided us with a subtile means for validating the computation. The effect has since been identified in many experiments.[16]

Ron Hardin doubled the wavenumber of the perturbation, and we observed a pattern similar to that shown in figure 5, except with two of everything per period. The surprise—which we saw in a computer-generated film from an overnight run that Hardin tended—was that this state was also unstable: After a sufficiently long time, the nutating, regularly spaced pattern "broke down" and the regions of like-signed vorticity merged—that is, we obtained a wavelength doubling.

When I visited Culham Research Laboratory in 1973 I found that Jess Christiansen had developed a computer code, using the vortex-in-cell algorithm for the periodic incompressible Euler equation (that is, equation 8 with $\nu = 0$). We observed similar effects when we started with a simpler wake-like initial profile.[17] Furthermore, if two positive and two negative finite-area vortex regions are placed asymmetrically in a periodic domain at the appropriate transverse-to-longitudinal separation distance ($h/l = 0.281$), the flow can be *stabilized* if the vortex regions have a sufficiently large area. This was a surprise, as flows with point vortices were known to be unstable.

Very recently, S. Kida, using a perturbation analysis, and Daniel Meiron, Philip Saffman and J. Schatzman, using a computer model, showed this stability from a linear point of view. Furthermore they showed that the flow is necessarily unstable, no matter what the area of the vortex regions, if h/l is far from 0.281 (in the last part of figure 5, for example, h/l is 0.47) or if h/l is 0.281 and the domain of the perturbations is not periodic (so that large-wavelength subharmonic perturbations can arise). They used a "contour-dynamical" algorithm to find steady-state solutions with piecewise constant vorticity in an asymmetric double-row configuration. This wake-like model was subjected to a linear perturbation analysis, which was performed on the computer because the shapes of the steady vortex states (which I call "V-states") are not well-known functions. The contour-dynamics representation[18] is a generalization of the "waterbag" model; it is both computationally efficient and mathematically lucid. It reduces the evolution of two-dimensional inviscid flows to the movement of contours (or interfaces) bounding regions of piecewise-constant vorticity. Recently Edward



Evolution of vortices downstream from a plate: contour lines of the vorticity ω at various times, from reference 15 (color added). The periodic boundary conditions in x let the simulation approximate a window that moves along with the fluid as it flows downstream from the plate. The flow at $t = 0$ (top) is a harmonically perturbed Gaussian profile. Eventually, the flow breaks up into primary (dark) and secondary (light color) vortex regions of positive (blue) and negative (red) vorticity. The horizontal and vertical scales are different; in the last figure, for example, the ratio of transverse to longitudinal distances between vortex centers is 0.47. Note the nutation of the primary vortex regions. Figure 5

Overman used an analytical–computational synergetic analysis to examine the "limiting" singular properties of rotating and translating V-states.

Hassan Aref and Eric Siggia continued the computer-simulation investigation of the evolution of wake-like structures with a "vortex-in-cell" code. They began with separated, symmetrically perturbed positive and negative vortex sheets. They confirmed the wake-breakdown results described above and also found another "breather" mode. That is, if the sheets are sufficiently close they evolve into a symmetrical dipolar structures, which loop away from the x-axis on trajectories of large radius and eventually return to the axis.

Recently, Glenn Flierl, Paola Rizzoli and I have used a more accurate pseudo-spectral code for similar wake studies, as well as ocean-related jet studies of models that include Coriolis terms in the equations of motion. These can model systems such as the Gulf stream. We now have a quantitative understanding of the wake flow phenomena which involve the shape and thickness of the wake and the wavelength of the initial small-amplitude perturbation. These insights are providing us with information for analytical progress on the formation of vortical structures in jets and wakes. However, we still are not sure if this wavelength-doubling mechanism accounts for Taneda's experimental results.

In the soliton and vortex studies there are many apparent missed openings, retreats or diversions. The creative process is one that Arthur Koestler has called[19] *"reculer pour mieux sauter."*

Supersonic jets

While vortices produced by low-speed flows past bluff bodies are a well-known and long-studied phenomenon, the study of supersonic jets is relatively recent. The earliest studies were carried out at low-supersonic speeds by Ernst Mach and Peter Salcher in the 1880s and 1890s. High-speed supersonic jets have recently become interesting because they may play a role in explaining some recently discovered astrophysical phenomena, such as the jet-like structures with "knots" one sees associated with some quasars and radiogalaxies.

