EXPERIMENTAL MATHEMATICS: THE ROLE OF COMPUTATION IN NONLINEAR SCIENCE

Dedicated to the memory of our friend and colleague, Stanislaw M. Ulam.

Computers have expanded the range of nonlinear phenomena that can be explored mathematically. An "experimental mathematics facility," containing both special-purpose dedicated machines and general-purpose mainframes, may someday provide the ideal context for complex nonlinear problems.

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It would be hard to exaggerate the role that computers and numerical simulations have played in the recent progress of nonlinear science. Indeed, the term *experimental mathematics* has been coined to describe computer-based investigations into nonlinear problems that are inaccessible to analytic methods. The experimental mathematician uses the computer to simulate the solutions of nonlinear equations and thereby to gain insights into their behavior and to suggest directions for future analytic research. In the last 20 years, the symbiotic interplay between *experimental* and *theoretical* mathematics has caused a revolution in our understanding of nonlinear problems [17, 25, 30].

Nonlinear science has become a discipline in itself, simply because nature is intrinsically nonlinear. The term *nonlinear science*, meaning the science of problems that are not linear, may seem odd at first: It seems to suggest that linear problems are the central issue, while in fact precisely the opposite is true. Both mathematically and physically, linear equations are the *exception* rather than the rule. Indeed, using a term like nonlinear science is, as the noted pioneer in experimental mathematics Stanislaw M. Ulam has observed, like referring to the bulk of zoology as the study of non-elephant animals. The reason for the nomenclature and for the strong bias toward the study of linear systems is expediency: In the past, *nonlinear* was nearly synonymous with *nonsolvable*. Today, thanks in large part to computers, many previously intractable nonlinear problems have been solved, and the field of nonlinear studies has come into its own.

We must distinguish two separate but related problems that occur in nonlinear science. The first of these is purely mathematical: Given an equation, what are its properties, and how can it be solved? The second problem involves what we call *modeling*: Given a process in the "real" world, how can we write down the best mathematical description or model? As scientists we want both to model the real world and to be able to solve the resulting models, and so we must address both problems, for the interplay between them is crucial. It is easy, for example, to write down the Navier-Stokes equations describing fluid motion; this does very little to reveal the nature of turbulent fluid flow, however. Similarly, intuition about the qualitative aspects of nonlinear behavior can be very valuable as a guide toward formulating the best set of equations to use as a model.

In mathematical terms, the essential difference between linear and nonlinear equations is clear: Linear equations are special in that any two solutions can be added together to form a new solution. As a consequence, there exist established analytic methods for solving any linear system, regardless of its complexity. In essence, these methods amount to breaking up the complicated system into many simple pieces and patching together the separate solutions for each piece to form a solution to the full problem. In contrast, two solutions to a nonlinear system cannot be added together to form a new solution. Nonlinear systems must be treated in their full complexity. It is therefore not surprising that no general analytic approach exists for solving them. Furthermore, for certain nonlinear systems that generate *chaotic* motion, in a sense we will discuss, there are no useful analytic solutions.

In modeling a real-world physical process, it is important to realize that a natural system that can be described by a linear model in some circumstances must be described by a nonlinear model in others. An example from elementary physics that illustrates this

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very clearly is that of a pendulum constrained to move in a plane. For small oscillations, the motion of the pendulum is well approximated by a linear model, and it can be shown that the pendulum's period is independent of its amplitude. This result was first observed by Galileo. For the full nonlinear equation, however, this result is not true: The period depends on the amplitude, and larger excursions take longer. Since in a real clock the amplitude always drifts slightly, a pendulum making large oscillations keeps very poor time.

A more striking illustration of the difference between a full nonlinear model of the pendulum and its linear approximation occurs when the effects of friction are included and a periodic driving force is added. In the linear model, a closed-form solution can still be obtained, and the motion can be described analytically for all time. For the nonlinear equation, the solution for certain values of the driving frequency is periodic and not too dissimilar from the solution of the linear model. For other values, however, the solution becomes chaotic and behaves in a seemingly random, unpredictable manner. As we show in the next section, the motion of the pendulum in this chaotic nonlinear regime defies analytic description.

That nonlinear equations can be chaotic has profound consequences in all of the sciences. The unpredictability and irregularity inherent in such diverse phenomena as fluid turbulence, neural networks, and weather patterns exemplify this chaotic behavior. Computers have played an essential role in elucidating the underlying nature of such chaos.

Computers have always been used for experimental mathematics; this approach has significantly shaped the modern perspective on fundamental problems. An important example is the understanding of the approach to thermal equilibrium. It has long been known that part of the kinetic energy created by colliding objects is converted into heat. More generally, the organized motion of a macroscopic collection of atoms is converted into the disorganized microscopic motions associated with heat, in accordance with the second law of thermodynamics. Although this may sound obvious, a direct demonstration of this seemingly simple fact is one of the outstanding problems in physics. An understanding of nonlinear processes and effects is necessary for the resolution of this problem, since it is fairly easy to show that a finite set of linear equations cannot model such behavior. It had long been assumed that the addition of nonlinearities would immediately solve this problem.

Shortly after the Maniac I computer was built at Los Alamos in the early 1950s, Fermi, Pasta, and Ulam [10] undertook a numerical simulation of a nonlinear system to study the approach to thermal equilibrium. They used the Maniac to simulate the behavior of 64 particles coupled together by nonlinear springs. Displacing a few of the springs from equilibrium, they fully expected to eventually see random-looking "thermal" motions, with the average vibration spread equally among all the particles. Instead, they were surprised to discover that the original configuration of particles recurred—there was no approach to thermal equilibrium! This discovery stimulated a considerable amount of further investigation, and now, through a closely interwoven combination of experimental and theoretical mathematics, we know that the underlying cause of this unpredicted behavior is *solitons*, remarkable pulselike waves that exist in certain nonlinear partial differential equations. Since then, with the aid of computers, we have found out more about how nonlinearities can cause an approach to equilibrium, through chaotic behavior, although the problem is still far from being resolved. We now know that nonlinear equations can generate either order or chaos; the trick is determining which to expect and when.

