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Scientific Visualization

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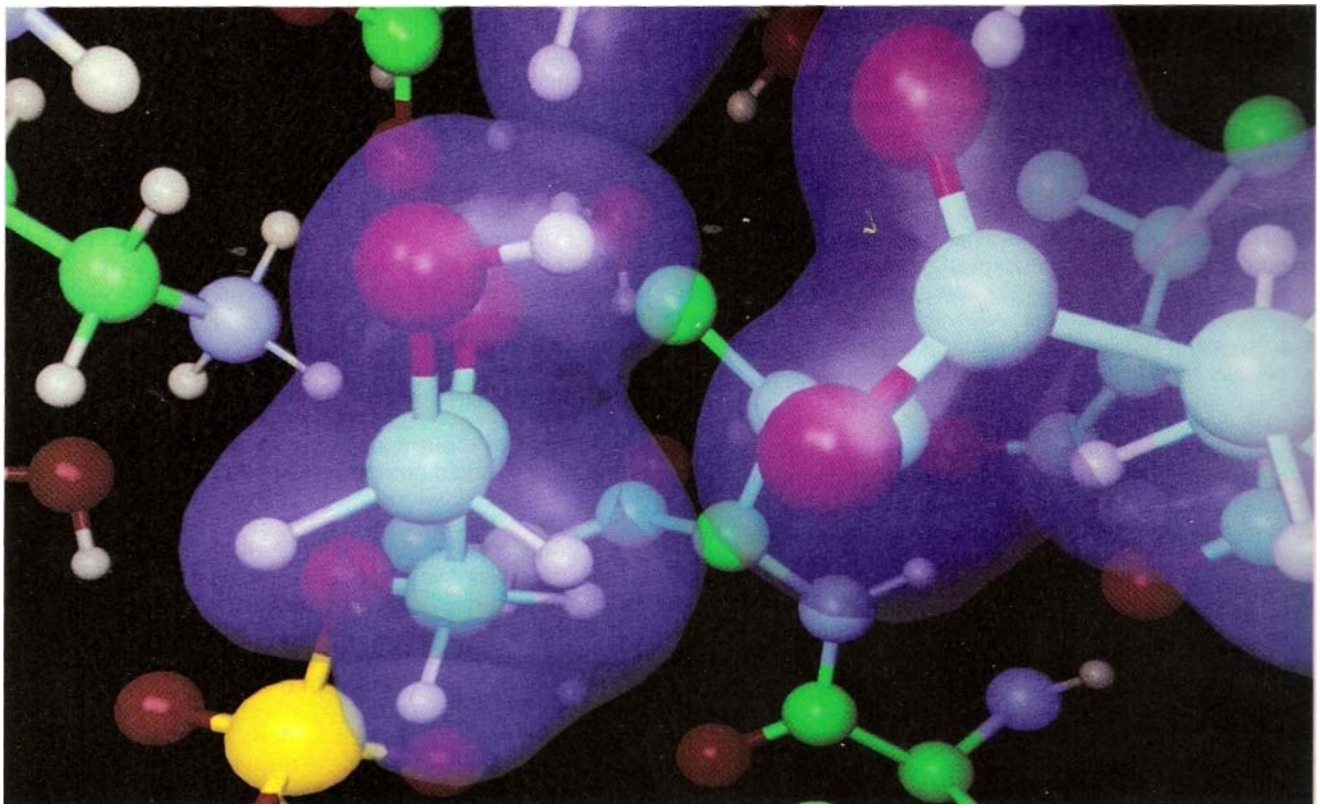
*v*isualization is the formation of mental images of what cannot be seen. It is seeing, in a way, that which is invisible, either because it is inaccessible to eye or camera, because its physical nature supports no real image formation or because its existence is abstract or hypothetical. Scientific visualization involves real images-drawings, photographs, holograms or video displays of graphs, charts, diagrams and other visual models-to serve as intermediate aids; it makes use of our real eyes to help our mind's eye in its task of grasping the structures, relationships and abstractions of science. The importance of real visual aids in scientific understanding may well be related to the fact that a very large proportion of our brains' neurons seem to be devoted to processing visual input.