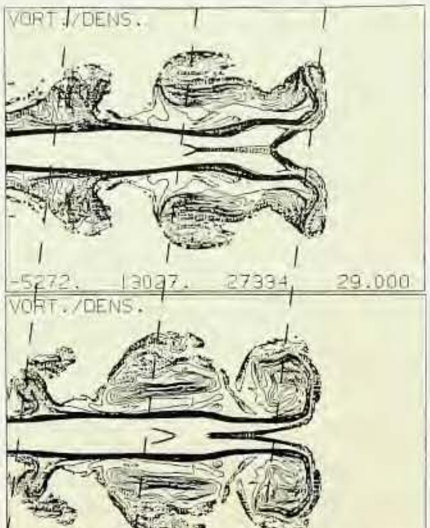
Undaunted by the sparsity of detailed experimental information—particularly for the astrophysical jets—Michael Norman, Larry Smarr and Karl-Heinz Winkler have performed[20] a detailed numerical simulation to study the evolution of these structures. To start, they introduce reasonable physical simplifications and assume that the observed phenomena are the result of nonionized, nonrelativistic and nonradiative hydrodynamics. Furthermore, because of the present limitations of computer size and speed, they also assume nonswirling axisymmetric flow (variables are a function of r, z and t only). Thus the model consists of the Euler equations for a compressible fluid

$$\begin{aligned}
&\partial_t \rho + \nabla\cdot(\rho u) = 0\\
&\partial_t(\rho \mathbf{u}) + \nabla\cdot(\rho \mathbf{uu}) = -\nabla p + \mathscr{D}\\
&\partial_t p + \nabla\cdot(p\mathbf{u})\\
&\quad = -(\gamma - 1)p\nabla\cdot\mathbf{u} + \mathscr{Q}
\end{aligned}$$

where $\mathscr{D}$ and $\mathscr{Q}$ have been inserted to model the effects of dissipation at discontinuous interfaces (such as shocks). In the future, these physical and geometrical constraints will be relaxed as phenomena are understood quantitatively and as better agreement with experiment and observation is sought. The control of numerical discretization errors will be a part of this synergetic approach. Note that, despite these simplifications, the parameters for Mach number M of the beam and the density ratio of beam to ambient ρ_b / ρ_m can be made much beyond those achievable in present-day laboratory experiments.

As shown in figure 1 and on the cover,[21] the jet enters the domain continuously at the left ($z = 0$) as a beam of constant density and unit radius; the undisturbed beam is clearly seen in figure 1a as a small, white, triangular region. The boundary at $r > 1$, $z = 0$ allows outflow, to accomodate the gas within the "cocoon" or sheath.

Figures 1a and 1b visualize the beam at $t = 60$ (in normalized units). Part a shows the "divergence" (blue) and "convergence" (red) of the flowing gas; note the alternating red and blue x-shaped regions, which are manifestations of oblique internal shock waves. Part b shows high-pressure regions as red and low-pressure regions as blue; here one sees the bow shock as a discontinuity in color (light-green to yellow followed by a structured high-pressure region in yellow). Part c is a space–time diagram



Specific vorticity for a supersonic jet continuously moving into a counterstreaming environment. The contours are for the specific vorticity ω_ϕ/ρ close to the bowshock and working surface of a beam moving at Mach 6 into an ambient fluid having 10 times the density of the beam. The times of the plots (in normalized units) are given in the lower right corners of the plots; the remaining numbers give details about the numerical values involved in the model. The ambient fluid is moving to the left at a sufficiently great speed to arrest the beam's progress. The dashed lines track vortical features as they are released into the backflow in a quasiperiodic manner. Note the wave-like modulation of the surface of the beam. (Courtesy of M. L. Norman, L. L. Smarr and K.-H. A. Winkler.) Figure 6

for $t = 0$ (bottom) to $t = 60$ (top) of the on-axis pressure. Note the coherent near-periodic (red–yellow) crests of high pressure, translating to the right at a speed slightly greater than the bow shock (green–yellow diagonal). Most important (perhaps the essential discovery) is the undulating *near-periodic* pattern of pressure on the axis, like colored beads on a necklace. The first intense-pressure (red) region near the axis, at the right side of the figure, is the region of the "working surface" where the incoming beam fluid is reversed in direction to form a counterflowing "cocoon." The near-periodic pattern is also evident in part a. Further back in the cocoon, that is closer to $z = 0$, one sees highly distorted or "shredded" axisymmetric vortical regions in white. These counterflowing vortical regions may be responsible for the x-shaped patterns—it's all a complicated nonlinear feedback process.

