26 April 1985, Volume 228, Number 4698 SCIENCE

An Approach to Complexity: Numerical Computations

Larry L. Smarr

Newton established modern mathematical physics in 1687 with the publication of his *Philosophiae Naturalis Principia Mathematica*, in which he showed how infinitesimal calculus could be used as the fundamental mathematical language of science. Since then, calculus has been instrumental in the discovery of the laws of electromagnetism, gas and fluid dynamics, statistical mechanics, and general relativity. These classical laws of nature have been described by partial differential equations (PDE's) for a continuum field.

The tools of calculus have also proved powerful for discovering exact analytic solutions of these equations. Indeed, for linear PDE's that are separable, and thus reduced to ordinary differential equations, such techniques as Fourier analysis can give all solutions of the equations. Much of theoretical physics is based on the results of such linear analysis. However, progress in solving the nonlinear PDE's that govern a great portion of the phenomena of nature has been less rapid. Here, exact analytic methods and linear perturbation methods have provided only a tiny subset of the set of all possible solutions (the solution space) of the equations. There are probably vast regions of the solution space in which the character of the solutions is qualitatively different from the character of the known analytic solutions.

Summary. The use of supercomputers and modern color-imaging techniques for numerical computation is beginning to fulfill von Neumann's vision that digital computers would become the most appropriate tool for solving nonlinear partial differential equations. An example of this approach, a model for the gas flow in the vicinity of a black hole, is described. From such calculations comes a realization that the multidimensional, dynamic solutions of nonlinear partial differential equations can exhibit complex behavior compared to what one normally encounters in analytic solutions. This complexity includes small-scale chaotic structure and large-scale persistently ordered structure. Computational methodology and the aesthetics that derive from it are discussed.

An alternative approach is to find approximate but general solutions for the nonlinear PDE's by the use of finite differences instead of infinitesimal differentials. In this approach, the space-time continuum is replaced by a discrete space-time lattice of events, and the PDE's are converted into a large set of coupled algebraic equations. The unknowns in the algebraic equations represent the field's values at each point of the lattice. With enough time, a computer can solve the algebraic system for the discrete solution. In principle, no symmetry or time independence need be imposed. As the spacing of the lattice is made smaller, the discrete solution should approach the one for the continuum.

Modern supercomputers—the computers with the largest memories and the fastest processors—are making this alternative approach quite practical. The result is a revolution in our understanding of the complexity and variety inherent in the laws of nature. Not surprisingly, these more realistic solutions are allowing a more constructive interplay between theory and experiment or observation than has heretofore been possible.

All this was foreseen by John von Neumann, who I believe occupies a position similar to that of Newton. The mathematician Garrett Birkoff makes this point strongly in a recent review article about numerical fluid dynamics. He paraphrases von Neumann's vision as follows (*1*):

> It seems clear . . . that von Neumann was envisioning fluid dynamics as a *mathematical science* as had Euler, Lagrange, Stokes, Riemann, and Poincare before him. His main point was that mathematicians had nearly exhausted *analytical* methods, which apply mainly to *linear* differential equations and *special geometries*. . . . In short, von Neumann's proposal was that, with high speed digital computers, one could substitute *numerical* for analytical methods, tackling *nonlinear* problems in *general* geometries.

Birkhoff notes that since von Neumann made these remarks, computing machines have increased in speed by a factor of one billion and become cheaper per computation by a factor of ten million. Assessing where we are today, he concludes (*1*):

> . . . numerical fluid mechanics has not and will not replace either analytical or experimental fluid mechanics as a research tool, but . . . it complements and supplements them invaluably.

Extending this view from a comment on fluid mechanics to a general conclusion, the mathematician James Glimm recently wrote (*2*):

> Computers will affect science and technology at least as profoundly as did the invention of calculus. The reasons are the same. As with calculus, computers have increased and will increase enormously the range of solvable problems. The full development of these events will occupy decades and the rapid progress which we see currently is a strong sign that the impact of computing will be much greater in the future than it is today.

The author is director of the National Center for Supercomputing Applications and associate professor in the Departments of Physics and of Astronomy at the University of Illinois, Urbana 61801.

