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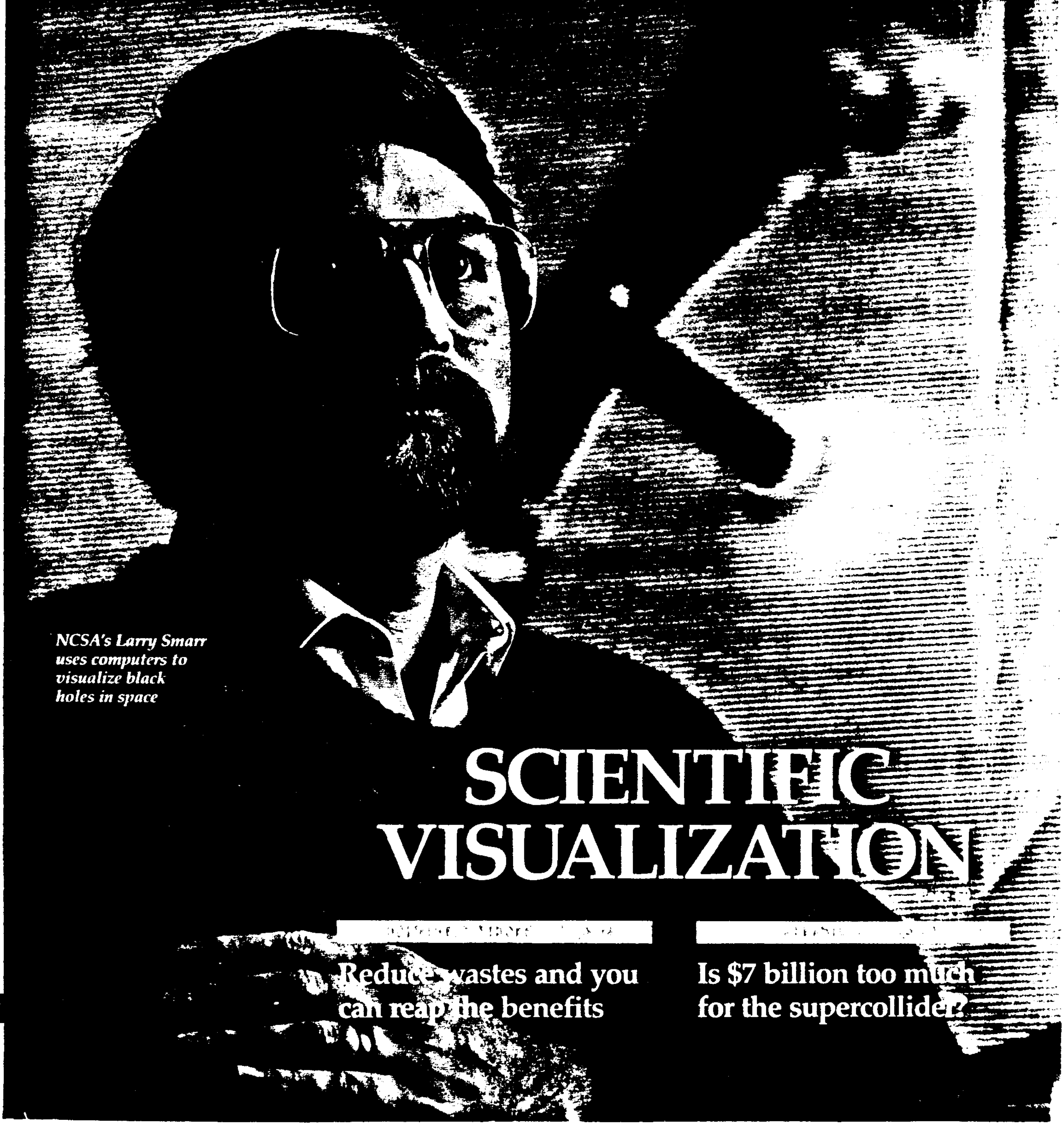
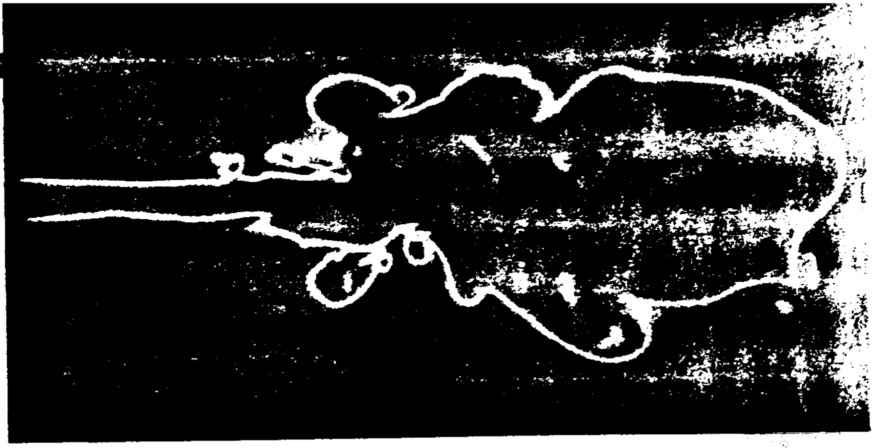