When I visited Garching in November 1983 we began to examine the vortex "shedding" process in the vicinity of the working surface. We boosted the ambient environment slowly from zero to a uniform leftward translation and were able to nearly fix the location of the bow shock in the computational domain. Figure 6 gives a contour representation of the specific vorticity (ω_ϕ/ρ) for a beam at normalized times 29, 30, 31 and 32. This covers a cycle of a near-periodic vortex shedding event: We can see the right-most of the coherent features growing ($t = 29$ to $t = 30$) and detaching between $t = 31$ and 32, as a new feature begins to grow at the front of the jet.

We have yet to determine how many of these space–time features are related to the physical assumptions described above. However, the quasiperiodic behavior we see in the figures may provide a possible explanation of the quasiperiodic emission structures observed in extragalactic jets.

Graphics

The benefits of the computational approach—that is, the heuristic usefulness of the computer—clearly depend on the availability of various graphical displays. As in a laboratory experiment, one must be alert to recognize small effects that may signal new phenomena. The discovery of the slow oscillation or "nutation" of vortex regions in the plots shown in figure 5 and the near periodic array of pressure maxima in figure 1 are clear examples of the importance of proper graphical displays. We would never have seen these behaviors in voluminous printouts of columns of numbers. The picture has clearly produced an insight into the physics.

As our analytical insight matures, the character of the graphical representation should be focused on particular events and their interaction. Fermi, Pasta and Ulam plotted waveforms and modal energies, as shown in figure 2. When it became clear that the progressive waves with periodic boundary conditions contained the same effect, we began tracking trajectories of waveform extrema; this proved informative, for it allowed us to see phase shifts arising from localized interactions. Following the trajectories of extrema turns out to be a generally useful technique, although the picture can sometimes be confused by fluctuations, as figure 4 illustrates. I have generally found that plots of energy and so forth vs. wavenumber do not provide information for making decisive progress but complement what has been learned in configuration (physical) space.

Oblique isometric projections were used for nonlinear waves by Robin Bullough, Chris Eilbeck and Philip Caudrey at Manchester in the 1970s. This has now become a ubiquitous mode of display. It provides a useful and artistically pleasing global summary of the nonlinear wave phenomena. It would, for example, be hard to imagine a clearer representation of the stability of a soliton than figure 7.

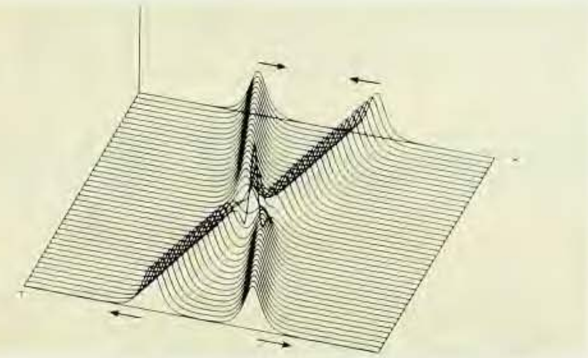
As I have already indicated, color can greatly enhance the perceptibility of small but essential details. Note that color is area-filling, so that color or gray-scale plots tend to draw the observer's eye to gross structures in the flow. Contour visualizations, on the other hand, emphasize details and give a better feeling for gradients, although the high density of information may obscure the essentials. A composite of both would be extremely useful!

Like color, ciné films or real-time video displays can greatly enhance the perceptibility of unexpected phenomena. In both cases, the added perceptual "dimensions" enhance the mind's ability to recall important features and to correlate old and new results.

With the advent of supercomputers, parallel processors and inexpensive memory, the computing power available to scientists and engineers has been increasing rapidly. However, the importance of interactive (via touch and voice), high-resolution color terminals for the perusal of computer-simulation results is just beginning to be recognized. Expert systems for this mode of study are in an infant stage. Robust and facile interactive graphics software still needs to be developed, to provide, for example:

▶ An ability to excise one-, two- or

Oblique projections of two-soliton interaction. The graph shows solutions of the nonlinear Schrödinger equation $i\partial_t\psi + \partial_x{}^2\psi + \kappa\psi|\psi|^2 = 0$ with two initial "sech" pulses. The analytic solution to this equation were first obtained by V. E. Zakharov and A. B Shabat, in Sov. Phys. JETP **34**, 62 (1972). The figure was produced for reference 4. Figure 7



three-dimensional regions containing extrema of some variable, so that we can easily track these extrema as a function of time (or some other parameter). The resulting diagrams will probably be "noisy," but informative.

