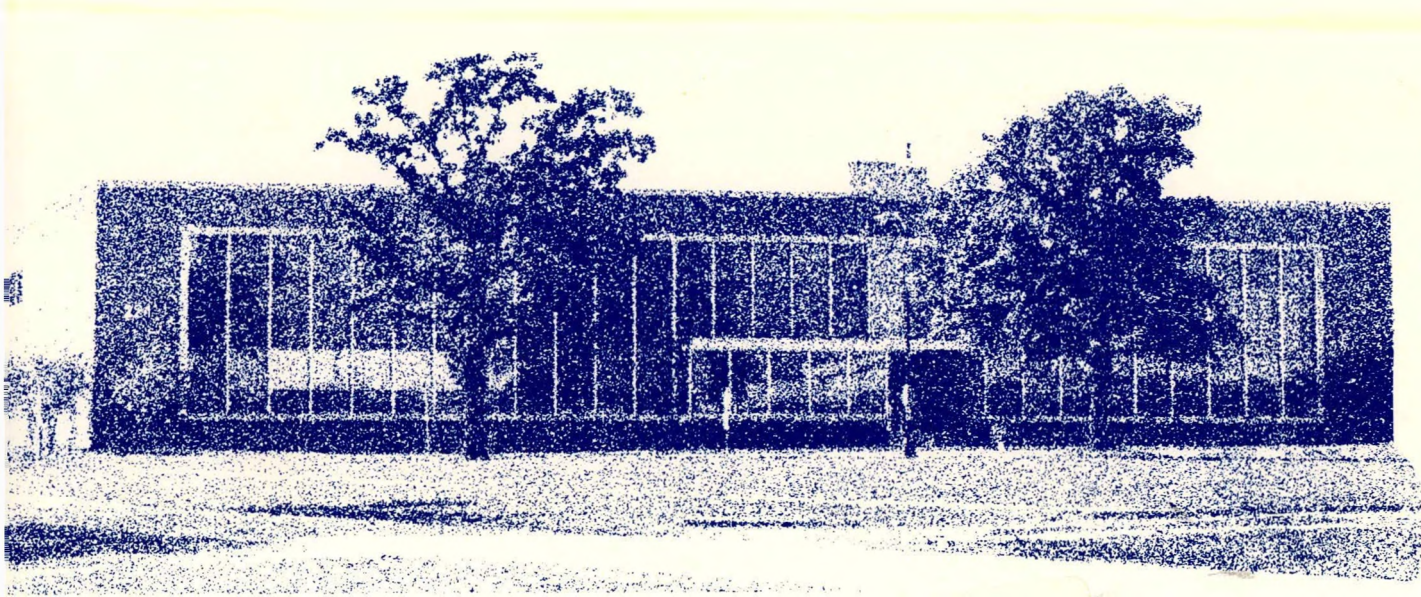


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# A Plan for Scientific Visualization

at ANL



Argonne National Laboratory  
Computing and Telecommunications Division

Operated by The University of Chicago for the U.S. Department of Energy under Contract W-31-109-Eng-38

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*A Plan for  
Scientific Visualization at ANL*

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March 1990

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(Intended primarily for internal distribution)

**MASTER**

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Fred Moszur (CTD) contributed to Chapters Two and Three. Mike Minkoff (CTD) contributed to Chapter One.

Cliff Caruthers (CTD), Doug Engert (CTD), Gail Pieper (MCS), Gary Schlesselman (CTD), and Dave Weber (CTD) reviewed various drafts.

Chris Opitz (CTD) formatted the original draft.

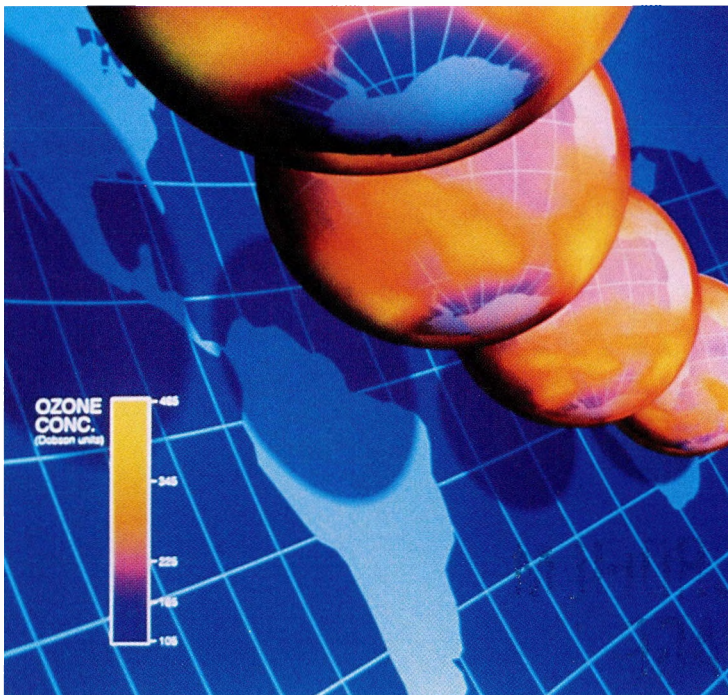
The graphic depicting the Antarctic ozone depletion was produced on Wavefront software by the National Center for Atmospheric Research.

# 1

## An Overview of Scientific Visualization

While humans casually continued to inject the skies with chlorofluorocarbons, aerosols, and numerous other chemicals throughout the 1970s, the Antarctic ozone level was drastically depleting, creating a hole in the ozone layer--a potential catastrophe threatening life on earth. Not until 1986 did a team of scientists at the British Antarctic Survey discover that the hole was enlarging, although this finding was implicit in raw data obtained from the Nimbus-7 satellite nearly ten years earlier.<sup>1</sup> Had scientists used visualization data analysis tools earlier, they might

have noticed the annual ozone depletion much sooner and begun efforts earlier to alert the world to this condition.



Ozone Concentration over the Antarctic  
(July through October, 1987)

<sup>1</sup> Lamhof, Olin et al., *State of the Art in Data Visualization: ACM SIGGRAPH '89 Course Notes* (Boston: ACM SIGGRAPH, 1989), pp. II 12-30.

## BASIC CONCEPTS OF SCIENTIFIC VISUALIZATION

Output from computer simulations, meteorological sensors, particle sensors, computed tomographic scans, or magnetic resonance scans often consists of exhaustive amounts of numbers that are difficult and time-consuming to analyze.

The complexity of such data generated by computers has produced a data glut in which researchers quite often use as little as 5% of the data generated or collected. In other words, computer storage capability has surpassed user retrieval capability. However, when researchers can translate numerical data into pictures, they can focus on structures within images, differentiate between important data and unimportant data, and sometimes they gain immediate scientific insight.

As a research tool, scientific visualization contributes greatly to scientific research by transforming quantitative scientific information into a qualitative global view for analysis of complex simulations or equations. Three-dimensional time dependent graphic representations and animation sequences can effectively portray dynamic processes, evolutionary progressions, and object interactions. For example, researchers can easily view the evolution of a fuel-combustion simulation with animated computer models by using "stop-frame" animation color-coded temperature fields.

Visualization enables researchers to view computational results in the natural geometry of the phenomena being analyzed. Conversely, visualization can use abstract models to emphasize selected characteristics. See Appendix B for a list of journal articles and books that discuss scientific visualization in detail.

Scientists require three types of visualization:

1. Analysis graphics allow researchers to interact freely with their data, observe time-dependent phenomena in real-time, interactively steer computations, and see immediate visual results on workstation displays. Analysis graphics require accurate data representation and interactive ability rather than image quality.
2. Communication graphics allow researchers to communicate scientific discoveries to colleagues in a clear and timely manner. Image quality is not as important as a clear visual representation of data.
3. Presentation graphics enable researchers to broaden their audience. This type of visualization allows researchers to illustrate formal presentations at conferences and articles in professional journals. Often, the higher the quality of the material, the more easily understood and effective the presentation. Visual information (e.g., animation) is often effective in conveying salient information, even to audiences unfamiliar with the topic.

## BENEFITS TO ANL SCIENTISTS

Visualization techniques have a broad range of use within computation for physical science and engineering modeling. Visualization provides a means to "see" globally the results of a computationally intensive simulation in a way that printed output cannot provide. Visualization provides new ways of debugging software, communicating results to others, and most importantly, seeing properties of a computation that were unknown before.

By investing in general purpose and customized visualization tools and techniques, Argonne researchers are able to use their time effectively when analyzing computational results and can effectively communicate information through visual models.

Among specific ANL activities that are appropriate for the use of visualization techniques are problems in chemical modeling, physical modeling, molecular modeling, atmospheric modeling, and fluid flow behavior in complex geometries.

# 2

## Current Scientific Visualization at ANL

Three-dimensional time-dependent graphics and animations can effectively illustrate dynamic processes, evolutionary progressions, and object interactions. A growing number of Argonne researchers are adopting these visual techniques for their analyses of complex simulations. However, as researchers obtain a substantial amount of scientific graphics with current ANL equipment, the acquisition of additional hardware and software graphics technology can dramatically improve effectiveness.

### GRAPHICS HARDWARE

The current graphics laboratory provides two-dimensional and three-dimensional imaging, video animation, and hardcopy output. Available hardware includes the Ardent Titan, the Sun 3/60, the Macintosh IIx, a stop-frame video animation system, and a Tektronix color printer.<sup>2</sup> This equipment is described below.

- The *Ardent Titan Graphics Supercomputer* creates interactive two-dimensional and three-dimensional models on its high resolution color graphics monitor and stereoscopic monitor through its software

packages and graphics libraries. It also produces video output.