With my colleagues (*3*), I have been practicing the "von Neumann approach" for the past 10 years on a wide variety of physical problems. Out of this research has developed a well-defined methodology for attacking a broad range of problems that occur in physics. Our approach to complexity complements other methods but has unique characteristics of its own. Many of the techniques and concepts that are described below were developed by M. L. Norman and K.-H. A. Winkler during our research on the modeling of supersonic gas jets (*4*). Since that research is well documented in the literature, I will illustrate the methodology with a more recent project I worked on with John Hawley (*5*).

This project explored what happens when gas falls toward a black hole. It is not my purpose to explain in detail the theory of black hole accretion; rather, I hope the description of this project will show the paradigmatic aspects of the methodology used in any computational approach to solving the PDE's that define the laws of physics. In addition, the black hole example exhibits those features of complexity that appear to be common to many solutions of these nonlinear dynamic PDE's, in particular, a large-scale persistently ordered structure, which imposes itself on the underlying gas flow. The coherent structure is spatially complicated and slowly changes with time, but the important point is that an approximate simplicity and certain morphological features appear at a higher level of complexity than might have been expected.

Numerical Modeling of Black Hole Accretion

Gas flowing toward black holes is believed to be the mechanism that drives the "central engine" in quasars and active galactic nuclei. Besides generating great luminosity in the vicinity of black holes, the gas flow may generate the bidirectional outflowing jets of gas that are often observed emerging from galactic centers (*6*). Because black holes are so small, direct observation of the gas dynamics around them is impossible. Therefore, our only hope for an understanding of this phenomenon is to solve the equations that govern it.

To this end, Hawley and I, in collaboration with James R. Wilson (*7*), developed a computer program that solves the general equations that describe relativistic gas dynamics in the fixed gravitational field of a black hole. The program requires the gas flow to be axisymmetric, but no other symmetry is imposed. The gas obeys the ideal gas law; however, shock discontinuities are allowed and are modeled by an artificial viscosity (*7*). No effects from real viscosity, heating or cooling, radiation, or magnetic fields are taken into account in the program. The nonlinear, coupled PDE's that describe the gas flow (*7*) closely resemble the standard Newtonian ones representing mass continuity, energy conservation, and the change in momentum caused by the effects of (relativistic) gravity. The solutions of these PDE's are the five functions needed to specify the density, the energy density (or, equivalently, the pressure), and the velocity fields on the static curved space-time continuum of the black hole.

Our goal was to discover what happens to a rotating gas flow as it falls toward a black hole. To this end, we performed a series of experiments numerically. We chose appropriate initial conditions and boundary values to represent such a gas flow, and then we used the finite-difference versions of the PDE's for relativistic gas dynamics to calculate the change in the gas flow with time. With modern color-imaging techniques, we could watch the flow develop as if we were watching an experiment in a laboratory.

We model space with a grid based on spherical coordinates. In the solutions exhibited here, there are 160 evenly spaced angular zones from the north pole to the south pole and 160 radial zones from the surface of the black hole to the outer spherical boundary (Fig. 1). The radial spacing is increased with distance from the hole to keep the grid zones approximately square. The PDE's are converted to finite-difference equations (FDE's) by replacing the differential operators in the PDE's with Eulerian finite-difference operators on the grid (*7*).

The resulting PDE's constitute a set of coupled, nonlinear algebraic equations. The unknowns are the $160 \times 160 =$ 25,600 values of the five physical variables at each time step. The computations are started at some instant of time by assigning all the unknowns initial values, and then the equations are solved for discrete steps in time. A typical experiment makes use of at least 10,000 time steps. Thus, the finite-difference solution is a set of five variables on a space-time lattice of 250 million points, that is, the solution is 1.25 billion numbers. One of the key issues I deal with in this article is how to translate this hopeless pile of numbers into recognizable science.

In the problem described here (*8*), we assumed that a new supply of gas had begun to fall toward a black hole that had previously consumed all the gas in its vicinity. To specify the rotation law for the gas, we assumed that all the gas had the same value of specific angular momentum. The calculation was started at the time when the inner edge of the infalling gas had reached a boundary radius 50 times the black hole's diameter, and the gas was assigned a radial free-fall velocity appropriate to gas that has fallen from infinity. Thereafter gas continually poured in across the outer boundary. If the gas reached the surface of the hole, it was removed from the grid.