FINITE DIMENSIONAL DYNAMICAL SYSTEMS AND DETERMINISTIC CHAOS

The pendulum is an example of a *dynamical system*, which can loosely be thought of as a system that evolves in time according to a well-defined rule. More specifically, a dynamical system is characterized by the fact that the rate of change of its variables is given as a function of the values of the variables at that time. The "space" defined by the variables is called the *phase space*. The position and velocity of a pendulum at any instant in time, for example, determine the subsequent motion; the pendulum's behavior can be described by the motion of a point in the two-dimensional phase space whose coordinates are the position and velocity of the pendulum. In a more complicated case, specifying the time evolution of a glass of water requires a knowledge of the motion of every drop of water in the glass. The phase space is constructed by assigning coordinates to every drop. Since the number of drops is very large, the *dimension* (i.e., the number of dimensions) of the phase space is enormous. Indeed, in the standard hydrodynamic description, the dimension is taken to be infinite.

The most interesting aspect of a dynamical system is usually its long-time behavior. If an initial condition is picked at random and allowed to evolve for a long time, what will the nature of the motion be after all the "transients" have died out? For dynamical systems with friction or some other form of dissipation, special features of particular initial motions will damp out, and the system will eventually approach a restricted region of the phase space called an *attractor*. As the name implies, nearby initial conditions are "attracted"; the set of points that are attracted forms the *basin* of attraction. A dynamical system can have more than one attractor, each with its own basin, in which case different initial conditions lead to different types of long-time behavior.

The simplest attractor in phase space is a *fixed point*. With fixed points, motion in phase space eventually stops; the system is attracted toward one point and stays there. This is the case for a simple pendulum in the presence of friction. Regardless of its initial position, the pendulum will eventually come to rest in a vertical position. Similarly, if a glass of water is shaken and then placed on a table, the water eventually approaches a state of uniform rest. This is true despite the fact that the water's phase space is effectively infinite in dimension.

A fixed point is the only possible attractor of a linear system. Nonlinear systems, however, have many more possibilities. For instance, motion may tend after a long time to an oscillation rather than to a state of rest. A good example is a metronome. No matter where the metronome is started, for a given setting it always ends up making a periodic motion with the chosen frequency. The limit or attractor of the motion is a periodic cycle called a *limit cycle.* Limit cycles represent a spontaneous sustained motion that is not necessarily explicitly present in the equations describing the dynamical system. Since linear systems are not capable of such behavior, the discovery by van der Pol [26] that nonlinear dynamical systems *could* possess limit cycles was both surprising and significant.

Van der Pol's studies were motivated by an interest in understanding and modeling the human heart, which can be thought of as a dynamical system, albeit an unconventional one. The normal rhythmic beating of the heart is a limit cycle. That this cycle is an attractor is indicated by its persistence under most perturbations, including sudden shocks or stress. Indeed the phrase "my heart skipped a beat" reflects both the existence of perturbations to the limit cycle and, implicitly but fortunately, the return of the heart to its normal pattern after the perturbation. Of course, if the disturbance is too large—a prolonged electric shock, for instance—the heartbeat will permanently stop. In impersonal mathematical jargon, the dynamical system has been forced into the attraction basin of a different attractor; in this case, the attractor is a fixed point—death.

In addition to developing a crude mathematical model for the heart, van der Pol also built an electric circuit to model the heart. With historical hindsight we can view this circuit as a primitive analog computer. Under normal conditions this computer produces a periodic heartbeat, but if certain parameters in the circuit are changed, the periodic beating is replaced by a sporadic, nonperiodic pattern, in which pulses are skipped at irregular intervals. The analogy to certain patterns occurring in heart disorders was striking. Although van der Pol did not realize it at the time, his observation of this transition to irregular, sporadic behavior, obtained through a combination of analytic and analog simulation, represented the discovery of a third type of attractor: a *chaotic* or *strange* attractor.

A trajectory on a chaotic attractor exhibits most of the properties intuitively associated with random functions, although no randomness is ever explicitly added. The equations of motion are purely deterministic; the random behavior emerges spontaneously from the nonlinear system. In standard mathematical models of random phenomena, randomness must be assumed to be present a priori. These models are a way of dealing with ignorance—the randomness summarizes what is unknown about the system. Deterministic chaos is strikingly different in that random behavior arises intrinsically from the geometry of the dynamical system and its attractor. Over short times it is possible to follow the trajectory of each point, but over longer periods small differences in position are greatly amplified, so that predictions of long-term behavior are impossible. The information originally contained in the initial conditions is lost, and the behavior of the trajectory becomes unpredictable. Consider a dynamical system where a real number is multiplied by two, its integer part is dropped, and then this sequence is repeated indefinitely. In a binary representation, this corresponds to a simple left shift. When this process is simulated on a digital computer, round-off errors replace the right-most bit with garbage after each operation, and the effect of each multiplication is to destroy the most significant bit. If the initial condition is known to 16 bits of precision, then this information is gone after only 16 multiplications, and the remaining number, generated entirely from round-off errors, is unrelated to the original initial condition. This is true even though multiplication by 2 modulo 1 is a completely deterministic operation. It is this amplification of noise or uncertainty that makes chaotic solutions effectively random and gives rise to the phenomenon known as *sensitive dependence on initial conditions*, which characterizes chaotic behavior.

The discovery, by meteorologist E.N. Lorenz [15, 16], of the mechanism by which *deterministic chaos* arises is an outstanding example of the effective practice of experimental mathematics. Lorenz believed that the unpredictability of the weather should be compatible with a deterministic description and embarked on a search for a set of equations to illustrate his point. He simplified several models of convection in the atmosphere and solved them on a small digital computer. After some experimentation, he found a chaotic attractor in the following seemingly innocuous set of nonlinear differential equations:

$$\frac{dx}{dt} = 10x + 10y,$$
$$\frac{dy}{dt} = -xz + 28x - y, \quad \text{and} \tag{1}$$
$$\frac{dz}{dt} = xy - \frac{8}{3}z.$$

A sample trajectory of this system of equations, projected on the xz plane, is shown in Figure 1.