- The *Sun 3/60 Scientific Workstation* allows for high resolution color graphics (primarily two-dimensional) as well as general purpose scientific computing.
- The *Apple Macintosh IIx* allows for high resolution color graphics as well as video input and output through its TrueVision NuVista video and graphics board.
- The *Stop-Frame Video Animation System* allows the computer to create smooth video animation of time-dependent phenomena by recording one frame at a time. Its components include:
  - An *Animation Controller* that synchronizes the activity between the Ardent Titan and the recorder.
  - An *NTSC Encoder* that converts component RGB video to composite videos.
  - A *Composite Video 3/4" Tape Recorder*.
  - VHS and Betamax Recorders*.
- The *Tektronix 4693DX Color Thermal Printer* provides medium-resolution color hardcopy.

The existing Stop-Frame Video Animation System is essentially a starter interim system to provide recording capability. The system requires a considerable level of skill (especially an understanding of video signal technology) to maintain and operate. The existing configuration is easily overwhelmed with any reasonable length video animation. Stop-frame recording involves three steps for each frame: (1) gathering the data, requiring 10 to 60 seconds, (2) rendering the data, requiring 10 to 120 seconds, and (3) recording the data, requiring approximately 20 seconds. Typically, the existing system would take 10 to 30 hours to record a 30 second animation. During this length of time, the video signal usually drifts and decreases the recorded image quality, and the recorder sometimes breaks during the mechanics of stop-frame recording.

While the Ardent Titan and the Macintosh IIx can be connected to the recording system, there is no capability for network access to the recording system. This limitation needs to be addressed to enable other computers to drive the recording system.

While the Ardent Titan has been used effectively to visualize several applications, it has a single-frame buffer and is essentially a single-user graphics system. The small number of appropriate graphics platforms constitutes a bottleneck for carrying out multiple visualization projects; therefore, more platforms are desirable.

<sup>2</sup> See Figure 8 in Appendix A for a complete configuration of the current Scientific Visualization Facility.

## GRAPHICS SOFTWARE

Argonne researchers use scientific visualization tools ranging from workstations to personal computer applications. While the available tools are certainly useful, Argonne recognizes that computational researchers need additional software capabilities to visualize scientific data more successfully and efficiently.

### NCSA ImageTool for Personal Computers

The National Center for Superconducting Applications freely distributes NCSA ImageTool, which is a computer application allowing computer users to analyze data visually on the Apple Macintosh II. NCSA also distributes ImageTool for the Sun workstation, and the PCShow program for the IBM Personal Computers. These programs allow researchers (1) to visualize data as raster images, (2) to use different color palettes, (3) to magnify images, and (4) to animate multiple raster images.

NCSA ImageTool uses color to analyze data stored in a two-dimensional array. It is a simple yet elegant user interface, and its public domain status makes it a popular tool for data analysis. However, applications that require the capability to view three-dimensional objects or volumes from arbitrary perspectives require more sophisticated capabilities than ImageTool provides.

### Ohio Supercomputer Center apE for Sun Workstations

The Ohio Supercomputer Center Graphics Project and the Advanced Computing Center for the Arts and Design has developed an Animation Production Equipment (apE) software toolkit that allows researchers the flexibility to examine data in both two and three dimensions. The apE system places an emphasis on animation and the integration of the visualization process into the scientific process.

The complete apE toolkit consists of tools, filters, and documentation. The tools (running with SunView) allow for interactive manipulation and examination of data while the filters perform the computations. It is available for the Sun 3 and 4 workstations.

### Disspla for Central and Distributed Computers

Argonne has invested substantially in code both on the central computers (Cray X-MP/14, IBM 3330s, VAX 8700) and on distributed minicomputers (VAXes) that relies on the Disspla graphics library. Researchers use Disspla to generate line plots, contour maps, surface plots, and three-dimensional plots mapped into two-dimensional space. Disspla can produce vector graphics for nearly any graphics terminal available and is beginning to introduce improved raster capabilities for the VAX version of Disspla. These improved capabilities are not yet available for the IBM, Cray, and Unix versions of Disspla. However, Disspla capabilities do not easily allow for the storage and manipulation (e.g., rotation, zoom) of three-dimensional objects.

The Computing and Telecommunications Division (CTD) will assist computer users who have invested substantially in programs that use Disspla. Doug Engert and Dave Leibfritz (CTD) have been modifying and testing the beta test version of the Disspla X-Window graphics driver. This driver enables Disspla programs running on the Cray X-MP to display images on a workstation running the X-Windows system. Any future video animation system incorporated into the ANL computing environment will need to accept images produced by Disspla programs. At the same time, CTD needs to acquire and explore systems and software with state-of-the-art capabilities.

Computer Associates plans to upgrade Disspla capabilities to benefit existing Disspla users. However, Argonne researchers who are developing new visualization applications should consider the most effective available alternatives.

### PV~WAVE for Sun and DEC Workstations

The Precision Visuals' Workstation Analysis and Visualization Environment (PV~WAVE) allows researchers to display, reduce, analyze, redisplay, and interact with multidimensional datasets. PV~WAVE can visualize up to five dimensions of data simultaneously, merging vector and raster image graphics. It also allows researchers to develop specialized applications, and to navigate through data by using built-in commands and macros or by creating their own commands and macros. PV~WAVE is available for the Sun or DEC workstations.

## SCIENTIFIC VISUALIZATION ACTIVITIES

A growing number of Argonne researchers are using scientific visualization to depict quantitative scientific information for analysis of complex simulations or equations. Establishing a Scientific Visualization Facility will assist these researchers by providing and developing visualization tools (e.g., animations to depict dynamic processes, evolutionary progressions, and object interactions; three-dimensional color-coded models; three-dimensional stereoscopic models; and two-dimensional raster images).

Most of the scientific visualization projects conducted at ANL involve the following steps:

1. Data originates from simulations on high-performance computers or from a wide range of sensing devices (e.g., ultra sound sensors, computed tomography scanners, magnetic resonance imaging devices).
2. The data to be visualized transfers to a computer with graphics capabilities. Typically, models requiring a complex three-dimensional visual paradigm are constructed on the Ardent Titan. Less complicated models are constructed on a Sun workstation or on a Macintosh IIx.
3. Effort is applied to develop visual models that convey multiple dimensions of data and to structure algorithms efficiently (sometimes in parallel) so as to reduce rendering time and enhance interactivity.
4. The interactive visualization program often enables researchers to explore the models from any desired angle, to change color maps, and to alter the scale. These capabilities make analysis and debugging easier.

Current Argonne visualization projects include combustion modeling, applying the theory of quantum molecular dynamics, analyzing electron momentum distribution, volume visualizing, simulating molecular structure, simulating phonon behavior in high-transition-temperature materials, and modeling Wakefield Accelerator electron fields. Unless otherwise indicated, visualizations for these projects have been developed by John Rowlan and Fred W. Dech (CTD). Descriptions of these projects follow.

## Combustion Modeling

Research in combustion involves the construction of numerical simulations to study the dynamics and structure of flames and combustion fronts in gaseous and solid fuel combustion. Numerical solutions are being generated on current vector supercomputers, but the volume of data generated inhibits understanding. The need to consider visualization techniques arises from (1) the need to analyze the volume of data, (2) the need to study problems in more than one dimension and view the solutions in the natural geometry, and (3) the need to preserve computed phenomena during data reduction.

One solution studied is a standing-wave solution characterized by the periodic appearance, disappearance, and reappearance

of luminous points on the surface of the solid fuel sample. To visualize the computed results, data was processed by a program developed on the Ardent Titan computer. The program minimized the physical model by displaying a three-dimensional cylindrical surface with a color map corresponding to the temperature field on the surface of the cylinder. The three-dimensional image can be analyzed interactively with the Titan's capabilities to rotate, translate, and magnify the model. Moreover, recording images with a video recorder in stop-frame mode enables researchers to use animation to see easily the time-dependent behavior of the simulation.

In the area of gaseous combustion, the cellular solution was computed for a two-dimensional model of gaseous combustion with a point source of fuel. In previous work, two-dimensional and three-dimensional line plots (generated with the

Disspla graphics library) provided a wire-mesh, three-dimensional-perspective surface plot to exhibit the temperatures. Time-dependent animation was not possible with this method. With the Ardent Titan, we create an abstract model using a solid rendering of a surface to illustrate the cellular structure more clearly in varying colors (see Figure 1). By extending this effort to animation, we are able to visualize the pulsating, time-dependent cellular solution. Future plans include creating variable-color palettes to emphasize and scale the color maps, in addition to enhancing the detail of the color maps and data sets.

Michael Minkoff (CTD) and Alvin Bayliss (Northwestern University) are the principal researchers.