NCSA's Larry Smarr uses computers to visualize black holes in space

SCIENTIFIC VISUALIZATION

Reduce wastes and you can reap the benefits

Is $7 billion too much for the supercollider?

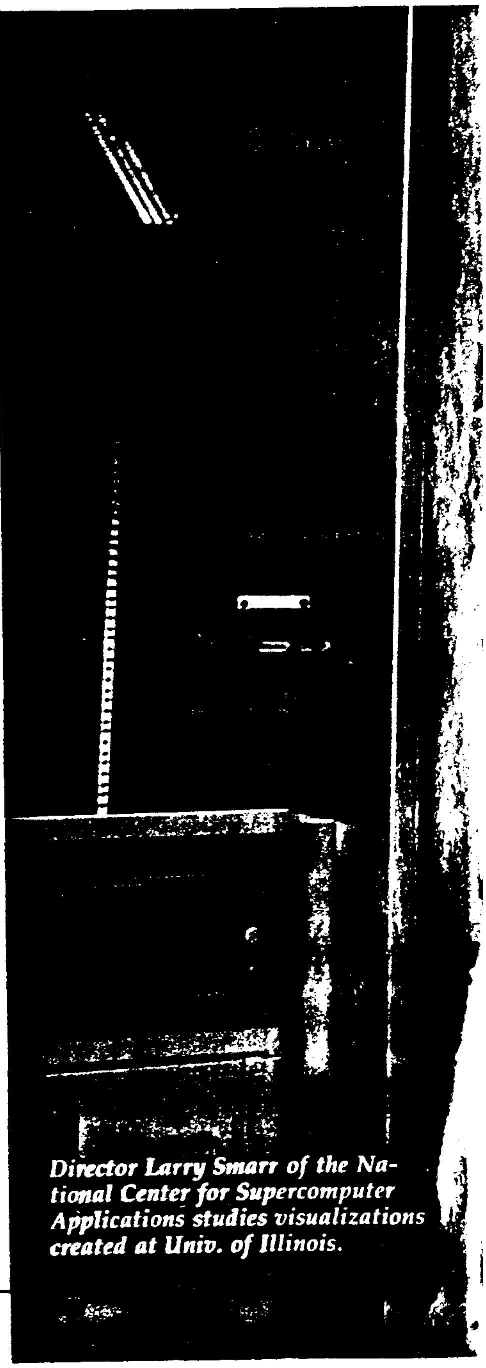


SCIENTIFIC

A New Computer Research Tool

Computer-generated images shed new light on complex scientific phenomena.

By Robert Cassidy, Editor-in-Chief, R&D Magazine



Director Larry Smarr of the National Center for Supercomputer Applications studies visualizations created at Univ. of Illinois.

LARRY SMARR SWEARS this story is true: "When I was starting college in 1966, my father told me, 'Do whatever you want, but look into these computers. I think they're going to amount to something.'"

