Special issue: Computational physics

Grappling with complexity

We are in the midst of a computational revolution that will change science and society as dramatically as the agricultural and industrial revolutions did. The discipline of computational science is significantly affecting the way we do hard and soft science. The articles in this special issue of PHYSICS TODAY demonstrate the vital growth of the infant computational physics. Supercomputers with ultrafast, interactive visualization peripherals have come of age and provide a mode of working that is coequal with laboratory experiments and observations and with theory and analysis. We can now grapple with nonlinear and complexly intercoupled phenomena in a relatively short time and provide insight for quantitative understanding and better prediction. In the hands of enthusiastic and mature investigators, intractable problems will recede on a quickened time scale in this computationally synergized environment.[1]

The theoretical, analytical and experimental modes of research go back to the beginnings of the scientific approach. By theory I mean the process of hierarchical and complementary modeling in which one describes concepts by mathematical equations. That is, mathematical models can overlap in their ability to represent the same phenomena and so complement one another. By analysis I mean both rigorous (theorem proving) and asymptotic (such as perturbation expansion) derivations. In the experimental and observational mode we have recently developed accurate and noninvasive diagnostics, as exemplified by laser and particle beam scattering and remote sensing of emitted electromagnetic radiation. Theory, analysis, experiment and computation may be considered manipulative processes. To put things in sharp relief, we may consider theory as concept and model manipulation, analysis as symbol manipulation, experiment as object and signal manipulation, and computation as number and image manipulation. (Of course processes overlap among the modes.)

The articles in this issue show that much of the domain of science and technology can be described theoretically by nonlinear, coupled evolutionary (time-dependent) equations. Fortunately, one can adjust this "topography" and find stationary or long-lived coherent structures to which one can apply the linearization approach. The stationary configurations and their responses to weak (linear) perturbations have provided insights into many problems in physical science. However, the essential nonlinearity of such problems has limited the usefulness of those insights beyond early times in a process. For example, laboratory and numerical experiments have shown that spatially localized structures like atoms or vortices can interact strongly to yield "inelastic" phenomena, including formation of other atomic species for the former and reconnection of vortex tubes for the latter.

In the realm of the physics of neutral fluids, discussed in the articles of William R. Holland and James C. McWilliams (page 51) and of Karl-Heinz Winkler and colleagues (page 28), the essential equations of motion were proposed in the 18th and 19th centuries. The task of determining their properties and relating them to observable phenomena proceeded slowly, so that until the mid-1960s very few useful (that is, nonlinear) time-dependent solutions were available. For the most part, scientific progress was confined to finding steady states in appropriate reference frames—such as boundary layers, shear layers, shock and solitary waves, and point or rectilinear vortex arrays—and to examining their linear stability. Engineers and applied scientists confronted with deadlines wrestled for solutions to practical problems by trial and error and by including large safety margins.

Consider the state of affairs at the dawn of the digital computer era and Theodore von Kármán's 1939 Gibbs Lecture to the American Mathematical Society on grappling with "nonlinear problems."[2] Although he ranged over model problems in elasticity and in incompressible and supersonic fluid dynamics, including a discussion of surface waves with finite amplitude (with reference to the Korteweg–deVries equation), most analytical results at the time were time independent and for the most part one and two dimensional in space.

Strong wave phenomena on the surface of a classical liquid have practical consequences, provide theoretically challenging problems and are also artistically beautiful. Katsushika Hokusai's marvelous woodblock print *The Great Wave off Kanagawa*, for example, which appears regularly in scientific books and articles, captures physical phenomena on at least three length scales. Although one can represent this type of stratified turbulence, where waves, vortex structures and mass irregularities (or bubbles) interact, by the Navier–Stokes equation (with appropriate surface physics), one can solve few problems and make almost no quantitative predictions. However, if one introduces a hierarchical modeling approach and takes it to a limit where functions depend on one space dimension, time and one dimensionless parameter, one obtains the Korteweg–deVries equation for shallow nonlinear water waves. Although Horace Lamb referenced the Korteweg–deVries paper in his classic monograph on hydrodynamics,[3] the equation was ignored as a vehicle for insight until Martin D. Kruskal showed that it arose as a model for describing the Fermi–Pasta–Ulam nonlinear lattice simulations. This led Gary Deem, Kruskal and me to make numerical simulations of the Korteweg–deVries equation and to discover the soliton concept. Almost immediately, a host of exactly integrable nonlinear evolution equations were found that describe a wide variety of physical processes. Although Scott Russell observed aspects of solitary wave interaction in canals in 1836, his work was forgotten until the numerical simulations quantitatively demonstrated the particle-like nature of solitons.[1]