Lorenz tells an anecdote concerning his discovery of chaos that illustrates what deterministic chaos entails in practical terms. Since his computer was printing out a list of the values of x, y, and z, he could stop the computer at any intermediate time, examine the series of numbers, and then restart it by entering the intermediate set of values. In doing this, he saw that the results very quickly began to differ from the original run. This difference increased as the simulation proceeded. Since the values were not printed out to full machine accuracy, there were very slight differences between the initial conditions in the two runs. The large difference in the subsequent results was caused by the rapid am-

This figure shows the projection onto the $x - z$ plane of a single orbit, that is, a single solution of the Lorenz equations (1). This orbit, which never closes on itself, defines the Lorenz attractor. The motion oscillates irregularly between the two lobes shown in the figure. If a trip around the right lobe is labeled "heads," and a trip around the left "tails," the resulting head-tail sequence has most of the properties of a random coin toss. (The figure was made at the University of Texas by Alan Wolf.)

FIGURE 1. The Lorenz Attractor

plification of the round-off errors. Lorenz's experience is a very precise illustration of the sensitive dependence on initial conditions phenomenon.

We should emphasize that the random character of chaotic solutions persists even in the absence of round-off errors or other external random influences. Chaos is spontaneously generated, creating randomness from purely deterministic origins. This seeming paradox explains the profound changes that have occurred in the way we think about random behavior since the discovery of deterministic chaos.

Lorenz went on to develop a geometrical picture of the underlying mechanism through which the unpredictability of chaotic dynamical systems can arise. In Figure 1, the attractor is roughly a two-dimensional sheet. Equation (1) can be viewed as stretching this sheet out and then folding it over onto itself, in the way a baker would fold bread dough. The process repeats itself over and over, and the attractor develops an infinitely folded structure. Objects of this type are now often called *fractals* [18]. The folding process in some sense thickens the sheet, giving it a dimension that is between two and three [8, 18].

Lorenz also reduced his system to a *one-dimensional map*. He observed that the behavior of eq. (1) is analogous to the chaotic behavior present in the *logistic equation:*

$$x_{n+1} = \lambda x_n(1 - x_n). \qquad (2)$$

This is a simple nonlinear rule that sends a point x_n to a new point x_{n+1} and can be thought of as a *discrete time* dynamical system, such as is produced whenever a system of differential equations is simulated on a digital computer. For any given parameter λ and initial condition x_0, a sequence of numbers $\{x_1, x_2, \ldots, x_n\}$ is generated. For $\lambda < 3$, x_n approaches a fixed point for large n. As λ is increased beyond three, the limit x_n begins to oscillate between two different values; in our previous terminology, the attractor of the equation is a two-point limit cycle. When λ is increased still more, the period of the limiting sequence successively doubles, yielding cycles of periods 4, 8, 16, 32, etc. This process finally stops when the period goes to infinity, at a value of λ approximately equal to 3.57. At many of the values greater than 3.57, the dynamical behavior is chaotic, and the resulting sequence of points $\{x_n\}$ generated by this equation never repeats itself.

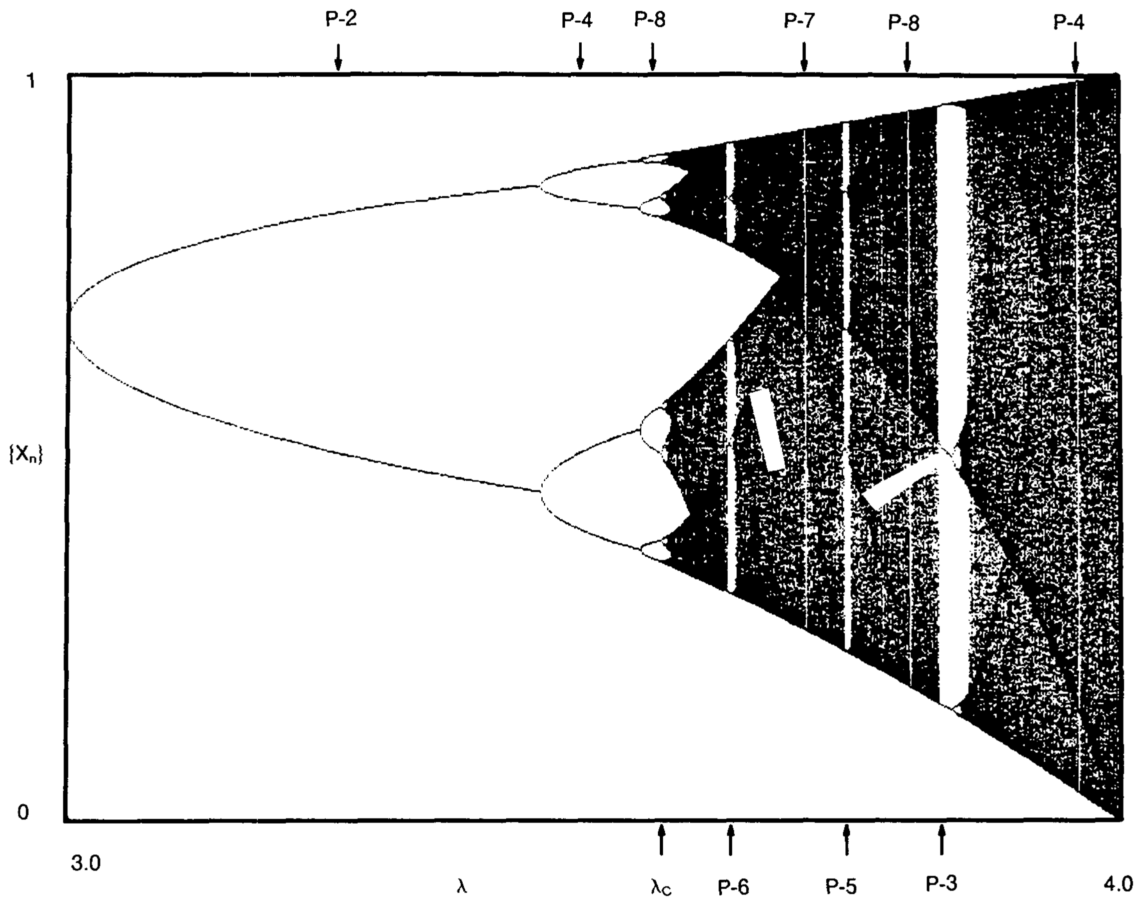
This series of events, referred to as a *period-doubling cascade*, is one of the standard routes from regular to chaotic behavior (see Figure 2). In numerical studies originally begun on a pocket calculator, Feigenbaum [9] discovered that the spacing of the parameter values where period doublings occur is universal in that, for a wide class of systems, it is independent of the details of the equations. Since then many of Feigenbaum's and Lorenz's results have been recast into a more rigorous mathematical framework. The crucial insights, however, were provided by experimental mathematics.