What was the final state of the gas flow? Before we made our calculations there had been little insight into the near-hole dynamics of nonspherical gas flow. However, a number of analytic studies (*7*) had given us clues to the character of any such flow. In the exactly soluble time-dependent, nonrotating, spherical case, the gas flow became supersonic before the gas fell into the hole. Therefore, as the flow became nonspherical in the general case, we expected that shock waves would become important.

In another exactly soluble case, for time-independent, nonspherical, rotating equilibrium, the natural state for a hot pressure-supported gas with constant specific angular momentum was an orbiting thick disk. Such a thick disk (Fig. 1) is shaped like a bagel with the black hole at the center of the bagel hole. The closed pressure-contour lines show how the pressure decreases with distance from a maximum near the surface of the black hole. Because constant specific angular momentum results in a vortex flow, the rotational velocity rises without limit as the axis is approached. Therefore, the centrifugal acceleration of the gas will always overcome the gravitational inward acceleration, resulting in an excluded funnel interior to this vortex flow. The static funnel wall threads through the opening in the bagel hole.

The first use of these analytic solutions was as calibrators for our program. We extensively tested (*7*) various differencing schemes in our program to determine which ones most accurately reproduced the analytic solutions. Second, the analytic solutions suggested features for us to look for in the general problem. For example, do shock fronts develop? However, analytic considerations could take us only so far. The detailed solution of the fully nonlinear, time-dependent, multidimensional, coupled PDE's was needed to see whether the incoming, nearly spherical, supersonic flow could form a highly nonspherical, subsonic, orbiting thick disk.

Exploring the Solution Space

Having set up our experiment, we began to explore the properties of the solution space. The first step was to define the dimensionless parameters that span the space. For a given value of one parameter specifying the flow, the specific angular momentum, the flow will change with the variation of another parameter, the ratio of the solid angle of the incoming flow to the angle subtended by the funnel wall. In Fig. 1, the boundary conditions for the two extremes of thick and thin inflow are indicated.

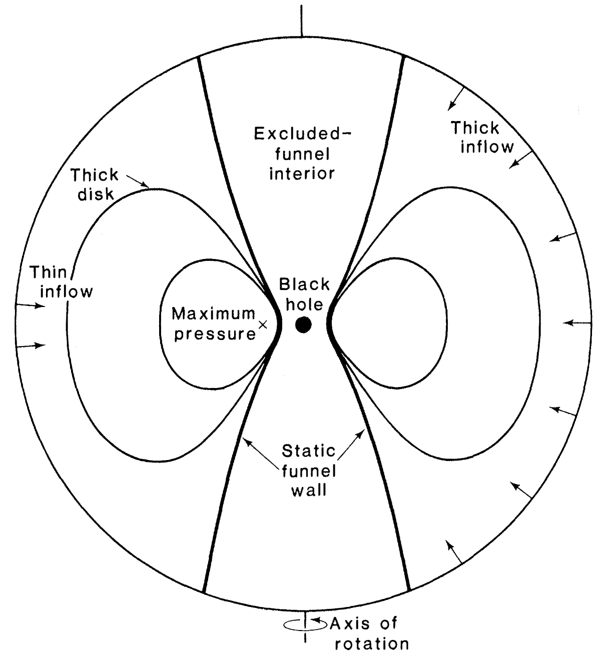

Fig. 1. A schematic diagram of the black hole accretion problem. The black hole in the center creates the gravitational field in which the gas flows. The gas is orbiting the hole with a constant value of specific angular momentum. The axis of rotation is vertical, and the equatorial plane is horizontal. The diagram is a cross section of the gas flow, and the contours of pressure for a thick disk at static equilibrium are shown. The pressure decreases outward from the pressure maximum near the hole. The static funnel wall is the closest to the axis the gas can come, given its angular momentum. Inside this wall the funnel is empty. There are two classes of boundary conditions: thin inflow, with gas only entering the grid near the equatorial plane, and thick inflow, with gas flowing in at all angles not excluded by the funnel interior.