The Fermi–Pasta–Ulam simulations were the first numerical molecular dynamics experiment on a nonlinear many-body system. In his article on page 68 Martin Karplus describes realistic three-dimensional molecular dynamics experiments for predicting the motions and interactions of macromolecules of biological interest. This work introduced conceptual changes in appreciating the role of internal atomic motions in protein function and has enhanced the analysis of experimental data. Understanding and controlling these motions present formidable challenges, but will provide payoffs in genetic engineering and drug design.

Other types of "coherent structures" and turbulence arise in different environments. For example, Winkler and his coworkers have made strides in supersonic vortex dynamics, a field usually studied by aerodynamicists seeking to understand shock waves intersecting with each other or impinging on solid objects. Winkler and his colleagues discovered how a supersonic vortex ring emerges from a classical experimental arrangement where a planar shock wave impinges on an axisymmetric spherical bubble. (See the figure on page 31.) Holland and McWilliams have found that an ocean basin can be adequately resolved by computational zones of one-third of a degree by one-third of a degree (about 6 km×6 km) with 20 vertical levels—a significant quasi-three-dimensional representation. They find that unstable streams such as the Gulf Stream spin off large (for example, 100 km in diameter) coherent structures called rings that may last for a significant time (for example, many months). The rings entrain biological materials and chemical tracers different from those of the surrounding water. In the near future Holland and McWilliams hope to extend this resolution to all the world's oceans. Realistic three-dimensional models will present formidable computing loads that only massively parallel processors will be able to deal with.

Understanding and communicating these evolving processes will require a substantial investment in visualization, diagnostic and networking hardware and software, as Winkler and his coauthors discuss. The sequence of figures on page 27, by Mogens V. Melander of the University of Pittsburgh, shows results of a three-dimensional pseudospectral simulation of the incompressible Navier–Stokes equation on a 64^3 grid. It begins at $t=0$ with two offset identical circular vortex tubes, each perpendicular to a different face. Initially a Gaussian function describes each vorticity distribution, and as time evolves the vorticity becomes distorted and intensified. We see in succession the close interaction and "binding" of oppositely directed tubes; hairpin "pulling"; strong core distortion; formation of a complex "core"; and finally "reconnection." Understanding mechanisms that contribute to these processes is an exciting challenge in the coherent structure approach to three-dimensional turbulence.

High-resolution, large-scale simulations on supercomputers are revealing insights often described as remarkable. The meanings of "high" and of "super" evolve as rapidly as technology permits. Ken C. Bowler and his coauthors, in their article on page 40, cover the implementation of some fast algorithms for doing problems in condensed matter and statistical physics on machines with massively parallel architectures. Nicholas Metropolis believes that the advent of massively parallel processors will introduce a more substantial positive discontinuity into the progress of computational science than came, for example, with the replacement of electromechanical by electronic devices! These machines will become more effective when we develop robust programming languages and compilers for the computational physicist that will not require a long time to learn and intensive concentration to debug. We must not underestimate the size of this task.