Chaotic dynamics has now been implicated in a variety of areas, ranging from the already mentioned examples of heart failure and meteorology to economic modeling, population biology, chemical reactions, neural networks, arrays of parallel processors, leukemia, and (more speculatively) manic-depressive behavior. In view of this daunting range of applications, two basic points are worth reiterating. First, dynamical systems need not be complicated for chaos to occur. Systems as simple as the driven, damped pendulum (shown in Figure 3) or the logistic equation can exhibit chaotic behavior. Second, the computer remains the essential tool for studying chaotic dynamical systems.

SOLITONS

Although simple dynamical systems with low-dimensional phase spaces can model much of the real world, the analysis of many physical phenomena requires a somewhat different approach. For example, in describing the motion of a glass of water, we stated that the phase space of this system is infinite in dimension. More precisely, to specify the behavior of every drop of water in the glass, we must specify the values of *functions*—the density $\rho(x)$ and the velocity $v(x)$—at every point x in the water. Deterministic rules for the evolution of these functions in time result in (nonlinear) partial differential equations involving derivatives both in time (t) and in space (x). Accordingly, the solution of these equations is mathematically even more complicated than that of finite-dimensional dynamical systems, and the insights provided by experimental mathematics even more crucial.

One such insight is the surprisingly widespread occurrence of an "orderliness" in nonlinear problems. This orderliness reflects the existence of highly stable, pulselike waves—solitons—in certain nonlinear partial differential equations. The discovery of solitons, which are an interesting and physically important phenomenon in their own right, demonstrates the success of the



The "bifurcation diagram" of the logistic equation (2) indicates the position of points in the attracting set on the x axis and the bifurcation parameter λ on the y axis. This figure was made by fixing the parameter λ and then iterating until transients had disappeared, so that x was near its attractor. The parameter λ was then changed, and the process repeated. For $\lambda < 3$ there is a unique attracting fixed point. Above $\lambda = 3$, at the bottom of the figure, the solution bifurcates into a period-two limit cycle. Following across the page, one can see the period doubling cascading eventually accumulating as the period goes to infinity at $\lambda_c \cong 3.57$. For values of $\lambda > 3.57$, chaotic solutions are intricately interspersed with limit cycles. (From Crutchfield, J., Farmer, J.D., Huberman, B. *Phys. Rep.* 92, 46 (1982)).

FIGURE 2. The Bifurcation Diagram of the Logistic Equation

synergistic interplay between computational and analytic methods that is experimental mathematics. Computer simulations led to a qualitative understanding of soliton behavior and directly stimulated the development of the analytic techniques that now give us a deeper understanding of most soliton-bearing systems.

Though solitons were discovered less than two decades ago [31], they have come to be associated with a wide variety of problems in mathematics and the natural sciences [24]. From DNA and α-helix proteins [7] to the Red Spot of Jupiter [19], from laser-plasma interactions [32] to gigantic ocean waves [20], solitons have been implicated in wide range of important and often beautiful natural phenomena. Indeed, the impact of this concept on nonlinear science has been justly termed the *soliton revolution* [26].

To define a soliton, we begin by considering the motion of a wave described by some general (not necessarily linear) wave equation. A *traveling-wave* solution to such an equation is one that depends on the space (x) and time (t) variables only through the combination $x - vt$, where v is a constant velocity. The traveling wave moves through space without changing its shape and in particular without spreading out or "dispersing." If the traveling wave is a localized single pulse, it is called a *solitary wave*. A soliton is a solitary wave with the crucial additional property that it preserves its form when it interacts with other similar waves. In a sense, these special solitary waves are like particles, and indeed the name soliton was chosen to resemble the names physicists traditionally give to atomic and subatomic particles [14].

Early in the 1960s Kruskal and Zabusky began the experimental mathematical study that led to the introduction of the term soliton [14, 17, 25, 30]. They were trying to understand the puzzling recurrences that had been observed in the computational simulations of Fermi, Pasta, and Ulam [10] a few years before.

Through a series of asymptotic approximations, they related the recurrence question for the system of oscillators studied in [10] to the nonlinear partial differential equation

$$\frac{\partial u(x, t)}{\partial t} + u(x, t)\frac{\partial u(x, t)}{\partial x} + \frac{\partial^3 u(x, t)}{\partial x^3} = 0. \qquad (3)$$

This "Korteweg-deVries" equation had first been derived in 1895 [13] as an approximate description of water waves moving in a shallow, narrow channel. To look for a solitary wave, one seeks a localized solution $u_s(\xi)$ that depends only on $\xi = x - vt$, thereby reducing the partial differential equation to an ordinary differential equation in ξ. For solutions vanishing at infinity, the resulting equation can be integrated explicitly to yield

$$u_s(x - vt) = 3v \operatorname{sech}^2 \frac{\sqrt{v}}{2}(x - vt). \qquad (4)$$

Intuitively, we understand the existence of this solitary wave as resulting from a delicate balance in eq. (3) between the "dispersive" term

$$\frac{\partial^3 u(x, t)}{\partial x^3},$$

which tends to spread out an initial pulse, and the nonlinear term

$$u\left(\frac{\partial u(x, t)}{\partial x}\right),$$

which tends to increase the pulse where it is already large and hence to bunch up the disturbance. This balance of dispersion by nonlinearity is the underlying mechanism in soliton-bearing systems. This dry mathematical description, however, obscures the beauty of solitons, which was eloquently communicated in one of the earliest recorded observations of the phenomenon. Writing in 1844, the British naval designer and amateur scientist John Scott Russell noted