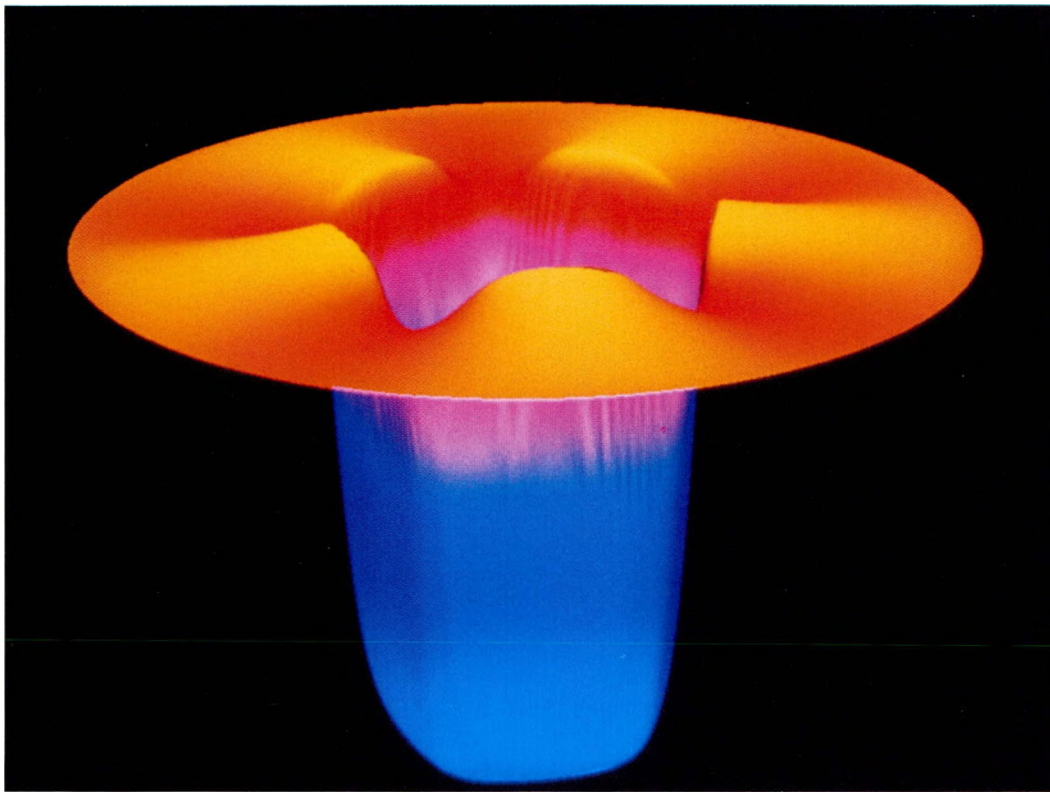


Figure 1: Abstract Model for Gaseous Combustion

## Applying the Theory of Quantum Molecular Dynamics

Quantum molecular dynamics applications use the Cray X-MP/14 computer to simulate the dynamic behavior of mixed quantum-classical particles. The physics and chemistry of materials involve systems that consist of light particles such as electrons interacting strongly with an ensemble of heavy particles evolving according to the time-dependent Schrödinger equation and the ions according to Newton's equations of motion. The real-time dynamics of electrons and ions can be simulated concurrently with the recently developed computer simulation technique called quantum molecular dynamics. The time-evolution operator for the electron-wave function is managed

by using a split-operator technique to accommodate the kinetic energy in momentum space and the potential energy in real space, while using three-dimensional fast Fourier transforms to make the transformation. The ions are simulated by classical molecular dynamics in the constant-temperature ensemble. This technique is the only one currently that can reveal the dynamic behavior of the quantum particle as well as the behavior of the classical system.

In previous work, we modeled the ions as simple two-dimensional projections on a Sun workstation. Now, we obtain simulation data from the Cray X-MP and develop a visual paradigm on the Ardent Titan to depict a set area (a box) containing three-dimensional opaque spheres (representing atoms) and transparent clouds (representing electron wave fields). The visualization program

on the Ardent Titan enables researchers to explore the electron field (the clouds) interactively from any desired angle. The program allows users to translate, rotate, and zoom into the model and to view the electron field in different intensities. Recent work depicts the electron field cloud as contoured transparent surfaces with the "Marching Cubes" algorithm (see Figure 2). Such modeling will increase visualization speed and also improve real-time interactivity. Future plans include time-evolution video animation to show the evolution of the electron cloud into the steady state.

Rajiv K. Kalia and Priya Vashishta (Materials Science Division) are the principal researchers.

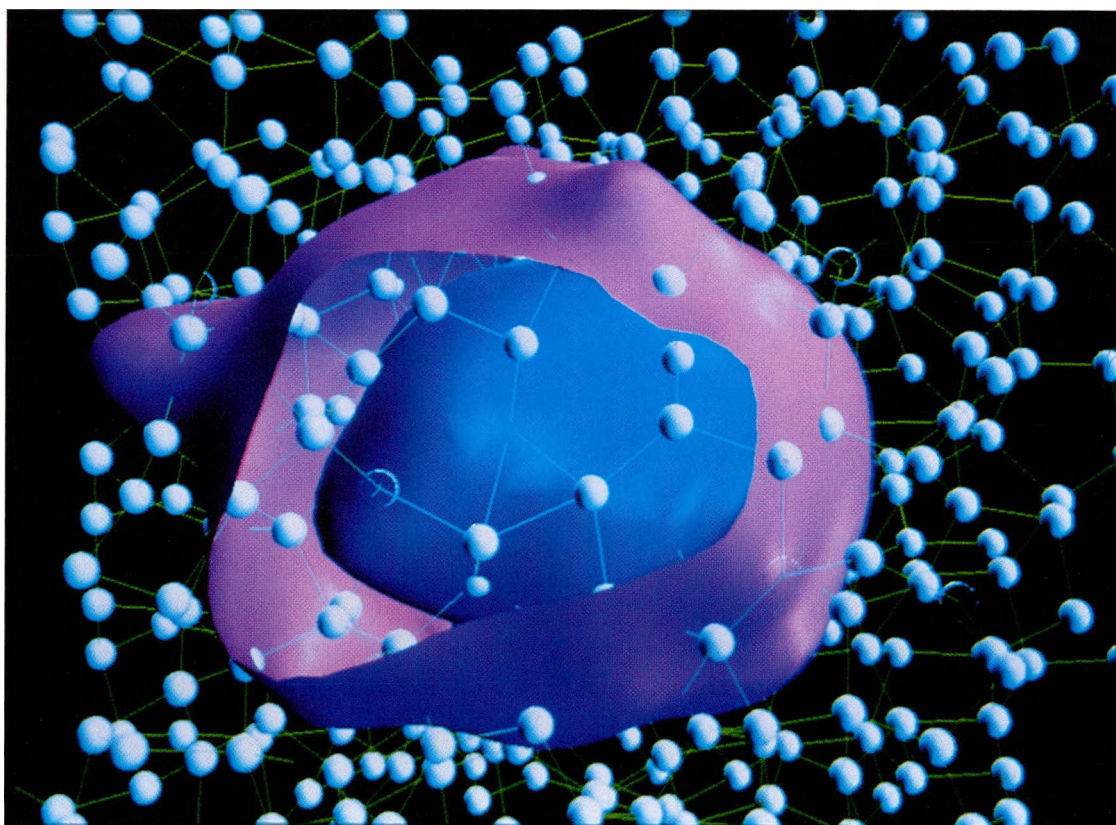


Figure 2: Electron Potential Within Dense Helium Liquid

## Analyzing Electron Momentum Distribution

A current two-dimensional positron annihilation study uses the Ardent Titan computer for graphics representation on two-dimensional positron annihilation data. Two-dimensional positron annihilation studies have led to detailed information about the electronic structure in materials such as metals and metal oxides. Scientists have recently used this

technique to study the new high-temperature superconductors and their electronic structure, particularly with regard to the existence of Fermi surfaces. Both the electronic structures and the data resulting from such measurements are highly complex and difficult to visualize with conventional graphics.

Using the Ardent Titan, these researchers have created three-dimensional abstraction with color coding (see Figure 3) that has proven effective for full comprehension and

use of the data, in addition to a three-dimensional color-coded surface (to model the electron movement distribution) and a stereo version of the model on the Ardent Titan stereoscopic terminal. Researchers are thus able to achieve real-time interaction with the model (with translation, rotation, and zoom options).

Daniel G. Legnini and Lars C. Smedskjaer (Materials Science Division) are the principal researchers.

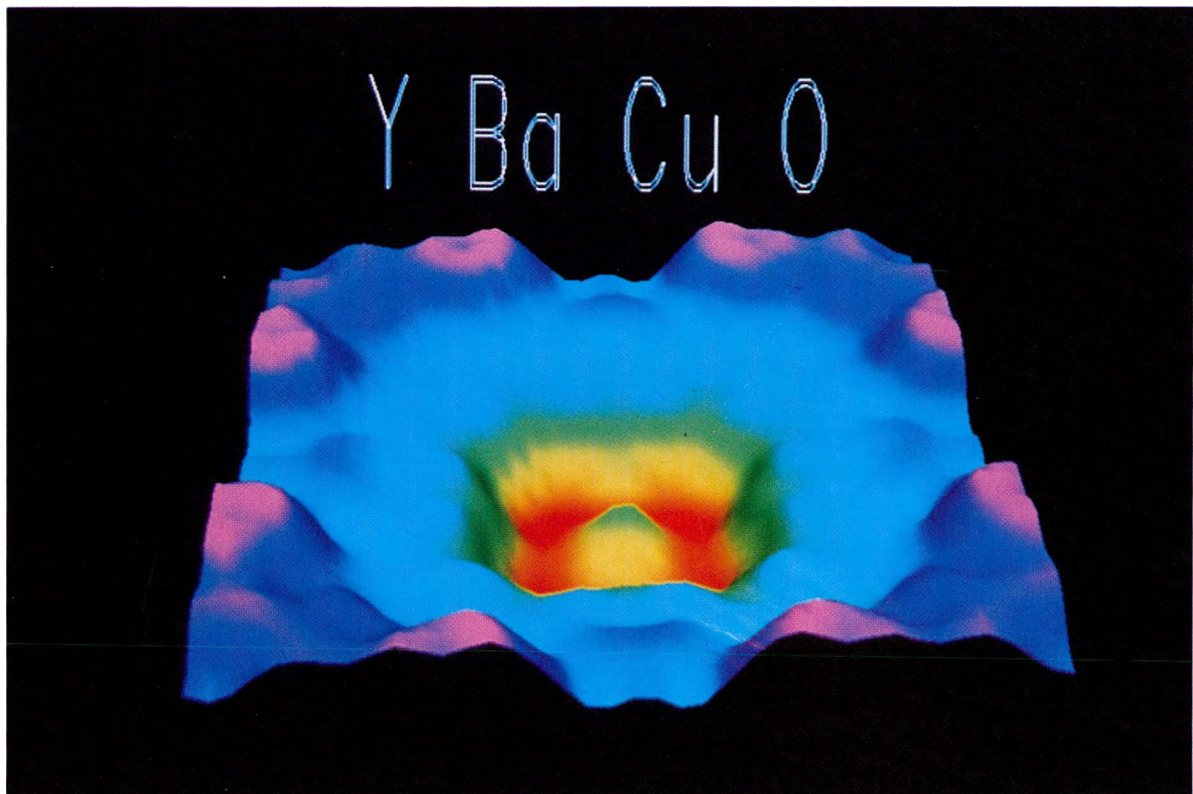


Figure 3: Electron Momentum Distribution Within Perovskite Superconductor

## Volume Visualizing

A recent volume visualization study develops nondestructive materials characterization methods by using equipment such as charged coupled device (CCD) cameras and computed tomography scanners to collect data for later image reconstruction and analysis. One particular application has involved collecting CT-scan data for a ceiling tile previously soaked in flame retardant solvent and assessing the effectiveness of the application of the process by studying how well the tile absorbed the solvent.