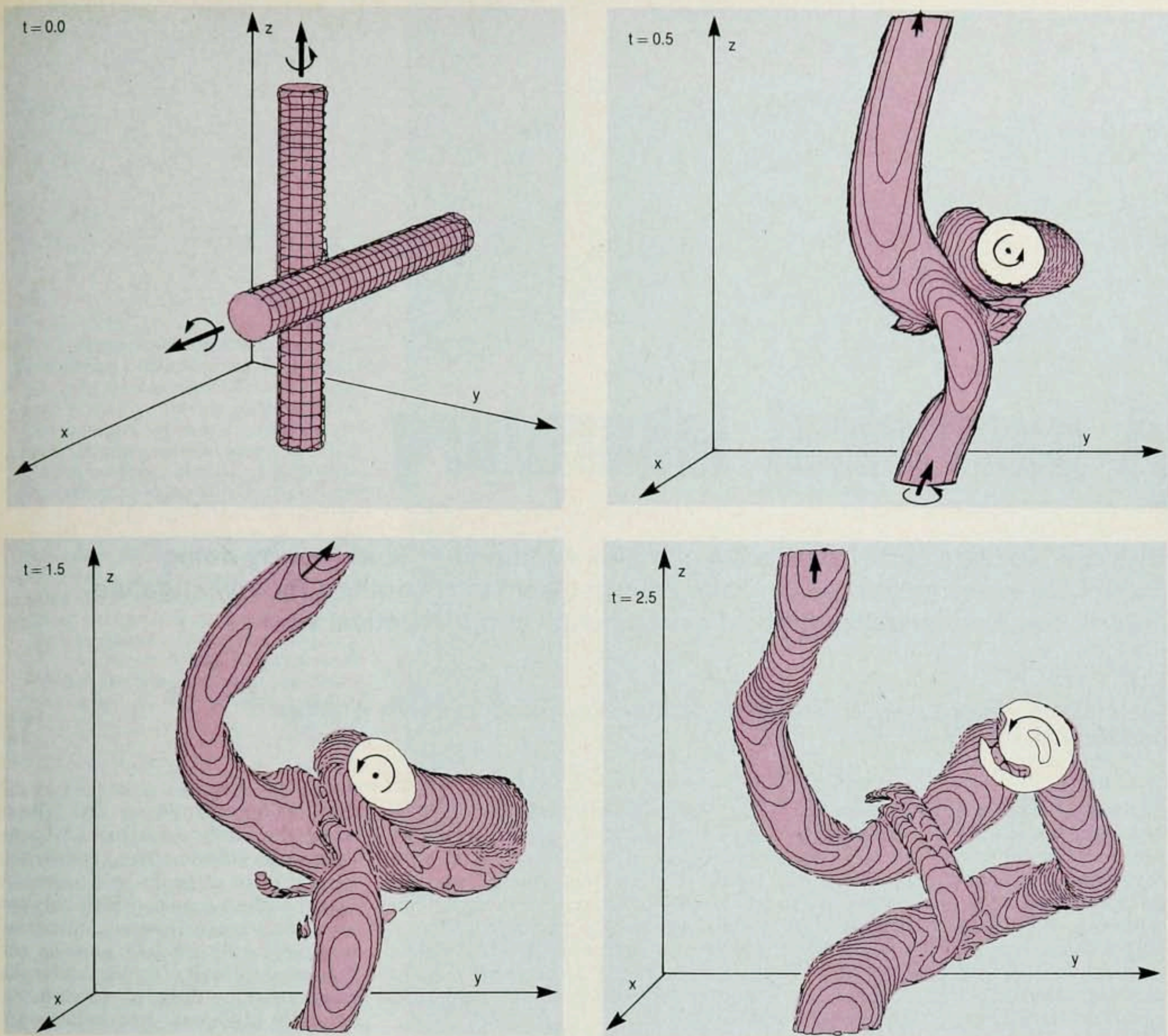
As the speed and rapid-access memory of computers increase, so will the range of length and time scales, degrees of freedom and physical processes that they can handle. We will be confronted with enormous quantities of information to assimilate, validate and disseminate. For evolution problems the data flood is portentous and must be dealt with in an *a priori* manner; otherwise we will arrive at the same situation we do in many experiments, ranging from geophysics to particle physics, where only a fraction of the data is studied. Winkler and his coauthors discuss some of the man–machine interaction problems that arise in storing and communicating with terabits of data from a two- or three-dimensional run. Winkler's "ultrafast" graphics system readily produces colored animated graphics with space–time zoom capability. As with early particle accelerators, his system will be emulated and augmented.