> I was observing the motion of a boat which was rapidly drawn along a narrow channel by a pair of horses, when the boat suddenly stopped—not so the mass of water in the channel which it had put in motion; it accumulated round the prow of the vessel in a state of violent agitation, then suddenly leaving it behind, rolled forward with great velocity, assuming the form of a large solitary elevation, a rounded, smooth and well-defined heap of water, which continued its course along the channel apparently without change of form or diminution of speed. I followed it on horseback, and overtook it still rolling on at a rate of some eight or nine miles an hour, preserving its original figure some thirty feet long and a foot to a foot and a half in height. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel. [23]

Although eq. (4) is by our definition clearly a solitary wave, is it a soliton? In other words, does it preserve its identity when it collides with another solitary wave? Here the analytic insight of the 1960s flagged, and to answer this question, Zabusky and Kruskal turned to careful digital computer studies of the interactions of these waves. The a priori expectation was that the nonlinear nature of the interaction would break up the pulses, causing them to change their properties dramatically and perhaps to disappear entirely [14, 17, 25, 30]. When the computer gave the startling result that solitary waves emerged from interaction unaffected in shape, amplitude, and velocity, Zabusky and Kruskal in 1965 invented the term soliton to dramatize their surprising and important discovery [31]. Figure 4 illustrates this behavior in the "sine-Gordon" equation, a well-known soliton system that can be viewed physi-

If a pendulum is both damped and periodically driven, at some parameter values, the resulting motion is chaotic. An impression of the motion can be obtained by making a stroboscopic picture. Imagine taking a snapshot once every cycle of the driving force. The result is shown here. The variable labeled "Position" plots the angle of the pendulum in units of 2π. The multiple images result from motions in which the pendulum swings over the top. The figure illustrates the intricate fractal structure of the underlying strange attractor. (From Huberman, B., Crutchfield, J., and Packard, N. *Appl. Phys. Lett. 37* (1980), 750.)

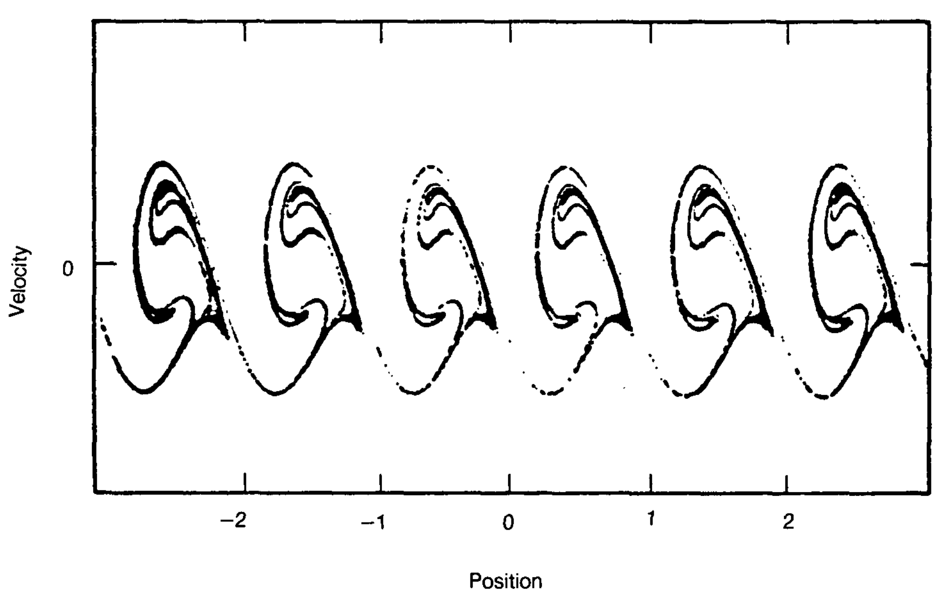
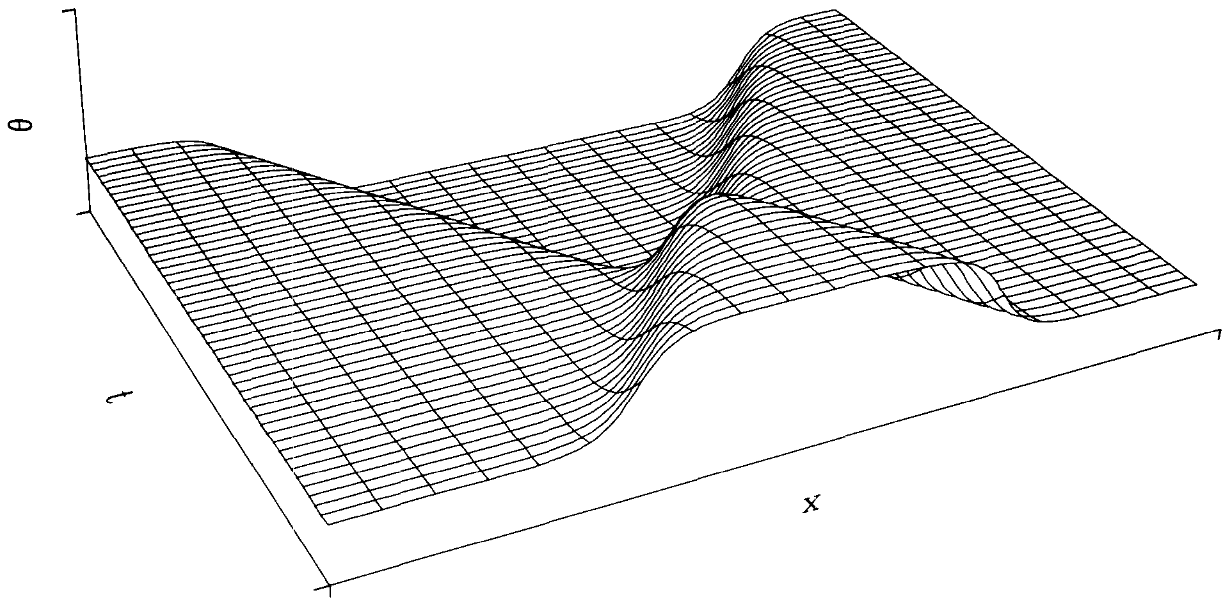


FIGURE 3. The Damped, Driven Pendulum



The remarkable robustness of solitons is indicated in this projected space-time plot of the interaction of two nonlinear waves in the sine-Gordon equation,

$$\frac{\partial^2\theta(x,t)}{\partial t^2} - \frac{\partial^2\theta(x,t)}{\partial x^2} + \sin\theta(x,t) = 0.$$

As time develops (toward the reader), the two steplike solitary waves—called *kink solitons*—approach each other, interact nonlinearly, and then emerge unchanged in shape, amplitude, and velocity. (This figure was made at the Los Alamos National Laboratory by Michael Peyrard of the University of Dijon, France.)