An existing X-windows volume analysis program has been adapted on the Ardent Titan that reconstructs a three-dimensional image and enables researchers interactively to peel away layers or slices of the image in any arbitrary orientation to see where the tile did or did not absorb the solvent (see Figure 4). Previously, they used two-dimensional slices depicted by a personal computer using NCSA ImageTool. By using this tool for volume analysis, researchers now have the flexibility to interactively select and visually study any portion of the object volume. Color variations in the images created by the volume

visualization program make it easy to detect variation in density that indicate where the solvent has absorbed. Researchers can also arbitrarily translate and rotate the volume and produce variable color maps. Future plans include using transparencies to filter out selected densities.

William A. Ellingson (Materials Components Technology Division) is the principal researcher. David Lifka (CTD) reformatted the CT-scan image data into a form suitable for the Ardent Titan and for NCSA ImageTool.

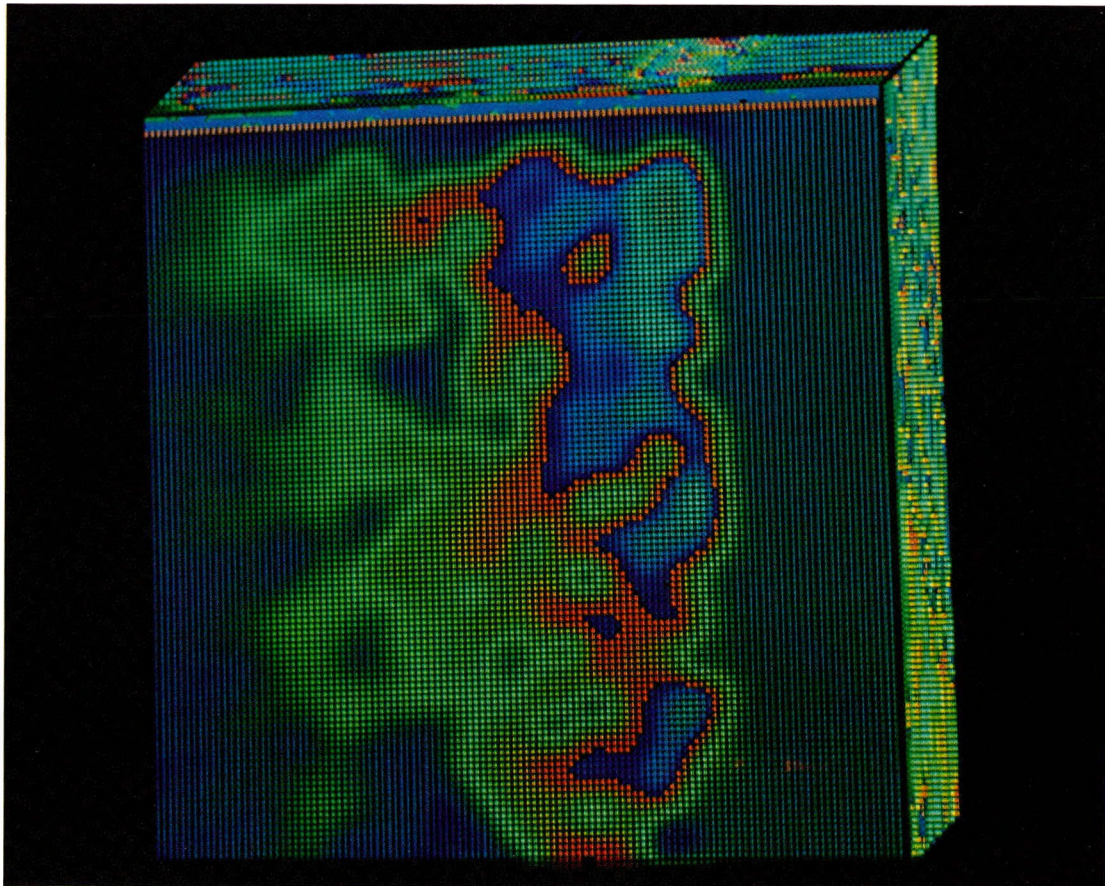


Figure 4: CT-Scan of Armstrong Ceiling Tile

## Simulating Molecular Structure

A recently developed interactive program on the Ardent Titan models molecular structures as ball-and-stick figures and space-filling figures. This program is sufficiently generic to model virtually any molecular structure and permits viewing from arbitrary angles. For this project, the program produces a three-dimensional model of silicon crystals that displays the crystalline structure and demonstrates the various states of the atoms. The model consists of ball-and-stick figures of a molecule silicon crystal rendered on the Ardent Titan from simulation results computed elsewhere.

Atomistic modeling in the form of molecular dynamics (MD) and in Monte Carlo simulations is a method of studying the cooperative and individual behavior of a system of atoms under well-prescribed conditions.

Through the use of interatomic interaction potentials and border conditions, simulations can be made to represent the physical state of a material at finite temperatures and pressures reasonably well. The results of such simulations are particularly valuable for the study of the relationship between the atomic structure of a system and its thermodynamic, mechanical, and transport properties. Because of these features, atomistic simulation is increasingly gaining recognition as a means

of probing complex physical processes at the atomic level.

The purpose of these simulations is to isolate more easily the effects of surfaces and interfaces, and to elucidate the kinetics of the melting process. To investigate the roles played by internal and external surfaces we have carried out a series of molecular-dynamics simulations of the melting of crystalline silicon, with and without such extrinsic defects, at elevated temperatures. See Figure 5 for an example of a molecular-dynamic simulation.

Simon R. Philpot (Materials Science Division) is the principal researcher.

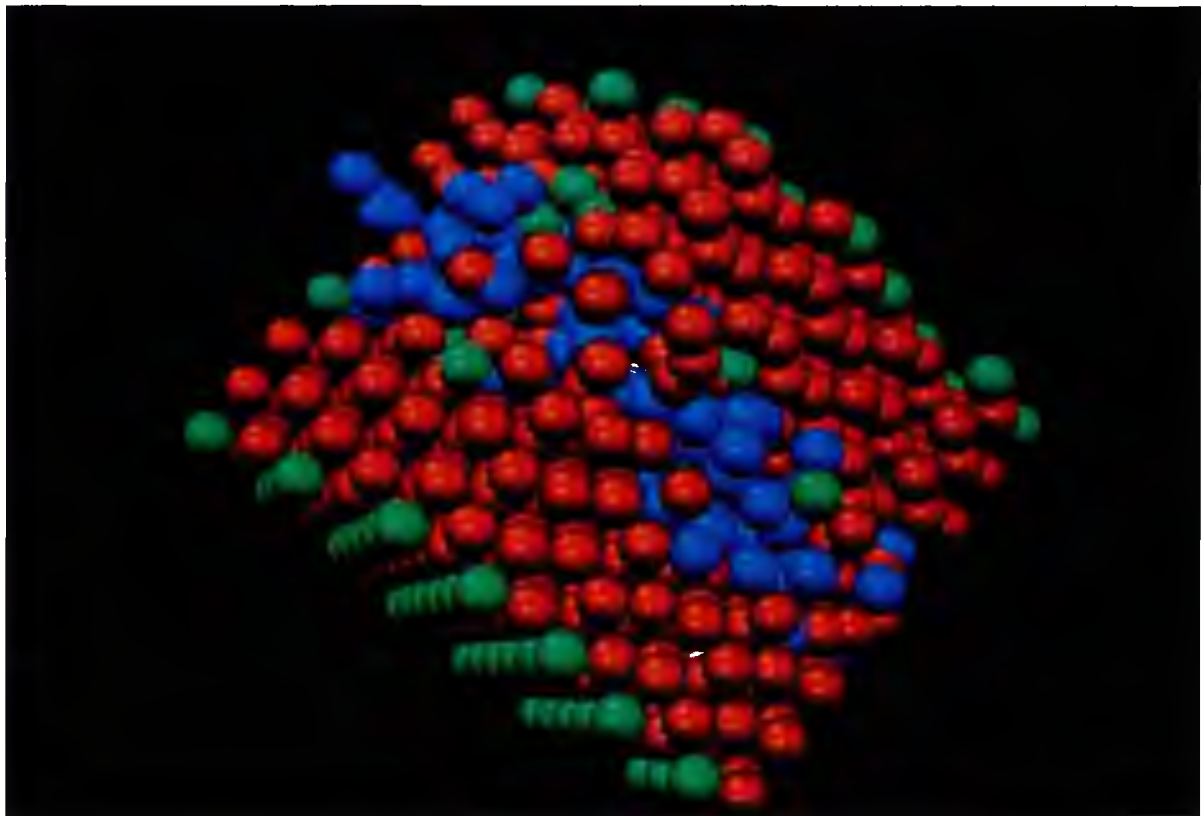


Figure 5: Silicon Crystal

## Simulating Phonon Behavior in High-Transition-Temperature Materials

A model developed on the Ardent Titan allows investigation of the thermal vibrations of atoms by means of a paradigm (a lattice structure with connected spheres) simulating dynamic collisions (ion-atom collisions) in solids (see Figure 6). The focus is on the channelling of energetic ions in single-crystal materials. The phenomenon of channelling deals with the steering of the energetic charged particles through the open channels along the crystallographic axial or planar directions, caused by gentle small-angle collisions with the atoms of the lattice. Since channelling is very sensitive to the displacement of the lattice atoms from their equilibrium position, the purpose of the present study is to investigate such displacements resulting from thermal vibrations or other causes across the superconducting transition in high-critical-temperature materials.