▶ An ability to make spatial and temporal correlations to obtain the histories of regions around the extrema. Such an ability should include capacity for rotating, displacing, stretching, smoothing or computing moments of dependent variables to facilitate comparisons.

▶ An ability to retain important summary or diagnostic variables in a diary to enable the investigator to optimize comparisons and to savor the physical and analytical essence of the results.

A new *modus operandi*:

To me it is clear that the examples of computational synergism I have described validate von Neumann's foresight. The soliton concept, for example, has given rise to much new activity[4,10] in pure and applied mathematics; it also has provided a new conceptual basis for applications in diverse areas of physics, providing an economy of thought in posing problems and obtaining solutions. I believe that computational studies will be as useful in the future development of nonlinear science as the accelerators of the past were for nuclear and particle science. It is only a historical accident that supercomputers became available later than the superaccelerators. An important asset of the computational physicist or mathematician is the will to use the computer resources to the limit when the algorithms are working and the physics is puzzling. It was, for example, a real high to be sitting at 3:00 o'clock one Sunday morning in the terminal room at the Max Planck Institute for Astrophysics in Munich and watch Winkler "fly" his jet calculations through the Cray-1.

Are we providing the kind of training in our universities that our students will need to undertake this style of work at the nonlinear frontier? I believe not. We will need to find new methods for teaching students to experiment with computers the way we now teach them to experiment with lasers or cyclotrons.[22]

Erwin Chargaff, in his review[23] of nucleic-acid research, notes, "It is in general true of every scientific discovery that the road means more than the goal. But only the latter appears in ordinary scientific papers." I have here tried to show concretely that the analytical–computational synergetic approach is a mode of working that is applicable generally in the natural sciences. It requires good analysis and good computation—but it also requires good graphics and other modes of computer expression.

Wolfgang Pauli collaborated with Carl Gustav Jung on an investigation of psychology and epistomology.[24] Among Pauli's contributions was an analysis of the influence of archetypal ideas on Kepler's work. He refers to the importance of images in creative science:

> . . . What is the nature of the bridge between the sense perceptions and concepts? All logical thinkers have arrived at the conclusion that pure logic is fundamentally incapable of constructing such a link. . . . The process of understanding nature as well as the happiness that man feels . . . in the conscious realization of new knowledge, seems thus to be based on a correspondence, a "matching" of inner images with external objects and their behavior . . . images [called by Kepler archetypal—*archetypalis*] with strong emotional content, not thought out, but beheld, as it were, while being painted. . . . As ordering operators and imageformers in the world of symbolic images, the archetypes [or "primordial images" of Jung] thus function as the sought-for bridge. . . .

On the basis of my own experience with computers, I would paraphrase his remarks in a contemporary vein by:

> The discovery of new knowledge in the natural sciences is a manifestation of a "matching"—that is, a linkage or a resonance—between data and an image of that knowledge in deeper levels of our consciousness. A proper picture or graph in the external domain can synergize the formation of images in our "nonconscious" mind and provide an alternative route for discovery.

With computers, the intuitive–geometric approach can be developed, taught to our students and made part of the scientists' *modus operandi*.

* * *

My debt to people and support organizations was described in reference 4. In recent years I have benefited from support from the US Army Research Office and the Naval Research Laboratory. In particular, I wish to acknowledge Martin D. Kruskal, Gary S. Deem, Edward A. Overman II, friends and collaborators over the years. Kruskal's deep mathematical insights and power with asymptotic formulations were always an inspiration. Deem passed away last year and I recall with pleasure his assistance in the early phases of the lattice and soliton work and our later mutual participation in analytical and computational studies of the evolution of fluid instabilities, vortices and "V-states" and enzyme membrane transport. Thomas von Foerster of PHYSICS TODAY *produced the initial version of the manuscript and assisted with many modifications thereafter. The final version was completed during my visit to the MIT Department of Earth, Atmospheric and Planetary Sciences.*

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