The above aspects of the computational revolution will affect not only scientific innovation and technological productivity, but also political, economic and military decision-making. For example, we are now being called on to forecast climate and health effects due to fossil fuel combustion and fluorocarbon emissions. Although this is a complex problem with large data sets, the experimental environment is relatively free and open, as it is also for oceanographic forecasting. Similarly, an important military issue is the ability to see, launch and communicate with weapons in an environment disturbed by nuclear explosions at a multitude of altitudes. Here, atomic, molecular, nuclear, and nonlinear neutral and plasma physics processes involve a gamut of phenomena, many of whose reaction rates or couplings have not been explored. However, unlike in atmospheric and oceanographic research, the experimental environment is restricted and the data sets are therefore smaller. Thus short-term (seconds to hours) nuclear explosion "weather" is much more difficult to forecast. The accuracy of weapons systems in such environments is uncertain and could probably be augmented through techniques described in some of this issue's articles.

The computational revolution raises still other questions:

▶ On the scientific side: How many physical effects, dimensionless ratios and length scales must we include to obtain the effects we seek? How do we address discrete vs continuous modeling of phenomena at long times? For example, for the Euler or weakly dissipative Navier–Stokes equation we may use the classical partial differential equations, the lucid contour dynamical equations[4] (a method for certain incompressible flows where the location of the boundary of a region is sufficient for determining the region's motion) or the recently proposed cellular automata approach. How do we quantify and control the errors that arise from various truncation, round-off and regularization techniques, including artificial dissipation, filtering and smoothing? How do these regularization techniques affect sensitivity to initial conditions and the development of real and numerical singularities and instabilities? How do results obtained with few-parameter models manifest themselves in more realistic models? How do we link the effects in the simulation data with the sparse experimental or field data to determine overlapping phenomena?

▶ On the human side: How do we build and sustain productive teams of scientists and technologists to solve complex problems? What short- and long-term career rewards should we provide for them? (For example, how do we handle tenure in an interdisciplinary computational group?) What new methods of communication do we



Evolution of two tubes of vorticity obtained with a filtered pseudospectral code of the incompressible Navier–Stokes equation on a 64^3 lattice. In these perspective projections, the lines are obtained by intersecting the vortex surface $|\omega(x,y,z,t)|/\max|\omega(x,y,z,0)| = 0.6$ with parallel planes. At $t = 0$ we see two surfaces, represented by lines resulting from planar intersections with two offset Gaussian vorticity distributions. The arrows show the direction of the vorticity vector in each tube. At $t = 0.5$, 1.5 and 2.5 we see the evolution of the vortex surface. At 1.5 oppositely directed tubes are in close proximity, and at 2.5 reconnection has occurred. (The color has been added.)

need to enhance transfer of knowledge? How are we to revise the teaching of natural science and mathematics to train computational researchers and practitioners? Philip J. Davis and James A. Anderson[5] and Lynn A. Steen[6] have addressed aspects of this problem for mathematics.

▶ Finally, on the resource side: How should the government allocate resources among large-scale projects? The NSF initiative to establish five supercomputer centers primarily for academic research was a major step forward. (See the news story on page 61.) These centers are capable of serving geographically dispersed users pursuing a variety of intellectual goals. They must be networked, be upgraded in a timely manner and include massively parallel machines and ultrafast visualization and diagnostic environments to deal with the enormous data sets that arise, for example, from evolution of three-dimensional phenomena. The major research funding organizations such as NSF, DOE and DOD will have to make choices that balance basic scientific inquiry with probable applied scientific and technological payoffs, particularly in the next five to ten years.

It is clear that computational science covers both the basic and applied modes; it is approaching a deeper understanding of and predictability for complex problems in the hard and soft sciences. Now is the time for computational scientists to unify their efforts, close ranks and lobby for new resources.

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