The young math and science whiz from Columbia, MO, took his father's words to heart. Today, the 42-year-old astrophysicist is director of one of the most advanced computer facilities in the world, the National Center for Supercomputer Applications (NCSA) at Univ. of Illinois, Urbana-Champaign.

Since its founding in 1985, NCSA, along with its sister facility, the Electronic Visualization Lab (EVL) at Univ. of Illinois, Chicago, has become a hotbed of scientific visualization, one of the most important technical advances in R&D of the past decade.

In simple terms, scientific visualization permits researchers to plot complex masses of raw data in several dimensions over time and to compare the images produced to theoretical models or simulations.

By comparing field data to theoretical formulations, researchers might

Instability in a supersonic gas jet. Early version (left) appears flat and undelineated. Later version shows greater detail and contour. Research by Michael Norman, Phillip Hardee, and David Clark; visualization: Donna Cox.

VISUALIZATION

Smarr wants to put the power of a supercomputer on the desk of every researcher in the world.

gain insights that confirm or refine their hypotheses—or they might discover anomalies that lead them in new directions.

Thus, through scientific visualization:

- Seismic researchers Gregory Lyzenga of Jet Propulsion Lab, Pasadena, CA, and Arthur Raefsky of Stanford (CA) Univ. can simulate the migration of stresses through Earth's crust after an earthquake.
- Computational chemist Harrell Sellers, an NCSA research fellow, can simulate the bond-cleaving activity of niobium metal clusters on the Apple workstation in his office.
- Univ. of Rhode Island, Kingston, zoologist Frank Heppner can visualize flocks of birds to determine if birds indeed follow a leader. (He believes their actions might be more chaotic than previously thought.)
- Using NCSA visualization techniques, scientists at the National Center for Atmospheric Research, Boulder, CO, have created a computer simulation video of global warming.
- Astrophysicists like Smarr and NCSA research fellow Michael Norman can visualize black holes in space.

But there is more to scientific visualization than pretty videos.

Another group of researchers is using massive computer power to "get inside" artificial worlds. At Carnegie Mellon Univ., Pittsburgh, Robert Thibadeau and Ping-Kang Hsiung have created a video that simulates what it's like to "pass through" a rectilinear lattice—at 99% the speed of light!

In Cambridge, MA, imaging researcher Alex Pentland has created a simulation to "teach" the basics of object recognition—edges, contours, shape, and shading—to computers.

Scientific visualization at this level is possible only because of the power of today's computers, says Thomas DeFanti, EVL's co-director. Pointing to a video of a fractal created by electrical engineer John Hart, DeFanti marvels, "Every frame of that film contains a teraflop of data—a million million bits."

Since 1985, some 20,000 researchers from 180 universities have tapped into the supercomputing facilities at NCSA and four other national supercomputing centers in Pittsburgh, San Diego, Ithaca, NY, and Princeton, NJ.

But that's not good enough for Smarr. He wants to give every researcher in the country who needs it access to supercomputing power. In particular, he wants researchers to benefit from the latest scientific visualization capabilities.

He sees the computer as the most important weapon in the armamentarium of today's scientist. "If you look at a mass spectrometer or a DNA probe or a scanning tunneling microscope, they're all absolutely wonderful technologies, but they are many orders of magnitude *less* useful than

Kodak's Lawrence Ray (above) with "glyphs" (left) used to simulate an injection molding process.

Visualization produces patents for Kodak

EASTMAN KODAK senior research scientist Lawrence Ray, 41, has no doubt that his company's $3 million investment in the Univ. of Illinois supercomputing center has paid off.

In two years, the Kodak team has developed two new processes that will add millions of dollars a year to the company's bottom line.

The first breakthrough was in injection molding. "Kodak produces a lot of plastic parts—camera molds, film spools, and so on," says Ray. "We were using a well-accepted injection-molding model based on research at Cornell Univ., but we were trying to simulate this on paper, the way you did in third grade."