Thus, with the initial conditions and these boundary values, we selected the solution space of the PDE's to be a two-parameter (thickness, angular momentum) family of gas flows in the fixed space-time of the black hole. Each computer run, which shows the development of the gas flow in time, is determined by one point in that two-parameter solution space. Our strategy was to spot-check the solution space by computing the results for both thick and thin inflows at a number of angular momenta.

The values of angular momentum were determined by the results of analytic theory. In Newtonian theory, any particle falling toward a $1/r$ gravitational potential finds a turning point at some radius. In general relativity, the gravitational pull increases faster than $1/r$; so for sufficiently small angular momenta, gravity overwhelms centrifugal acceleration, and the particle falls into the black hole, even though its Newtonian turning point would be outside the surface of the black hole (*7*). There is a critical value of specific angular momentum at which this effect first occurs. Therefore, for our computations we chose values of angular momenta that were more than, about, and less than this critical value, expecting qualitatively different behavior in the resulting solutions.

I will describe in detail only one computer run (*8*), which resulted from the choice of one point in the two-parameter solution space. My description will focus on the scientific results only insofar as they illustrate the scientific methodology used in this approach.

As gas pours onto the grid from the outer boundary, it begins to fall toward the hole (*9*). Figure 2 (*10*) represents a cross section of the density field at an early stage in the development of the flow, when the gas has just bounced off the centrifugal barrier near the hole. A single computer run would be represented by thousands of such images. The spectral order of colors creates a color scale (subdivided into 73 intervals) that we chose to be proportional to the logarithm of density, with blue representing the lowest value and red the highest value. In each image, each grid zone is assigned a color from this scale to represent the density of the gas in that zone at that moment. No color smoothing is done (the individual zones can be seen near the edge of the grid), so the color image accurately represents the results from the computation.

The central black hole and the evacuated funnel north and south of it are visible. From the outer boundary to smaller radii, the color gradually shifts from orange to redder colors, representing the adiabatic compression of the gas. There is a black, empty region surrounding the outside of the funnel wall bordered by thick red lines in an hourglass shape. The sudden jump from orange to red denotes a funnel-wall standoff shock front. This shock front is caused by the centrifugal deceleration of the incoming supersonic gas. It causes the gas to turn abruptly and slide down the inner edges of the standoff shock front.

When the two sliding gas flows (whose density has become so high that they are shown as dark red) meet at the equatorial plane, the gas is diverted inward and shoots toward the hole. As this rotating gas flow nears the hole, its centrifugal acceleration increases faster than the intense gravitational attraction of the black hole. At the last moment, the gas splashes backward off the centrifugal barrier. To avoid the continually incoming gas, the gas that splashes back must flow above and below the equatorial plane. During this process, some of the gas begins to build up a thick disk in precisely the region predicted by analytic theory. Remarkably, very little gas flows into the hole.

The color image on the cover shows the density field of the flow at a later time, after a quasi-steady state has been established; Fig. 3 shows the pressure field at that time. Because a strong shock front causes a much larger jump in pressure than in density, the color image of the pressure field is ideal for locating shock fronts (the color scale is proportional to the logarithm of the pressure). An abrupt jump from dark blue (lowest pressure) to bright blue or green across the funnel-wall standoff shock front is shown. Figures 2 and 3 also show that the shock front migrates to a larger radius with time. This is caused by the continual buildup of a high back pressure in the thick disk (the red heart-shaped region), which pushes the shock front outward.

In Fig. 3 the arrows represent the direction of the flow. Note that the shape of the thick disk is distorted from the equilibrium form shown in Fig. 1 by the ram pressure of the inflowing gas, just as might be expected intuitively. The inflowing gas is pushed away by the high pressure of the thick disk; however, it is trapped between the static funnel wall, where it is excluded by centrifugal acceleration, and the standoff wall shock. Its only means of escape is to flow out vertically as a hollow biconical jet. In doing so it adiabatically expands, and the pressure decreases, as shown by the colors changing from red to green to blue. The key features of the flow are the quasi-stationary patterns shown by the colors; the arrows show that gas continually flows through those patterns.