To simulate the passage of the energetic incident ion through a crystal lattice, one must first have a three-dimensional crystal structure of the required material stored in computer memory. We have achieved this step in a general way, so that the structure of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  can be obtained. We must then identify the interaction energy of the moving ion and a lattice atom and compute the deflection at each interaction. We simulate the thermal vibrations of the lattice atoms by giving a random displacement to each lattice atom (assuming a Gaussian distribution). In this way, the response of the crystal lattice to the motion of the incident ion is depicted, and the complete trajectory of the ion along a crystallographic direction is projected.

The visualization model developed on the Ardent Titan provides a way to investigate the correlated collisions of the incident ion along a crystallographic direction. The model is a preliminary version that simplifies the particle interactions to reduce the complexity of computation but renders reasonably accurate

trajectories. The complexity of the crystal structure requires defining a "unit cell" (by using functions within the Dore' library) that can be replicated to represent an entire lattice structure. This model can simulate the trajectory of a particle through a crystal lattice from three perspectives (a view parallel to the initial trajectory, a view perpendicular to the initial trajectory, and a view representing a "fly through" following the particle through the lattice). One can thereby visualize the oscillatory motion of the incident ion through the axial or planar channels and also investigate the effect of atomic displacements in the lattice on this trajectory. The results assist us in understanding the mechanism of superconductivity in high-critical-temperature materials.

Lynn E. Rehn (Physics Division), Rajeshwar P. Sharma and Loren J. Thompson (Materials Science Division), and Peter Sigmund (Odense University) are the principal researchers.

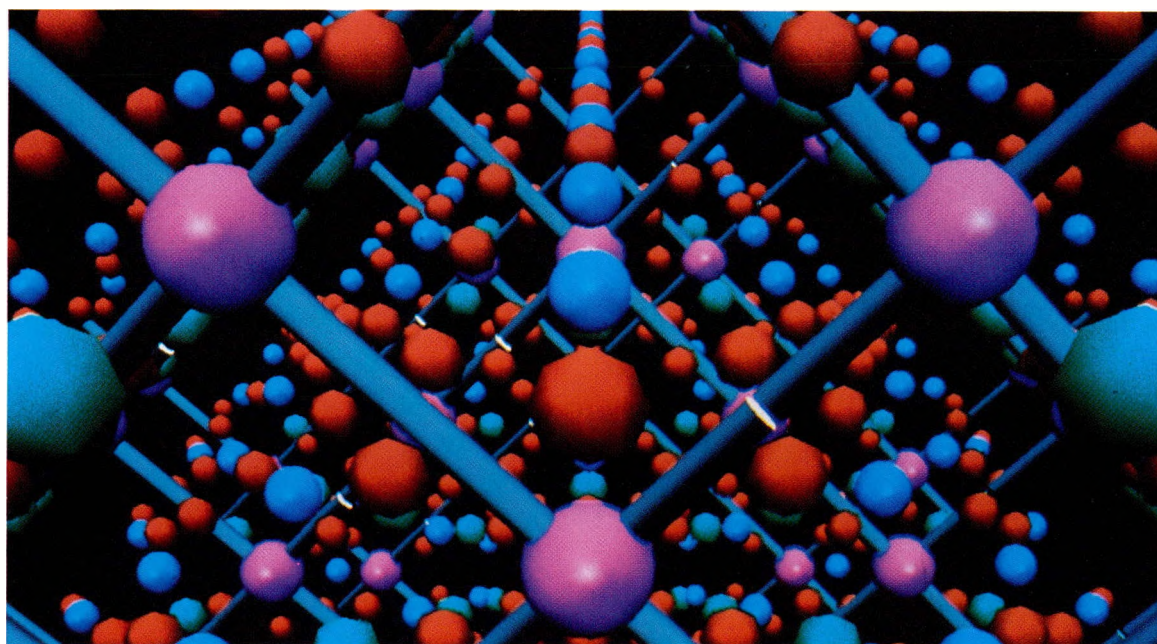


Figure 6: High-Temperature Superconducting Crystal

## Modeling Wakefield Accelerator Electromagnetic Fields

Another recently developed program models the time evolution of electromagnetic fields of the dielectric Wakefield Accelerator (see Figure 7). The Wakefield Accelerator is among the new particle acceleration techniques being developed by the ANL Advanced Accelerator Group. An intense electron bunch excites electromagnetic fields in a dielectric tube, which can then be used to accelerate a trailing electron bunch to high energies. A code has been developed to calcu-

late the fields in these and in similar devices which are driven by an external radio frequency source.

The code (ARRAKIS) is a finite difference time domain Maxwell equation solver based on the two-step Lax Wendroff method. The present version is restricted to an axially symmetric geometry but allows essentially arbitrary dielectric properties to be specified. Of particular interest is the case of a non-linear dielectric, where analytic solutions are not available, and which can exhibit nonlinear wave steepening effects. The source of the fields may be either a rigid relativistic electron bunch traversing the device axis of a dipole radiator.

We are animating the time evolution of the radial electric, longitudinal electric, and azimuthal magnetic fields with the NCSA ImageTool program on an Apple Macintosh IIX with a NuVista graphics board. The animations consist of Radial-Z coordinate displays of electric and magnetic field strength in the device at successive time steps. The result is a timely and economical way of analyzing captured data.

Paul V. Schoessow (High Energy Physics Division) is the principal researcher.



Figure 7: Longitudinal Electric, Azimuthal Magnetic, and Radial Electric Fields (from top-to-bottom) of the Wakefield Accelerator

# 3

## *Projected Plan for Scientific Visualization at ANL*

The projected Scientific Visualization Facility would provide an increasing variety of services for Argonne researchers. Initially, the staff of the Facility would share the responsibilities for production, education, and research. The Facility would focus its software development in such areas as “real-time” interactive visualization and volume visualization. The Facility plans to acquire equipment and develop visualization tools as required by the visualization needs of ANL scientific disciplines.

### **SCIENTIFIC VISUALIZATION SERVICES**

The Scientific Visualization Facility would offer both centralized and decentralized services, as well as instructional and specialized services.

#### **Centralized Services**

The Scientific Visualization Facility would provide Argonne researchers with high-end graphics and image processing hardware and software to solve difficult scientific visualization projects, to produce presentation graphics, to develop and test visualization software, and to research advanced scientific visualization techniques.

Argonne researchers will need production services (requiring specialized equipment) that include creating presentation quality hardcopy output suitable for public conferences, publications, and presentations.

Computer artists and scientific visualization specialists would develop visual paradigms to present data in forms in which researchers can more effectively analyze and describe physical phenomena. The Facility would provide the necessary equipment for producing computer-generated scientific film, video, slides, photographs, and printed output.

#### **Decentralized Services**

The Scientific Visualization Facility would develop and distribute graphics software that operates on workstations (e.g., Sun, NeXT, Silicon Graphics) or personal computers (e.g., IBM PS/2, Apple Macintosh IIx). Some visualization projects will require specialized graphics computers, and researchers may need to acquire such equipment themselves or arrange to use the Facility’s high-end graphics machines.<sup>3</sup> Pilot projects and software development often would be done initially on the Facility’s machines, and the software would then be sent to the researcher’s graphics computer.

<sup>3</sup> See Figure 9 in Appendix A for further information on proposed equipment.

A remote visualization environment would use inexpensive scientific workstations (e.g., Sun and NeXT) and give researchers the ability to use local visualization analysis tools and to store and transfer images between workstations and personal computers. This environment would also allow researchers with inexpensive recording equipment to produce locally short segments of animation videotape and high-quality hardcopy output.

A remote interactive visualization system would connect a researcher’s workstation or personal computer with high-end graphics running on supercomputers or specialized graphics machines. The researcher would be able to manipulate a computation while watching the graphic evolve. Installing an interactive distributed system would require high-speed networking (e.g., ULTRAnet) and the development of techniques allowing users to synchronize the computation with the rendering process.

#### **Instructional Services**

Argonne researchers who need scientific visualization may also need advice and instruction on the selection and use of equipment. The Facility staff will recommend and maintain a number of graphic workstations and can assist users with the configuration, installation, and integration of distributed systems.

To make researchers more aware of the various contributions that scientific visualization can offer to their research, the Facility should offer introductory and advanced courses on in-house visualization

hardware and software. Associated colloquia and seminars would provide the opportunity for physical science researchers who have benefitted from scientific visualization to share their insights with Argonne researchers.

## **STAFF ORGANIZATION AND RESPONSIBILITIES**

Ideally, the Scientific Visualization Facility would provide (1) animation, rendering, and production services, (2) education and training, and (3) research and development. Space requirements for the Facility include a room for workstations, programmers, visitors and various output devices, a smaller room for the sensitive digital framestore equipment and computer hardware, and offices for staff and students.

### **Animation, Rendering, and Production Services**

The Animation, Rendering, and Production Services staff would install algorithms developed by the Research and Development staff and would work with computational scientists at ANL. They would also produce large-scale animation projects and create high-quality scientific visualization hardcopy.

In the future, the staff should consist of at least two software specialists and one computer animator-artist skilled in digital imaging and animation techniques. They would be responsible for the day-to-day production of computer video animations and hardcopy images and would provide the necessary expertise for transferring

computer images from networks or workstations to various media for producing color computer hardcopy images and for editing computer digital animation.

The computer animator-artist's responsibilities would be:

- To help organize and define images by selecting visual paradigms that best illustrate the underlying data.
- To assist in the construction of color palettes and color maps that make the morphology of a scientific event more visible.
- To define visual representation of phenomena that does not exist in nature or are not readily observable (e.g., reactor core, collision of two neutron stars).
- To organize and create effective animations.

### **Education and Training**

The Education and Training staff would communicate the benefits of scientific visualization to Argonne researchers by offering courses and arranging colloquia and seminars featuring graphics and visualization specialists. The staff would also suggest various graphics workstation configurations according to user needs and budgets, provide assistance for graphics configurations, and provide instruction and maintenance for selected graphics hardware and software.

The staff would also provide information about:

- Available hardware and software.
- Available methods for producing videos, slides, etc.
- Macintosh tools.
- Network connections.
- Visualization choices for specific tasks.