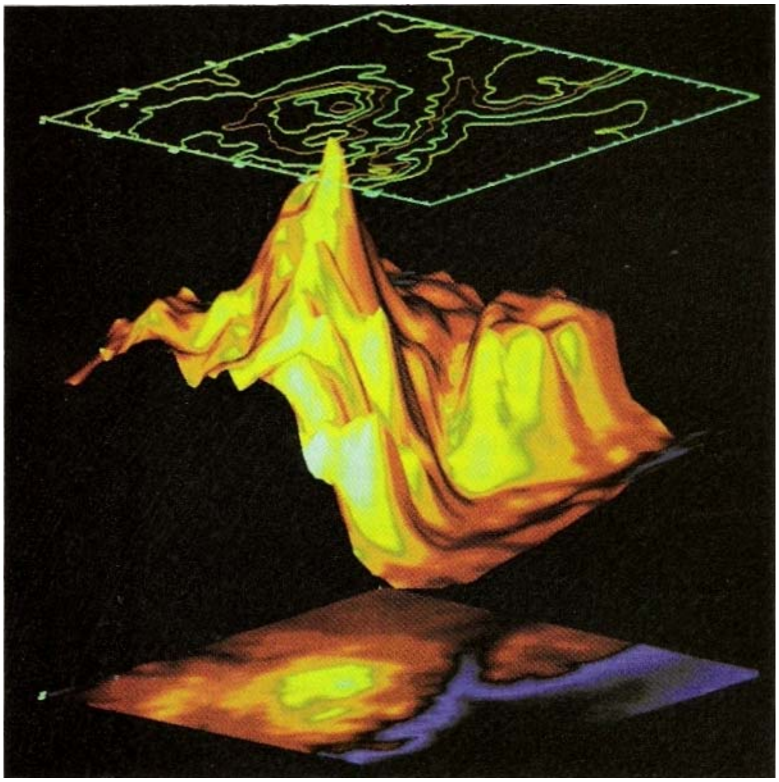
Presently, the workstation revolution, together with the associated proliferation of supercomputers and near supercomputers into academic and industrial environments, is giving rise to a rapid and dramatic revolution in the art and practice of scientific visualization. The supercomputer centers create a demand for powerful, efficient visual presentation methods simply because of the immense volume of the data produced by supercomputer simulations. On today's machines the solution of a single, 3-D continuous-field simulation, as frequently carried out in such computational scientific domains as fluid dynamics, structural mechanics, meteorology, seismology, cosmology, molecular modeling and others, may well contain some hundreds of millions of numerical values. There is no hope of digesting such large data sets-of finding their essential features and exposing their hidden details-without the application of high-resolution, high-speed computer-based visualization tools.

High-resolution graphical rendering is computationally expensive in the sense that a large number of arithmetic operations are required to produce a picture from model data. However, these graphical computations are stereotyped and repetitive, so they may be performed by special dedicated processing circuitry with a high degree of parallelsim. The



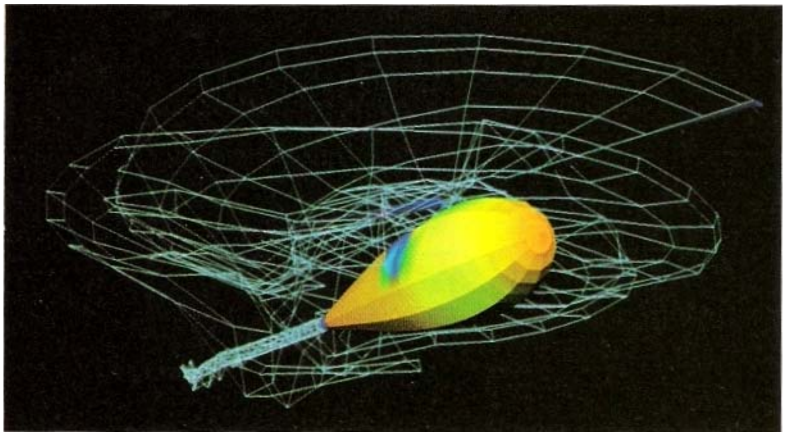
Active site of the enzyme triose phosphate isomerase, together with its natural substrate dihydroxyacetone phosphate. Atoms are represented as colored balls (red = oxygen, blue = nitrogen, green = carbon, yellow = phosphorus and white = hydrogen) with associated chemical bonds depicted by cylinders. The transparent blue surface represents a level surface of the electron density calculated quantum mechanically.