The question now becomes which of the features of the particular flow we have computed are generic. To answer this we have performed many computer runs, varying first one parameter and then the other (*8*). We have found that as long as the inflow is thick, the standoff shock fronts occur. As the angular momentum decreases, the general relativistic effect mentioned above opens a "spillway" from the inner edge of the thick disk into the hole [an effect predicted from analytic calculations by Paczynski (*11*)]. As more and more gas flows into the hole, the flow out of the jet is reduced. Finally, when the angular momentum is close to the critical value expected from general relativistic theory, all the gas inside the standoff shock fronts goes into the hole, and no thick disk or jet forms.

With thin inflow, a similar sequence of structures occurs in the thick-disk region. However, outside of the disk, no standoff shock fronts form and the narrow jet becomes a wide billowy wind. A black and white image of this configuration can be seen in a previous issue of *Science* (*12*). In the extreme case of thin inflow and very low angular momentum, the gas falls steadily into the hole.

In summary, we have found that the two-parameter solution space decomposes into regions within which the solutions share common morphological features. These features are not details of the flow but rather large-scale coherent patterns in it. For each distinct region of the solution space one can make a paradigmatic cartoon film of the solution. This procedure for characterizing a numerical function is not so different from what one does with analytic functions. Consider a sine function. One can draw a periodic, oscillatory, constant-amplitude graph to represent it without worrying about the particular values of the two parameters, period and amplitude. In both the analytic and numerical case, the important feature is the form of the function.

One of the key differences between numerical functions and simple analytic functions is that numerical functions have multidimensional spatial forms that are dynamic. That is, both Figs. 2 and 3 are frames from the same solution; the behavior in both figures must be included in the cartoon film representing this portion of solution space. The only way to understand the solution is to watch the color films that represent the solution in terms of different physical variables (*13*).

In summary, our approach is to compute discrete solutions to the finite-difference PDE's and then to convert these numbers into color images that change in time. In these images we can observe coherent large-scale structures in the flow. By performing additional computations, we can determine which of these structures are generic and over how large a region of solution space these structures are present. The boundaries between qualitatively different structures can be identified by this procedure. Finally, analytic methods and intuition are used to explain why the structures should be there. In some cases, this process reveals new phenomena for which complete analytic theories can be worked out.

I call this practical approach "exploring the phenomonology of solution space." This approach has a long history that was recently summarized by Zabusky (*14*). He terms the interplay between computing, analytic methods, and graphic visualization "computational synergetics." It is an important methodology of science and one that is becoming more widespread.

Fig. 2. The gas flow, in the thick-inflow case, at the moment the gas begins to splash back from the funnel wall near the hole. The quantity represented is density. The color scheme and features are explained in detail in the text.

The Ubiquity of Complexity

Just how prevalent is the phenomenon of complexity? Wolfram (*15*) gives an excellent overview of this question with particular emphasis on why the computer is so well matched to the study of complexity. It seems that most systems in nature can exhibit both simple and complex behavior. To date, theoretical physics has mostly concerned itself with simple behavior, since analytic tools were well matched to that study. However, as computational resources become more powerful and accessible, more studies are being performed on the complex behavior of simple systems.

A clear statement of the ubiquity of complexity, with examples from theoretical physics, can be found in "Prospectus for Computational Physics" (*16*), commonly referred to as the Press Report. This report shows that complexity can arise in a variety of ways: in moving from a few degrees of freedom to many degrees of freedom, from ordinary differential equations to PDE's, from simple or one-dimensional models of physical processes to multidimensional models, from low-order to high-order expansions, from scalar systems to vector or tensor systems, and from linear systems to nonlinear systems.

In summary, the Press Report concludes:

> One sees, then, that complexity arises not from 'bad taste in the choice of problems', but inevitably as theory advances . . . .

A similar statement could be made in every field of theoretical science. Ultimately, this is because nature is complex. Consider the dynamics and formation of galaxies, where a hundred billion stars interact gravitationally to produce the beautiful spiral arms familiar from astronomical photographs. At the opposite extreme of scale, the macromolecules that underlie life itself perform their biological functions largely because of the manner in which their thousands of component atoms arrange themselves in highly ordered large-scale structures. We are beginning to acquire the computational tools and scientific methodology that will allow us to attack these and other complexities head on.