Ray's colleague, Richard Ellson, asked NCSA's Donna Cox to help him visualize how plastic flows in an injection-molding system. Cox came up with glyph images, which animate the temperature, flow direction, magnitude, and pressure of plastic being injected into a mold. The visualization led to the new process.

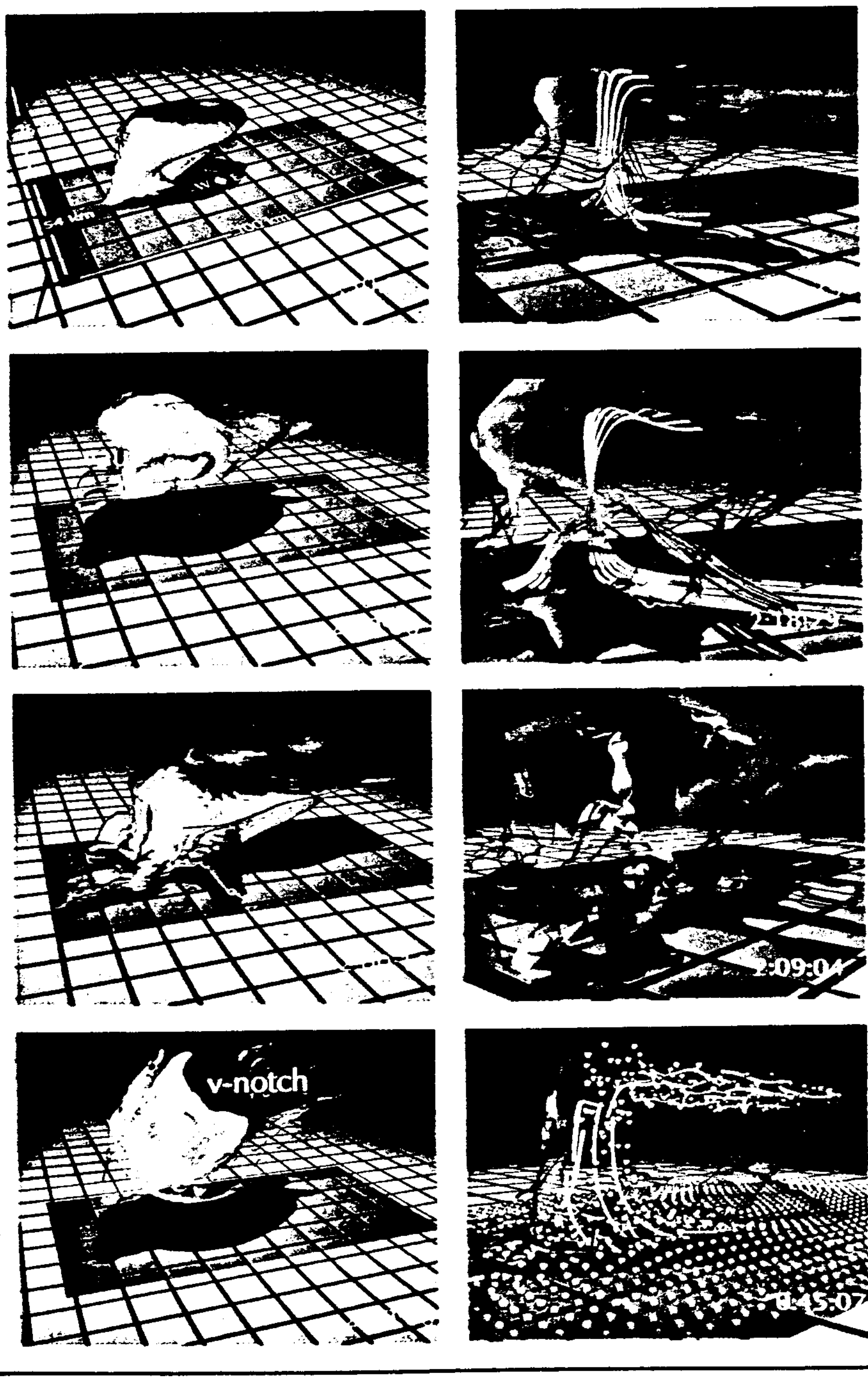
Another advance came in electronic imaging, which resulted in a new process for producing halftones with laser printers. "What would have taken nine months on a VAX 8550, we did in 34 hours on the Cray," says Ray. "We had a patent application filed before we would have finished the run on the VAX."