This image is a frame from a computer graphic movie, generated by Stephan Fangmeier at the National Center for Supercomputing Applications, from a simulation carried out by Paul Bash and Martin Karplus of Harvard University, using the original enzyme structure determined by Robert Davenport and Gregory Petsko of the Massachusetts Institute of Technology.



Three different but correlated bivariate distributions are represented using three kinds of visualization functions. In the middle, terrain elevation data around Pike's Peak is rendered as a shaded surface. Above, a correlated distribution of temperatures is depicted by a contour curve plot. Below, a correlated distribution of snow pack depth is represented by a color shaded contour plot. This image was produced using the software package PV Wave, a toolkit which gives scientists the capability of interactive construction and viewing of visual representations of functions and data sets.

Display of the results of a supercomputer simulation of the dynamical interaction of the wake of the rotor blades with the body of a helicopter. The vortex sheet created by the blade motion is depicted in wire frame style. Colors on the helicopter body denote pressure. The high-pressure spot (blue) on the starboard side is caused by the blade tip vortex, and is seen running rapidly aft in phase with the blade rotation in the movie of which this represents one frame. The fluid dynamical simulation was performed using the USAERO program from Analytical Methods, Inc. This image was produced using Ardent Computer's CFD Viewer.



development of application-specific VLSI circuits for advanced graphical processing (chips which can be produced relatively cheaply and ganged in parallel or pipelined fashion in order to multiply performance) has been a major factor enabling widespread affordable access to previously unheard of levels of graphics functionality in the new workstations and image computers. These hardware platforms have the potential for supporting highly innovative modes of scientific visualization.

Visualization innovations will not come automatically with the hardware, however, but will require further inventiveness. While the rendering of images from surface models may be regarded as stereotyped computation, there remains considerable freedom for choosing the methods of associating geometric objects (for example, curves, surfaces, volumes) and their visually relevant properties (color, opacity, illumination), with the abstractions of any particular computational science (pressure, velocity in fluid dynamics). And, of the possible methods of mapping physics to graphics, call them visualization *functions,* we have, in general, no way of knowing a priori which will be best in any particular case.

Moreover, we have to contend with the terrible 2-D bottleneck: until computer holographics becomes a widely available technology, all graphical display media are essentially 2-D surfaces, including the retina of the eye. There is no way to project a general 3-D model scene to a single 2-D view without losing information, in fact, most of it. For simple mechanical models a few views, as in drafting, may suffice to communicate all the relevant 3-D information, but the situation is much more difficult in the case of continuously varying spatial distributions, or in the case of very large biomolecular models, more serious still when these complex systems also vary in time. But it is these complex cases which give rise to the largest solution data sets and so are most in need of efficient visualization modes.

Even in the static case, whatever visualization functions and rendering algorithms are used, it is clear that many 2-D views are needed to get the 3-D picture. The researcher is obliged to view them in some sequence in time and then must somehow mentally integrate these viewing experiences to form his picture of the static 3-D situation. This process is aided considerably when the viewer has interactive control over the view selection. This means he is able to vary viewing parameters (for example, view point, view direction, etc.) smoothly and at will and see the corresponding views appear without noticeable delay. In the ideal case, using a joystick or other natural and comfortable control device, he would be able to roam about in his massive 3-D data set rotating objects to see their shapes from all sides, choosing section planes, panning to search for features of interest and zooming in to inspect them. Another dimension of assistance to the process is added when the researcher is also given interactive control of the selection of visualization functions.

Interactive graphics is, of course, a principal raison d'être of the workstations and it is also one of the primary characteristics distinguishing this visualization revolution from the earlier modes. The illustrations on these pages, while attractive and informative, do not begin to convey the power of interactivity. And even though these illustrations all have markedly different visualization functions, they will probably look trite in comparison with the newer styles of scientific visualization which will appear during the next few years as the workstations and minisupercomputers become available to workers in more and more diverse scientific and engineering areas.