Coexisting Aesthetics

Finally, let me turn to a disturbing feature of the revolution in computing techniques. Too often misunderstandings arise between scientists trained in classical analytic methods and those for whom numerical methods are the primary research tool. One often hears: "Numerical solutions are inelegant," or "Analytic solutions are simplistic." Such comments reveal a clash between two coexisting aesthetics derived from the nature of the computational tools that are used. Rather than define precisely the principles of both camps, I will give examples of their calculational goals.

Much scientific effort in the three centuries since Newton has been directed toward discovering the form of the basic laws of physics. Analytic methods have been precisely the right tool for that job. However, although analytic solutions have given us a skeletal view of the content of those laws, they have not revealed the true complexity of the solution space. Therefore, the search for form is shifting from the laws to the solutions of the equations describing those laws. Computational methods are the appropriate tools for this latter search.

Many of the classic analytic solutions are for fundamental static equilibria. What is becoming clear in many areas is that there is a new class of dynamic equilibria which are just as fundamental. These are large-scale coherent structures with long lifetimes compared to the underlying system's dynamical time scales. Although many are being studied observationally (for example, Jupiter's red spot), a growing number are being discovered numerically. As is the case for the soliton (*14*), the prototype of dynamic equilibria, for most of these structures some underlying mathematical principle is at work. It seems to be a general property of nonlinear systems that they "lock on" to coherent structures that are far from the linear regime.

Many analytic solutions exhibit high degrees of spatial or internal symmetry. Indeed the power of group theory in science attests to symmetry being a fundamental property of nature. However, many of the phenomena of nature are inherently unsymmetrical and time-dependent. The beauty of the ever changing three-dimensional structure of clouds is surely as great as the beauty of a perfect crystal. To explore such phenomena as the clouds requires the ability, which numerical tools give us, to probe complexity.

Much of the beauty of analytic functions comes from their encoding what is visually beautiful. For example, the periodic and oscillatory nature of the sine function is better perceived by a graph of the function than by looking at its name. Just so, the eye can perceive fundamental properties of complex solutions by using color images or other computational devices in situations where closed analytic forms are impossible. Thus, the visual representation of mathematical functions may become the common bond between simple analytic functions and complex numerical ones.

As I have attempted to show in my example of a black hole, scientists need to have an intuition formed from both aesthetics. There is no inherent conflict