FIGURE 4. The Interaction between Two Solitons

cally as a set of simple pendulums coupled together in a particular manner.

The remarkable results in soliton research raise two questions that are central to nonlinear science. First, since models possessing solitons are quite special mathematically, how relevant is the concept to the real world? Second, if the robustness of the soliton is a reflection of a very orderly and coherent phenomenon, quite in contrast to the erratic and chaotic behavior discussed above, then how can order and chaos be reconciled?

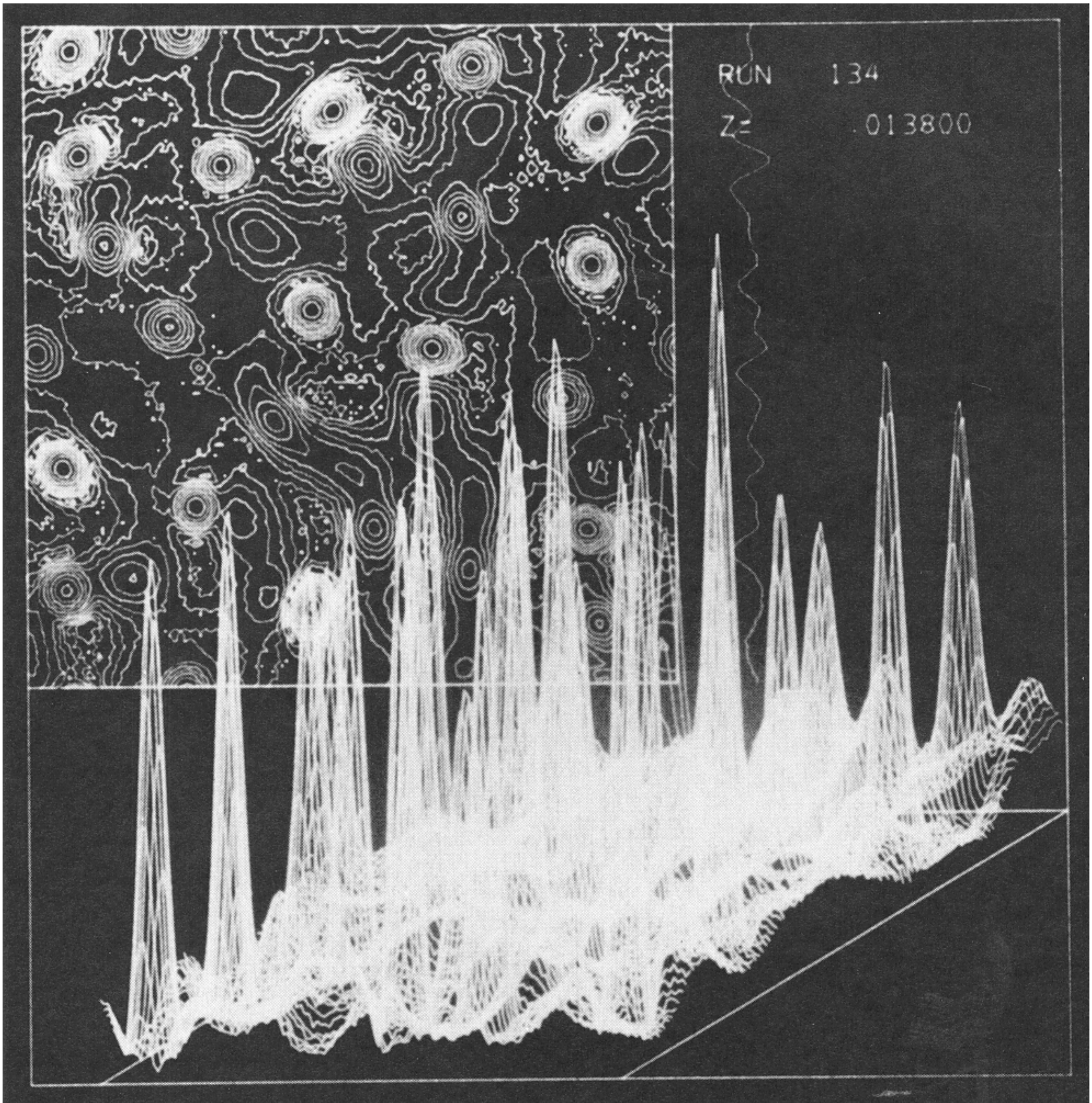
For the first question, it has already been shown that a surprisingly large number of models for natural phenomena possess solitons. More important, an even larger class of phenomena is described by models that are, in a mathematical sense, "close" to soliton systems. There now exists a variety of numerical and analytic perturbation techniques for studying these "nearly" soliton systems, and it is known that solitons still play an important role in many perturbed systems. In these nearly soliton systems, the nonlinear wave solutions should more properly be called solitary waves, since they generally have complicated interactions that destroy the strict solitonic character of the waves. Indeed, recent studies [1, 22] of these interactions provide yet another illustration of the dialectic of experimental mathematics. In several nearly soliton systems, the interactions among solitary waves showed an interesting and remarkable resonance phenomenon first observed in rough numerical simulations. More precise numerical studies revealed obvious regularities in the resonance structure and eventually led to a surprisingly simple analytic explanation of the apparently very complex behavior [1, 22].

For the second question, by analogy to the results of finite dimensional dynamical systems such as the damped, driven pendulum, we would expect that adding damping and a periodic driving force to a soliton-bearing nonlinear partial differential equation would set the stage for a struggle between order and chaos. Indeed, recent computer studies [11] have shown that a soliton system can be driven to chaotic behavior in time, while retaining some of its ordered spatial structure. Figure 5 illustrates this "order in chaos" in the context of an equation that models the interaction of a laser beam with a plasma. Understanding the implications of this order in chaos and, more generally, of nonequilibrium nonlinear phenomena, has emerged as one of the central current challenges for experimental mathematics.