- Image data formats for displaying, recording, etc.
- Graphics hardware evaluations.

## **Research and Development**

In response to the needs identified by ANL research, the Research and Development staff would conduct advanced research and development in scientific visualization (e.g., in volume visualization, real-time interactive environments, image processing, graphical networking, multiprocessor architectures, and modeling natural phenomena). These future activities will require the skills and expertise of at least two computer specialists (Ph.D.s), doctoral candidates, or highly skilled and experienced masters level researchers.

Since scientific research often requires the development of specific visualization tools, new algorithms and techniques will need to be developed. This type of visualization research is an integral part in the development of visualization tools.

### **Projected Three-Year Staffing Plan**

Table 1 outlines a plan for staffing the Scientific Visualization Facility over the next three fiscal years. In addition to regular staff, a number of highly skilled graduate students would be added.

**Table 1**  
**Staff Acquisition Plan**

<i>Year</i>	<i>Quarter</i>	<i>Staff Acquisition Plan</i>	<i>Students</i>
FY1990	Q1	-	1
	Q2	Applications programmer/education coordinator	2
	Q3	Computer animator-artist	2
	Q4	-	
FY1991	Q1	Software specialist	2
	Q2	Ph.D. researcher	2
	Q3	-	3
	Q4	-	3
FY1992	Q1	Software specialist	2
	Q2	Ph.D. researcher	2
	Q3	-	3
	Q4	-	3

## THE SCIENTIFIC VISUALIZATION ENVIRONMENT

The optimum environment for diverse needs in scientific visualization includes distributed workstations, high-performance computers, and high-speed networks. To address this broad range of application needs, CTD will offer easy-to-use general purpose visualization software ranging from tools for animation and volume analysis to custom tools for specialized applications. These available alternatives will enable researchers to derive immediate benefits from visualization with a small investment of effort. With an increase in that investment, researchers can migrate to more sophisticated tools and techniques. However, the more effective visual analysis tools for a researcher's specific application often require collaboration with visualization specialists.

## Workstation-Based Visualization Software

Visualization software running on a researcher's workstation can offer an effective method for analysis, but few vendors currently supply visualization software applicable to the types of research done at the Laboratory. Argonne researchers need interactive graphics tools for workstations and personal computers that will allow image processing, two-dimensional and three-dimensional rendering, palette construction and manipulation, image compositing, and presentation.

These tools will provide Argonne scientific visualization specialists with a general framework from which they can develop more specific tools for specific scientific disciplines. These visualization tools will include algorithms for image processing and manipulation,

programs to create two-dimensional and three-dimensional animation of complex objects, and graphical interfaces to window managers to link workstations and supercomputers.

Close involvement with Laboratory researchers and cooperation with other national laboratories and universities will help the Facility avoid unnecessarily duplicating other development activities. CTD is aware of such tools as the NCSA ImageTool program, the LBL Scry animation utility, the NCAR CGM X-Windows viewer, the Ohio Supercomputer Center apE toolkit, and the PV~WAVE program. CTD will make these tools available at ANL as appropriate.

## The Distributed Scientific Visualization Workstation Environment

Ideally, researchers should be able to communicate their discoveries, as well as their simulation codes and visual displays, to other researchers on remote computers. Therefore, researchers who have workstations and personal computers will eventually need:

- Memory-to-memory image transfer (i.e., supercomputer-to-personal computer frame buffer).
- Image compression and decompression algorithms to aid in image transfer.
- Remote visual access to centralized computers with high-end graphics capabilities.
- Local animation and video recording on videotape equipment.
- Color image conversion algorithms to enable conversion of image files to different formats, so they can be viewed on a variety of frame buffers.

This environment would allow researchers to view displays that were originally generated locally or with remote supercomputers. Researchers would be able to produce slides, photographs, and animation as easily as sending text files to a laser printer. Film recorders or video recording equipment would be connected to workstations and would allow users to produce scientific animation with little effort.

The Scry program from Lawrence Berkeley Laboratory is one example of a distributed environment. Peter Bertocini (CTD) has written an interface that animates GKS metafiles (produced by Displa programs) on Sun workstations. The recording capabilities of Scry have yet to be explored.

## “Realtime” Interactive Visualization

Computational researchers want “realtime” interactive visualization to see immediate results and to manipulate the computations as they watch the graphical display evolve. For complex simulations (e.g., fluid flow and molecular dynamics), researchers will need supercomputers and massively parallel computers to drive the computations.

It is therefore important to couple supercomputers closely with graphics displays. Ideally, a memory-to-memory bus would link the Cray X-MP, the Connection Machine, and other advanced computers to workstations with graphics capabilities. A possible way of achieving high bandwidth links would be to incorporate an HSX channel on the Cray X-MP with HSC interfaces on graphics workstations running on a high-speed network such as ULTRAnet. Such high-speed links would give Argonne researchers a direct visual connection between their workstations and advanced computers.

To achieve interactive visualization for complex simulations, either a powerful rendering engine (a super graphics workstation) or a powerful computational engine (a vector or parallelizing supercomputer) with a high-speed network attachment (or both) is necessary. However, many applications will probably continue to exist with calculations so time-consuming that interactive visualization will not be feasible. These applications must resort to stop-frame animation—a post-processing activity rather than an interactive one.

## Network Access to Scientific Visualization Devices and Services

The use of the Laboratory-wide TCP-IP Ethernet and Network File Systems will make user images available to Scientific Visualization Facility output devices and user data available for rendering by Facility staff. As the Laboratory upgrades Ethernet capabilities with the Fiber Optic Distributed Data Interface (FDDI) ring, the increased transmission speed can be used for visualization services. In particular, the higher FDDI network transmission speed will enable researchers to transfer longer sequences of animation to the video animation recording system. Similarly, higher network speeds will benefit the interactive visualization discussed earlier in the preceding paragraphs.

## Volume Visualization and Image Processing

Scientific visualization requires tools to reconstruct, display, manipulate, and analyze images based on data collected from magnetic resonance imaging, ultrasound, x-rays, and other sensors. The development of graphical representation of three-dimensional volumes is new. Projects under consideration include magnetic resonance imaging, computed tomography imaging, ultrasound imaging, and volumetric representations that model stress and strain of reactor components.

Related areas of scientific visualization to be researched include algorithms for rendering surfaces and volumes into volume memories, anti-aliasing of volumes, hidden volume removal, three-dimensional sculpting programs, general utility programs for arbitrary scaling and rotation of volumes, and volume compositing.

## **The Interactive X-Window Environment**

The X-window interface requires the development of compatible visualization tools to allow researchers to distribute graphic capabilities to many different computers. Potential near-term projects would include enhanced user interfaces for scientific simulation programs and workstation-to-super-computer links.

## **Animation Routines**

Animation of complex objects and scenes is becoming important in scientific applications because animated sequences convey more information than still scenes and evoke special interpretive capabilities in the human visual system. Available staff would develop basic animation routines to control the motion of many objects moving and interacting with one another and to interpolate object location. Visualizing fluid flow with the COMMIX program is one possible application at ANL. Other applications include the tracing of parallel

and vectorized computer algorithms and time simulations of fuel combustion and molecular dynamics.

## **FUNDING**

We will look to Laboratory discretionary funds to develop the infrastructure of this new organization and to enable pilot projects to visualize selected Laboratory applications. We will use the General Purpose Equipment (GPE) process to acquire initial equipment configurations. However, the Facility will need to secure sponsors for long-term research activities. CTD will pursue joint proposals with ANL divisions for visualization of scientific applications. Table 2 lists possible funding sources for the Scientific Visualization Facility.

Funding earmarked for collaborative CTD visualization projects will enable the desired expansion of staff and equipment to create the "critical mass" required for a viable organization. Table 3 outlines a funding plan for FY1990, FY1991, and FY1992 with the possible funding sources.

## **Equipment and Approximate Costs During Phase 1**

Phase 1 constitutes the minimum configuration of equipment necessary to expand the Scientific Visualization Facility. This equipment comprises the foundation from which the organization can grow; it includes video animation, input and output of computer images, and low-end personal computer-based graphics workstations. Table 4 outlines the approximate costs of equipment to be acquired in FY1990.

## **Equipment And Approximate Costs During Phase 2**

Phase 2 emphasizes the acquisition of high-end graphics workstations and specialized graphics architectures such as image processing computers and high-speed parallel processing graphics machines. Table 5 outlines the approximate costs of equipment to be acquired for the Facility in FY1991 and FY1992.

**Table 2**

**Possible Funding Sources for the Scientific Visualization Facility**

<i>Activity</i>	<i>Possible Funding Vehicles</i>
Applications research	Laboratory discretionary funds. Cooperative research and application projects from other ANL research divisions. State of Illinois proposals. NSF proposals. DOE proposals. Cooperative research with industry. Cooperative research with universities.
Production visualization services	Laboratory discretionary funds. Cooperative research and application projects from other ANL research divisions. State of Illinois. Industry collaboration. Internal service requests. Chargeback for cost recovery.

**Table 3**

**Possible Funding Plan**

FY1990

- Submit an Exploratory Research Funds Proposal to ANL management to fund staff and equipment identified in FY1990 activities and equipment.
- Submit proposal to outside agency for visualization of specific projects.

FY1991/92

- Extend ERF funding.
- Establish "steady state" of
  - funding from outside agencies
  - funding from outside users
  - service requests from internal divisions.