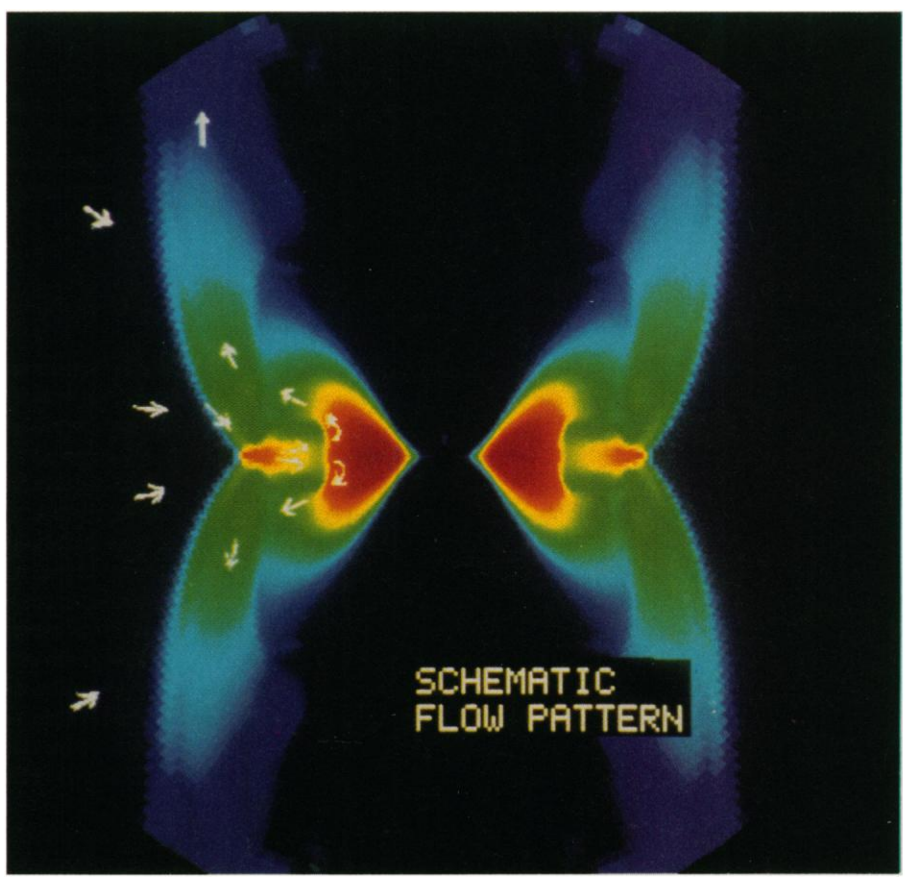

Fig. 3. The gas flow at a later time for the same conditions as in Fig. 2. The colors represent the pressure gradient. The arrows indicate the direction of the flow.

between these two views; both are useful for discovering parts of the whole. I hope that students today are being trained with equal emphasis on analytic and numerical methodologies.

Prospectus

In summary, the prodigious growth in computing power is ushering in new approaches to complexity in many areas of science. Although the shift of methodology and aesthetics was foreseen by von Neumann over 30 years ago, the fulfillment of his vision is only beginning. For his vision to be realized, there are two major requirements. First, computers must continue their rapid rate of increase in speed so that more and more complex problems can be attacked on human time scales. Second, there must be much greater accessibility to the full range of computational tools that are needed so that a "critical mass" of scientists can work in each field of interest. Both of these requirements are likely to be met.

References and Notes

1. G. Birkoff, *SIAM Rev.* **25**, 1 (1983).
2. J. Glimm, in *Frontiers of Supercomputing*, N. Metropolis *et al.*, Eds. (Univ. of California Press, Berkeley, in press).
3. These colleagues include J. Centrella, B. DeWitt, P. Dykema, K. Eppley, C. Evans, J. Hawley, J. LeBlanc, M. Norman, J. Wilson, and K.-H. A. Winkler.
4. M. L. Norman, L. Smarr, K.-H. A. Winkler, M. D. Smith, *Astron. Astrophys.* **113**, 285 (1982); M. L. Norman, K.-H. A. Winkler, L. Smarr, in *Astrophysical Jets*, A. Ferrari and A. G. Pacholczyk, Eds. (Reidel, Dordrecht, 1982), p. 227; M. L. Norman, L. L. Smarr, K.-H. A. Winkler, in *Numerical Astrophysics: A Festschrift in Honor of James R. Wilson*, J. Centrella, J. LeBlanc, R. Bowers, Eds. (Jones and Bartlet, Portota Valley, Calif., 1985), p. 88; L. L. Smarr, M. L. Norman, K.-H. A. Winkler, *Physica D* **12**, 83 (1984); M. L. Norman, K.-H. A. Winkler, L. L. Smarr, in *Physics of Energy Transport in Extragalactic Radio Sources*, A. Bridle and J. Eilek, Eds., in preparation.
5. This work was performed while J. Hawley was a graduate student in the Astronomy Department at the University of Illinois. He is currently the Bantrell Fellow at the California Institute of Technology.
6. M. C. Begelman, R. D. Blandford, M. J. Rees, *Rev. Mod. Phys.* **56**, 255 (1984).
7. J. R. Wilson at the Lawrence Livermore National Laboratory was the first person to write a computer program that solved the general relativistic hydrodynamics equations for this problem; see J. R. Wilson, *Astrophys. J.* **173**, 431 (1972). Hawley, Wilson, and I wrote an updated version of the program and carefully calibrated it; see J. Hawley, L. L. Smarr, J. R. Wilson, *Astrophys. J.* **277**, 296 (1984); *Astrophys. J. Suppl. Ser.* **55**, 211 (1984).
8. J. Hawley, "A numerical study of nonspherical black hole accretion" [thesis, University of Illinois (1984)]; J. F. Hawley and L. L. Smarr, *AIP Conf. Proc.*, in press. Only black and white images are in these two sources.
9. In this discussion we assume that the black hole is nonrotating. Our program also handles the case of a rotating black hole. See (*8*) for details.
10. K.-H. A. Winkler developed the color-image algorithm for presenting the supercomputer solutions. J. Hawley adapted the approach and rewrote the algorithm for our project. The calculations were made on the Cray-1 supercomputer at the Max-Planck Institute for Physics and Astrophysics, Institute for Astrophysics.
11. B. Paczynski, *Astron. Astrophys.* **34**, 161 (1974).
12. M. M. Waldrop, *Science* **223**, 575 (1984).
13. The movie was made at the Max-Planck Institute for Physics and Astrophysics, Institute for Astrophysics.
14. N. J. Zabusky, *Phys. Today* **37**, 36 (July 1984); *J. Comp. Phys.* **43**, 195 (1981).
15. S. Wolfram, *Sci. Am.* **251**, 188 (September 1984).
16. W. H. Press, "Report by the Subcommittee on Computational Facilities for Theoretical Research to the Advisory Committee for Physics, Division of Physics" (National Science Foundation, Washington, D.C., 1981).