RIGOROUS MATHEMATICAL RESULTS FROM COMPUTERS

From the mathematician's perspective, experimental mathematics may seem suspect. Yet there are by now many examples of rigorous results that would have been impossible without the aid of computers. Perhaps the most familiar is that of the "four-color" problem, for which the computer was used to search through the enormous number of cases needed to establish the theorem. More typically, however, the interplay between computational studies and mathematical theorem proving proceeds as a classic dialectic. At each stage of the process, the fundamental question is, Do the computer results represent interesting new phenomena inherent in the real-world problem being studied, or are they computational artifacts resulting from limitations in numerical methods or modeling? This question stimulates careful mathematical analysis.

An example from the study of hyperbolic conservation laws illustrates the interplay between computational and mathematical research. A conservation law asserts that the time evolution of a system being studied naturally keeps a particular physical quantity at a constant value. For linear conservation laws, such as



Highly localized nonlinear pulses have emerged from a random initial background in this computer simulation of the self-focusing instability of a laser beam passing through a plasma. The localized peaks, although not strict solitons, do show a substantial robustness, and the interplay of the order they individually represent with the temporal chaos in the driven, damped laser-plasma system is the subject of considerable current research. (From a computer-generated film made at Los Alamos by Fred Tappert of the University of Miami.)

FIGURE 5. Spatial Order in Temporal Chaos

those governing the propagation of weak disturbances in continuous media, smooth initial data imply the existence and uniqueness of smooth solutions. For a nonlinear equation, however, smooth initial solutions often "blow up," that is, approach infinite values in finite time. Hence it is necessary to consider *weak solutions*, which possess discontinuities (representing, for example, abrupt jumps in pressure, density, or velocity), but satisfy an integral version of the original partial differential equation. As there is an infinite number of weak solutions to the initial value problem, however, an additional condition known as an *entropy condition* is necessary for identifying the unique physically relevant solution. Since analytic techniques for laws of conservation are not generally available, the problem is to solve the equations numerically and to guarantee that the solution obtained is physically correct.

In 1965, Glimm [11] formally proved the existence of a solution for all time for nonlinear systems of laws of conservation with nearly constant initial data. Chorin [2] used the concepts of Glimm's proof to devise a numerical scheme for solving such systems. In particular, Chorin adopted Glimm's idea of random sampling from the analytic proof and thus departed radically from previously existing numerical techniques. Somewhat surprisingly, the scheme has been found effective even for problems that do not satisfy the original assumptions of the existence proof. The unexpected success of the Glimm/Chorin random choice scheme has motivated mathematicians to derive not only new results on the convergence and correctness of approximation techniques, but also broader proofs of existence for solutions of conservation laws.

We have seen that the contribution of computers to mathematical progress has not been limited to the fields of numerical analysis and approximation theory. A further area where significant results have been obtained on the basis of computational studies is the analysis of scale invariance, that is, the analysis of phenomena whose mathematical properties repeat on all length scales. In particular, the work of Collet, Eckmann, and Lanford [3] provides a proof (using computer-generated estimates) of the existence and convergence of a scaling function introduced by Feigenbaum for one-dimensional maps; this scaling function is the underlying factor producing the "universal" behavior mentioned briefly in the section on finite-dimensional dynamical systems. It has now been shown rigorously for dissipative systems that the universal behavior characterizing one-dimensional maps can occur even when the phase space dimension becomes infinite. Results on the mathematics of scale invariance have also been obtained in such other problems as hierarchical models in statistical mechanics and renormalized quantum fields.

In a wider context, computers have drastically expanded the range of nonlinear phenomena that can be explored mathematically, and motivated the development of techniques specifically designed to handle nonlinearities. Mathematical problems that may become tractable with computer-generated insight include the solution of equations with widely varying time and length scales, the global description of a nonlinear system's dependence on the values of its associated parameters, and the analysis of the effect of random fluctuations in the coefficients of partial differential equations [4]. The techniques used in studying such problems usually attempt either to isolate or simplify the inherent nonlinearities. For example, *continuation* methods approach an intractable nonlinear problem $F(x) = 0$ by attempting to treat it as the limit of a sequence of related solvable problems. Specifically, the objective, if possible, is to define a "family" of problems, $H(x, \lambda) = 0$ for $0 \leq \lambda \leq 1$, where $H(x, 0)$ represents an easily solvable problem, $H(x, 1) = F(x) = 0$ represents the original nonlinear problem, and a computable path $x(\lambda)$ exists that connects the solutions for $0 \leq \lambda \leq 1$. As yet, the techniques for such problems are ad hoc, though their analysis and continued application should yield a rich mathematical theory.

PRESENT AND FUTURE TOOLS OF EXPERIMENTAL MATHEMATICS

By its very nature, experimental mathematics is serendipitous: A hint provided by a numerical simulation sparks an intuitive insight that points the way to a detailed numerical check that eventually leads to an analytic understanding. This step-by-step process illustrates the need in experimental mathematics for a wide range of computing resources, from special-purpose dedicated machines to advanced general-purpose mainframes. In this final section, we reflect in more detail on the tools of experimental mathematics as applied to nonlinear science.

Digital computers, at both mainframe and minicomputer levels and in the conventional sequential or partially pipelined architecture, remain the general-purpose tool of experimental mathematicians. Massively parallel digital machines, with either single instruction or concurrent processor architecture, offer an exciting future alternative. Special-purpose digital computers, designed for a narrow class of problems, are an important new tool, and their use in nonlinear science should increase dramatically in the future [21].

The future use of analog computers in experimental mathematics has not been as well covered as digitals, and so we begin by outlining their advantages and limitations, and then conclude by peeking into the laboratory of a future experimental mathematician. Although it is difficult to give a general definition of an analog computer (since, as van der Pol suggests, any circuit built from well-characterized components should be included), it usually consists of a moderate to large number of function modules, based on operational amplifiers, that perform such operations as summation, inversion, integration, and nonlinear function generation. To program an analog computer, these modules are "patched" together in a configuration imitating the actual connections in the model system. The behavior of the voltages in the computer represents the time evolution of the variables in the equation under study.