**Table 4**

**Phase 1:  
Equipment and Approximate Costs for FY1990**

<i>Equipment</i>	<i>Cost</i>
Output Devices	
Digital video framestore.....	\$ 65,000
Digital signal converter.....	4,500
Component videotape recorder.....	27,000
High-resolution color printer.....	11,000
High-resolution color scan converter.....	18,000
RGB animation film recorder.....	28,000
High-resolution color monitor.....	4,500
Input Devices	
Color image scanner.....	6,000
Interactive input devices.....	5,000
Graphics Workstations	
High-performance graphic workstation.....	120,000
Scientific workstation.....	11,000
TOTAL EQUIPMENT COST.....	300,000

**Table 5**

**Phase 2:  
Equipment and Approximate Costs for FY1991 and FY1992**

<i>Equipment</i>	<i>Cost</i>
Output Devices	
Portable video projection system.....	\$ 28,000
Input Device	
Digitizing camera.....	10,000
High-end Graphics Workstations	
Parallel processing graphics computer.....	230,000
General purpose Unix-based scientific workstations (4).....	40,000
TOTAL EQUIPMENT COST.....	308,000

## EQUIPMENT

The Scientific Visualization Facility staff would be able to develop visual paradigms to find new ways of representing data that will (1) analyze and describe physical phenomena and (2) develop visual representations that best quantify data more quickly. The staff would also create presentation-quality hardcopy output suitable for public conferences, publications, and presentations. The equipment selected for the Scientific Visualization Facility would represent the best available for each function.

The typical visualization programs for displaying an image can be installed on any number of computer systems with dedicated graphics hardware. Most of the equipment available to the Scientific Visualization Facility staff would reside initially in the Mathematics and Computer Science Division Graphics Laboratory (Building 203, Room C229). CTD has requested General Purpose Equipment (GPE) funds to acquire equipment such as graphics workstations, scientific workstations, an image processing machine, digital video frame stores, video tape recording equipment, and personal computers.<sup>4</sup>

### Software

A purchased collection of graphics application packages would reduce the need for software development by the Scientific Visualization Facility staff. Software items to be acquired would include scientific visualization software (e.g., Preci-

sion Visuals PV~WAVE, Cray Research MPGS), animation software (Wavefront), graphics language source code (e.g., Dore'), paint systems (e.g., Artisan and Lumina). The software would be selected to run on many different platforms and work with many types of output devices.

### Workstations

Workstations and personal computers will be a major component of the ANL scientific computing environment. They offer a wide range of application software and provide a cost-effective visual interface to the computational processes running on high-end computers. Table 6 lists types and examples of workstations and briefly describes their functions.

#### *Graphics Workstations*

Graphics workstations combine the specialized graphics software and hardware with number-crunching ability. High-end graphics machines in this class include the Ardent Titan, the SGI 4D/240, the AT&T Pixel, and the Stellar GS2000 workstations. Medium-end graphics workstations include the Silicon Graphics Personal IRIS. More of these machines will be needed as the workload increases, since a machine can work on only one project at a time.

#### *Scientific Workstations*

The generic scientific workstation has a display resolution on the order of 1,280 by 1,024 pixels and 8-to-24 bits of color, is connected via networks to other workstations and larger computers, has substantial

processing power for improved response, and can accept specialized graphics hardware and software. Typical examples of this machine are NeXT machines and Sun Sparkstations.

#### *Image Processing Machines*

Image processing machines such as the Pixar II are powerful computers that have specialized image processing hardware and software to serve a wide range of image applications not available on conventional workstations. These applications include image enhancement and manipulation, image filtering and edge detection, volume visualization, 48-bit color images, analysis of computed magnetic resonance imagery and ultrasound images, and realistic surface rendering.

#### *Personal Computers*

When configured with appropriate graphics boards (e.g., the TrueVision NuVista board), personal computers (e.g., Apple Macintosh IIX) become powerful graphics platforms adequate for many low-end visualization applications while costing much less than specialized graphics workstations. A great deal of graphics software is becoming available for these machines.

<sup>4</sup> See Appendix A for a complete configuration of the proposed Scientific Visualization Facility.

**Table 6**  
**Workstations**

<i>Workstation</i>	<i>Function</i>
High-performance graphics workstation SGI 4D/240 AT&T Pixel Machine	High-speed parallel computing with state-of-the-art graphics
Medium-performance graphics workstation SGI Graphics Personal IRIS	Cost-effective workstation platform for two-dimensional and three-dimensional graphics
Scientific workstation NeXT Sparkstation	General purpose computing machine with good two-dimensional graphics
Image processing machine Pixar II Image Computer	Image processing applications
Personal computer platforms Apple Macintosh with NuVista graphics board	Low-end graphics workstations video in/out

## Output Devices

Output devices will include the Digital Video Framestore System, video recorders, film recorders, color printers, a high-resolution scan converter, digitalizing cameras, video cameras, and image scanners. Table 7 lists types and examples of output devices and briefly describes their functions.

### *Digital Video Framestore System*

A networked digital video framestore system allows images to be sent directly from any computer and will allow image editing, compositing, and overlaying text, symbols, scanned images, and paint system images. The framestore permits random access to stored images.

The required configuration of this equipment will include a digital video framestore, (e.g., the 50-second Abekas A-60 Digital Disk Recorder) with a digital character generator, (e.g., the Abekas A72 Digital Character Generator). A digital signal converter (e.g., the Abekas A20 Signal Converter) would convert the RGB signal into a digital image.

### *Video Recorders*

Video recordings of animation are easy to use and offer short turn-around time between image recording and viewing. Commercial grade equipment such as the Sony BetaCam SP and Sony D1 digital recorder would be used to produce presentation-quality video recordings. It is possible to configure

distributed low-end graphics workstations with video recording equipment.

Research is necessary in high definition television (HDTV), which promises major improvements in image quality and color in video recording.

### *Film Recorders*

The preferred medium for high-quality imaging is film, because of its unrivaled resolution and color definition. A typical device for producing films is the Matrix QCR, which has an 8K by 8K resolution, 16.7 million colors, and interchangeable film formats. An inexpensive desktop film recorder would allow users to create hard

copies of the images on their display at the touch of a button and would produce 8 by 10, 4 by 5, and 35 mm formats.

### **Color Printers**

High-quality color printers are evolving rapidly. Some of these printers currently produce photographic quality, and their quick turnaround time makes them useful for prompt visual analysis.

### **High-Resolution Scan Converter**

A high-resolution scan converter would convert the RGB picture of most computer displays to NTSC video necessary for standard video recording.

### **Digitalizing Cameras, Video Cameras, and Image Scanners**

Digitalizing cameras, video cameras, and image scanners integrate computer-generated models with pictures from the real world and with scanned images of complicated diagrams or portions of other documents.

### **Input Devices**

Devices such as tablets, pedals, mice, switches, spaceballs, and knob boxes are an important part of the interactive visualization process, since it allows more natural and convenient interaction than traditional keyboard input. Tablets aid in image editing and compositing; knob boxes and the new 6-dimensional spaceball and Data-Glove might be used to control the orientation of a model or process occurring on the computer screen, such as rotation, translation, yaw, pitch, and roll. Table 8 lists the types of input devices and briefly describes their functions.

**Table 7**  
**Output Devices**

<i>Output Device</i>	<i>Function</i>
RGB analog film camera Matrix Multicolor	Single image film recording
Pin register film recorder Matrix/Oxberry	Animated film recording
Component analog video tape recorder Sony BetaCam SP	Stop-frame animation video recording
Component digital video tape recorder Sony DVR-1000	Digital recording and archival of computer animation
Monitors, encoders, sync generators	System peripherals
High-resolution color laser printer	Hardcopy output
Digital video framestore system Abekas A60 digital disk recorder Abekas A20 signal digitizer	Networked image generation, playback, and editing

**Table 8**  
**Input Devices**

<i>Input Device</i>	<i>Functions</i>
Digitizing video camera Color image scanner	Full color input of real-world images, charts, photographs, and complex diagrams
Tables, Spaceball, Mouse, Knob Box, DataGlove	Interactive input

## LIAISONS WITH OTHER RESEARCH INSTITUTIONS

Collaboration with other scientific visualization groups stimulates the communication and exchange of useful ideas, minimizes redundant efforts, and leads to greater productivity.

The Scientific Visualization Facility at Argonne National Laboratory and the Electronic Visualization Laboratory at the University of Illinois at Chicago have agreed to collaborate on scientific visualization activities. Joint research activities are currently in the planning stage. Graduate students from Electronic Visualization Laboratory are spending summer semesters at

Argonne working in the Scientific Visualization Facility and are bringing with them valuable expertise and knowledge in the area of computer graphics and scientific visualization.

A collaboration with the National Center for Supercomputing Applications in Urbana, Illinois, is also in the planning stage.