17. I thank J. Hawley for permission to use the unpublished color images in this article. My colleagues have been instrumental in the development of the ideas expressed in this article. In particular, I thank J. Centrella, C. Evans, J. Hawley, M. Norman, W. Press, R. Wilhelmson, K. Wilson, J. Wilson, K.-H. A. Winkler, and N. Zabusky. The hospitality and support of the Max-Planck Institute for Physics and Astrophysics, Institute for Astrophysics, and its director, R. Kippenhahn, are greatly appreciated. The images were made both at the Institute for Astrophysics and at the University of Illinois VAX and Image Processing Center. This work was partially supported by the National Science Foundation and the Alfred P. Sloan Foundation.

Computer-Assisted Analysis in Organic Synthesis

E. J. Corey, Alan K. Long, Stewart D. Rubenstein

The chemical synthesis of organic molecules has proceeded at an accelerating pace for more than a century and a half. Since the Wöhler synthesis of urea in 1828, organic synthesis has had an enormous impact on civilization and on the development of science itself. Advances in the understanding of chemical structure, chemical reactivity, stereochemistry, and biochemistry have been due in no small part to discoveries in organic synthesis. Yet all of the syntheses of the 19th century and most of those of the first half of this century were developed from a relatively primitive conceptual base. Many syntheses, especially in the 19th century, were discovered serendipitously (or opportunistically) in the sense that they were accomplished as unplanned results of exploratory studies of chemical interactions between different types of molecules. Other syntheses used a series of established reactions to convert a basic structure into a somewhat larger molecule. Such syntheses involved the successive attachment of functional or substituent groups through the use of replacement, condensation, or coupling reactions. Thus, the dyes alizarin (1869) and indigo (1890) were synthesized by elaboration of anthracene and aniline, respectively, and the alkaloid tropinone was made from cycloheptene (1901). In contrast to the vast majority of these early syntheses, which were based on the availability of starting materials that contained a major portion of the final atomic framework, a few syntheses emerged whose design depended on the knowledge of certain ring-forming reactions that could be used to build an atomic framework. Among the best examples of these are the syntheses of α-terpineol (W. H. Perkin, 1904), camphor (G. Komppa, 1903; W. H. Perkin, 1904), tropinone (R. Robinson, 1917), and equilinin (W. Bachmann, 1939) (*1*).

In the post–World War II period, synthesis attained a different level of sophistication partly as a result of the confluence of five stimuli: (i) the formulation of detailed electronic mechanisms for the fundamental organic reactions, (ii) the introduction of conformational analysis of organic structures and transition states based on stereochemical principles, (iii) the development of spectroscopic and other physical methods for structural analysis, (iv) the use of chromatographic methods of analysis and separation, and (v) the discovery and application of selective chemical reagents. As a result, the years 1945 to 1960 saw the accomplishment of a number of highly sophisticated syntheses of complex molecules, including vitamin A (O. Isler, 1949), cortisone (R. Woodward, R. Robinson, 1951), strychnine (R.

E. J. Corey is a professor, Alan K. Long is a research associate, and Stewart D. Rubenstein is a graduate research assistant in the Department of Chemistry, Harvard University, Cambridge, Massachusetts 02138.