In the qualitative studies of finite dimensional dynamical systems, analog computers have several advantages over conventional digital machines. First, because their modules can be connected in a parallel architecture, they are typically much faster than digital computers costing many times more; further, assuming that there are a sufficient number of modules to implement a given system, simulation speed is independent of the number of system variables simulated. In contrast, the speed of a conventional digital computer simulation is proportional to the size of the model system. Second, analog computers are ideally suited for extensive interactive programming. The parameters of the system, including the speed at which the solution is generated, can be varied in real time as the simulation proceeds. This is essential for a qualitative search through the wide range of parameters necessary to probe the whole phase space of a dynamical system. Third, analog computers solve coupled nonlinear equations by mimicking a physical system. The error properties of a particular digital integration scheme need not ever be considered. Indeed, within the range of accuracy limited by the tolerances of the components, the *unsystematic* errors caused by the thermal fluctuations and electronic noise in an analog simulation can actually be useful; this is the case, for example, in qualitative studies of chaotic dynamical systems [5, 6]. Specifically, these fluctuations obliterate the detailed fine structure found in the mathematical description of chaos and thus effectively mimic the coarse-grained behavior that is observed in actual physical experiments in, for example, convecting fluids or nonlinear electronic circuits.

Against these advantages must be weighed the disadvantages of a restricted dynamic range for variables, a limited accuracy for the final solutions, and the need to repatch (instead of rewriting) computer code when a new system is studied. These obvious compromises suggest that analog computers should be used not in isolation but in conjunction with digital machines. It is precisely this kind of hybrid machine that is used in dynamical systems laboratories that have been designed expressly to study chaotic behavior. The digital computer, often a microcomputer, is the "front end" to the conventional analog computer. The digital machine is useful for configuring the analog computer for simulation—it sets initial conditions, parameters, and nonlinear functions in lookup tables. Since no commercially available hybrid computer as yet automatically patches the desired simulation, these values must be entered by the analog programmer. The most important role of the digital computer is to record statistics from the analog simulation and to generally "observe" it. The digitized data so obtained are then down-loaded to a larger minicomputer for statistical analysis.

This hybrid configuration resembles our conception of the experimental mathematics facility of the future. To bring this conception into sharper focus, we should recall the three general requirements imposed by the nature of nonlinear science. If we want to study nonlinear problems in toto, instead of piecing together solutions to separate parts, we must consider them over wide ranges of initial and boundary values in essentially all regions of phase space. This means generating and analyzing massive amounts of data. To meet these requirements, a computational facility should provide three key features: (1) It should be extremely fast and highly interactive, to permit broad but efficient parameter searches and to generate and manage a large amount of data; (2) it should have extensive graphics capabilities, to display data and to stimulate intuition; and (3) it should be user friendly, to encourage the widest participation by researchers from the many different disciplines that can utilize nonlinear science.

An extensively parallel architecture seems essential for interactivity and speed. Although a massively parallel general-purpose mainframe could be used, a more efficient synthesis of the digital and analog worlds for the simulation of nonlinear differential equations would seem to be the digital differential analyzer (DDA), first introduced during the late 1950s. The architecture of a DDA, like that of an analog computer, is a parallel configuration of function modules. The difference is that these modules and the signal pathways are completely digital. The parallel architecture brings high speed to ordinary differential equation simulation; for high accuracy, one would want the basic data type to be 32- or 64-bit floating-point numbers. The use of the floating-point format would almost entirely eliminate the dynamic range problems routinely encountered in traditional analog programming. We would provide a general-purpose digital computer as a host or "front end" for the floating-point DDA, as per already existing hybrid systems. The host would maintain real-time user interaction with the simulation by controlling the solution displays, initial conditions, and parameters.

We should not underestimate the size of the parallel structures needed to attack the important problems in nonlinear science. In the analysis of three-dimensional time-dependent fluid flow, 1000 modules are necessary just to introduce 10 mesh points in each spatial direction; for applications requiring several dynamic variables per mesh point, such as magnetohydrodynamics or lattice gauge theories, this number is even greater. At this point, one naturally begins to think of using VLSIs in the floating-point DDA to reduce cost and size. With the relative simplicity of the function modules and the relatively low speed required for each, one can easily imagine an entire floating-point DDA with several dozen modules and a switching network integrated on a single chip.

The second desired feature—extensive graphics capability—facilitates the manipulation and the rapid assimilation of the overwhelming masses of data generated in studies of nonlinear problems. Imagine a central console consisting of several high-resolution color displays. For input the user would have a standard keyboard, a scientific (equation) keyboard, and a mouselike pointing device. The output, virtually all in graphical form, would be provided by the displays. The main console display would show immediate user input, while a simulation monitor would provide a listing of the differential equation's parameters, the initial conditions, the run time, and other simulation control information. The output color displays would be completely programmable to show (for the example of ordinary differential equations) various time series, phase space projections, and cross sections of solutions, and various dynamical systems theory statistics such as power spectra and correlation functions. This sophisticated interface would be even more important in simulations of nonlinear partial differential equations where it is necessary to follow functions of several spatial dimensions as well as the dimension of time. We expect furthermore that movie animation capabilities will play an increasingly important role for the presentation of results to the world at large.

The third feature of our future facility—user friendliness—is essential for attracting researchers from a wide range of disciplines. Some of these researchers might have little or no desire to understand, let alone work with, the elegant architecture that underlies the computer facility. Although we could make many specific suggestions, one example relevant to an architecture based on coupled DDAs will suffice. Here, it is clearly essential that a switching network should be provided to allow for automatic "patching" of the DDA module to simulate a given equation. Ideally the host computer would have both an *ordinary differential compiler* to generate the patching for the individual DDA units and a *partial differential equation compiler* to link the individual DDAs together appropriately.

Our proposed experimental mathematics facility synthesizes highly focused but restricted special-purpose machines and general-purpose mainframes. Its architecture is tailored for a class of problems that encompasses the bulk of nonlinear science. Although we cannot hope to foresee all the exciting developments that will result when such facilities are available to the experimental mathematician, we can be confident that the insight recorded by von Neumann in 1946 remains true today:

> 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.
> ... we conclude by remarking that 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. [12]

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