# APPENDIX A

## Scientific Visualization Equipment Configurations

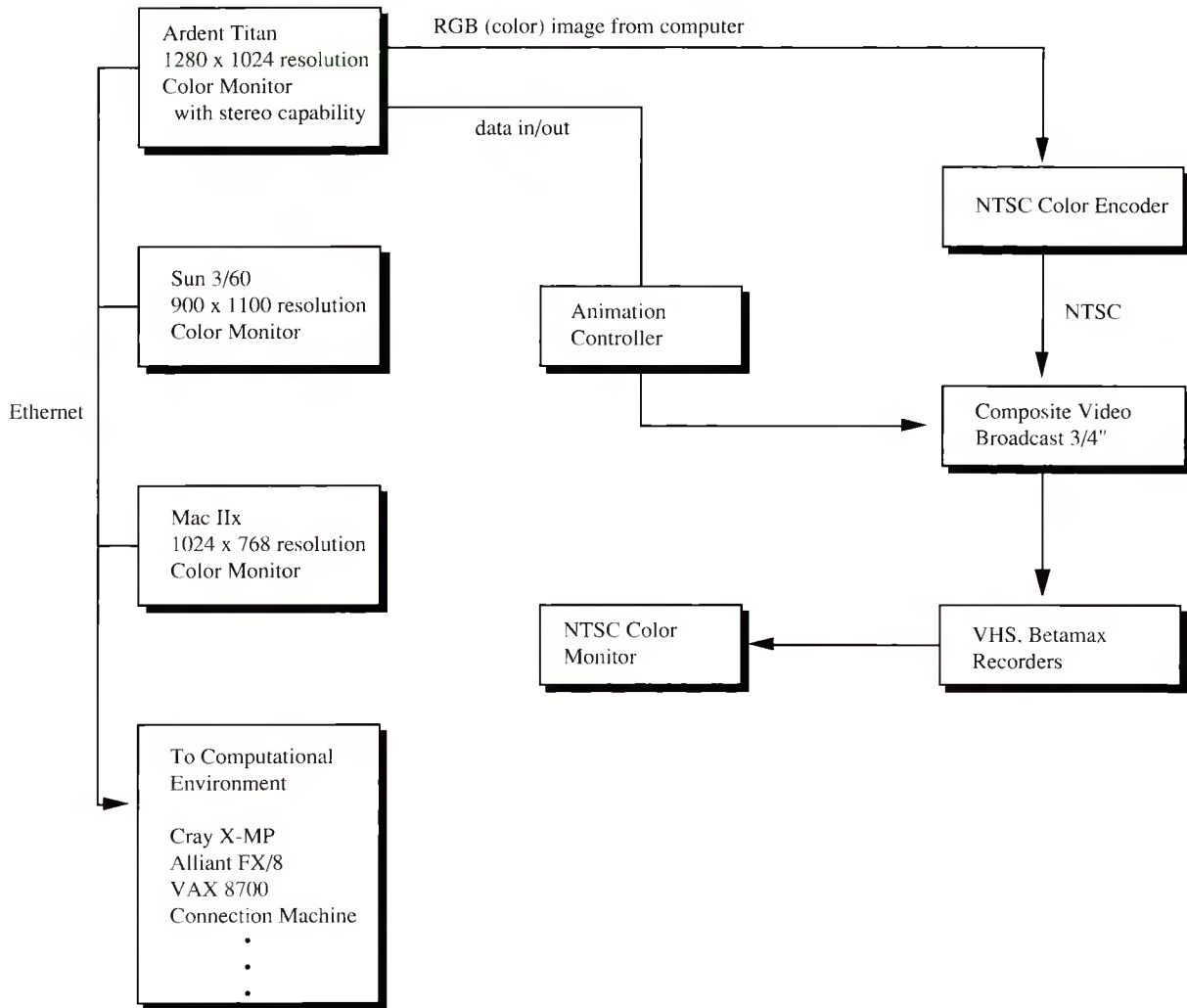


Figure 8: Current Scientific Visualization Equipment Configuration

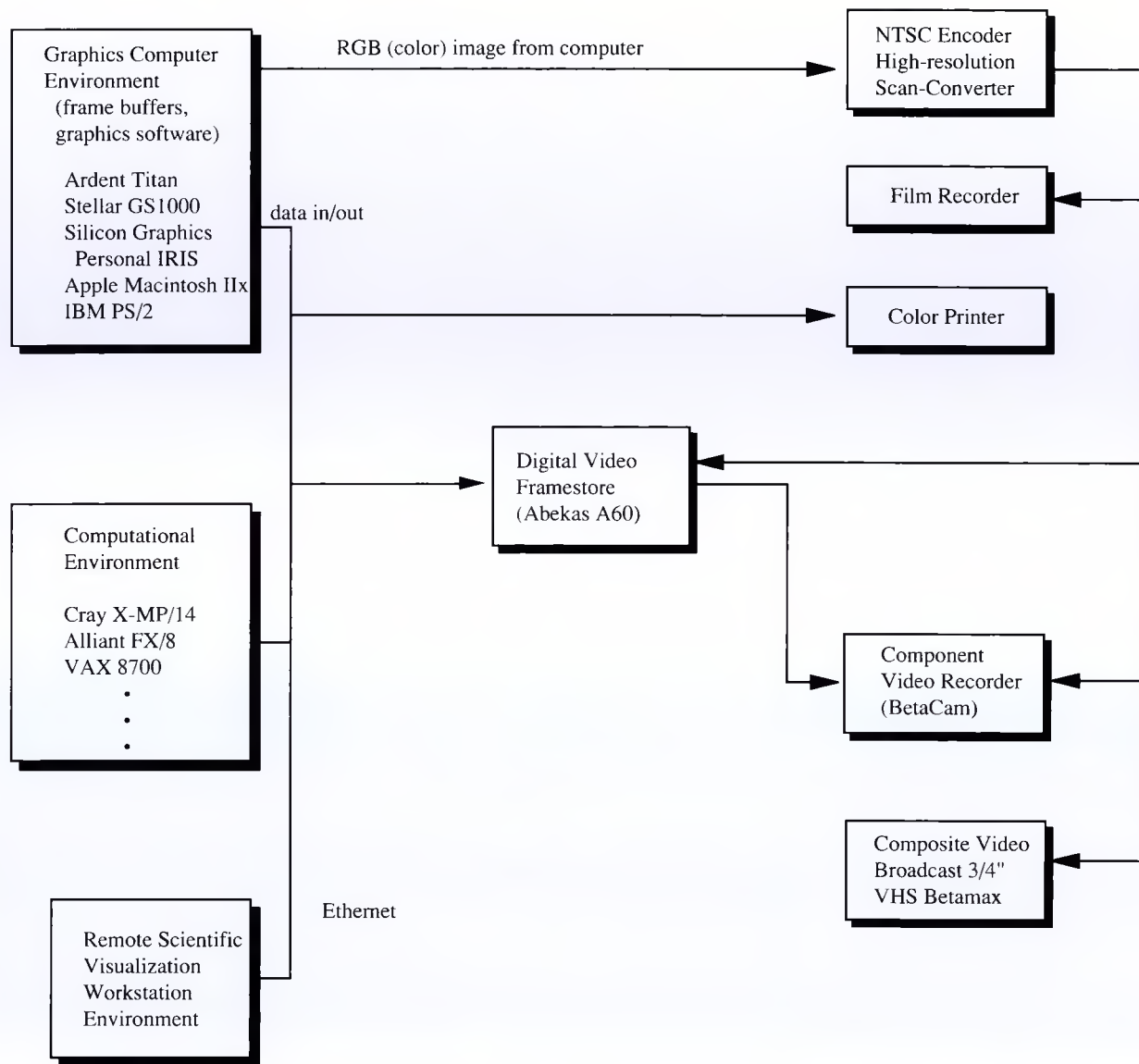
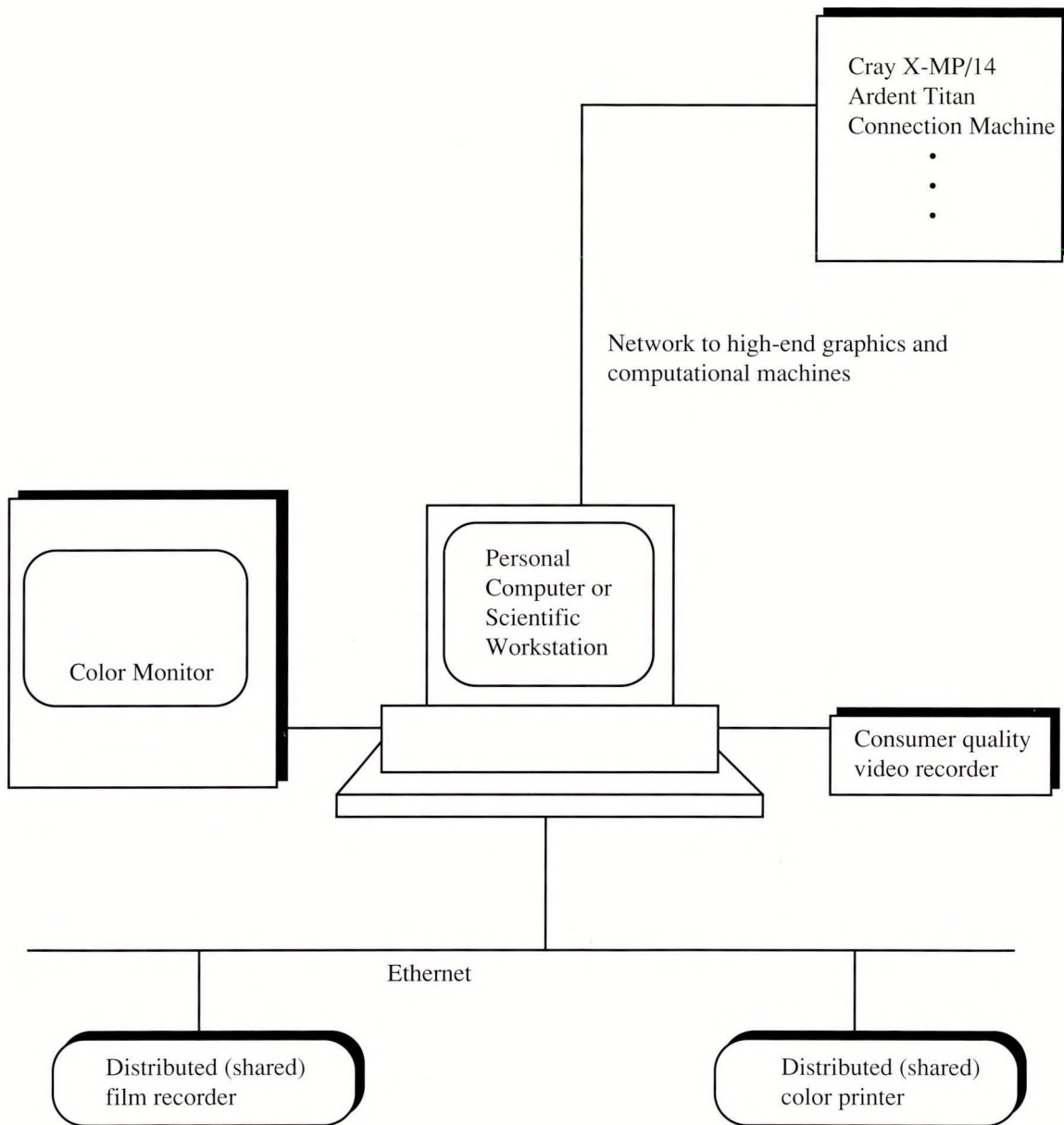


Figure 9: Proposed Scientific Visualization Equipment Configuration



**Figure 10: Remote Scientific Visualization Equipment Configuration**