Storm windows

ATMOSPHERIC research scientist Robert Wilhelmson with still frames from his NCSA visualization of a numerically modeled severe storm.

The arrows represent wind vectors. The floating balls simulate moisture.

Next task: including surface boundary layer physics in the computer model to simulate a tornado.



the computer," he says.

Researchers in the field don't consider Smarr's dream a fantasy. "The notion that you'll have a computer laboratory on your desk or in the next room is not that far off," says senior research scientist Lawrence Ray of Eastman Kodak, one of NCSA's seven industrial partners. (The others: Amoco Corp., Caterpillar, Dow Chemical, Eli Lilly, FMC Corp., and Motorola.) "The concept is in its infancy, but I'm very bullish on high-performance computing," says Ray.

How fast is scientific visualization advancing? "When we first came to NCSA in 1988, a frame would take us six minutes to draw," says Ray, who holds a PhD in mathematics from Univ. of Rochester. "Now we can draw that same frame in three-quarters of a second—same information, same everything. We used to save every frame we drew. Now we dump them. It takes longer to retrieve them from disk than to redraw them.

"We can take a simulation that runs on our Cray X-MP, download it to my Sun [workstation] with an AT&T Pixel Machine, and have the capability of near-real-time animation under full user control," says Ray, who learned computers doing antisubmarine warfare research for the U.S. Navy. "You've got to play a lot of games to make this system work, but the performance is there, and it will only improve. The idea is to be able to run your model and see your results instantly."

Everyone in the field agrees that Smarr gets much of the credit for creating a national supercomputer program. After earning his PhD from Univ. of Texas, Austin, in 1975, Smarr took a summer job at Lawrence Livermore (CA) National Lab, while holding another position at Harvard Univ., Cambridge, MA. He needed to get access to Livermore's supercomputer.

"At Livermore, I would see complex visualizations of the hydrogen bomb going off, but I couldn't talk about them at Harvard because they were classified," he recalls.

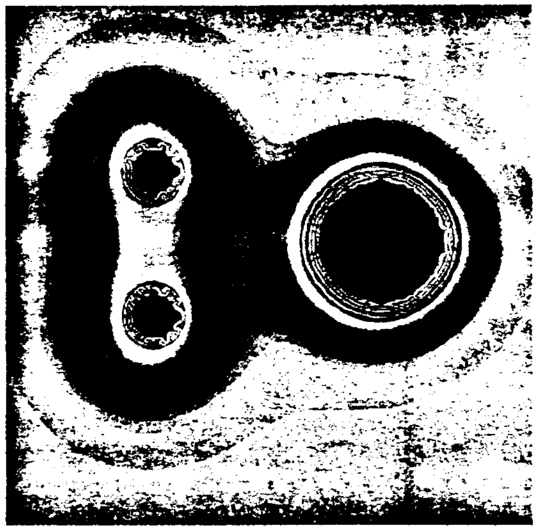
In 1980, Karl-Heinz Winkler (now NCSA's deputy director) invited Smarr to the Max Planck Institute in Munich, where he met Michael Norman (now an NCSA research fellow) and other international research "stars." "It was crazy," says Smarr. "Why were all these guys in Munich?

'Why were all these researchers in Munich?' Smarr wondered. 'Because of the supercomputer.'

Because of the supercomputer!"

During the next three years, while an associate professor at Univ. of Illinois, Smarr documented what he called "the supercomputer famine in America." In 1983, he asked the National Science Foundation to set up supercomputing centers around the country. Amazingly, within six months, NSF not only approved the program, but Congress allocated $43 million in start-up funds—twice what was requested. The first such center, NCSA, was opened in 1985.

To get an idea of how Smarr's vision is becoming a reality for scientists, let's take a look at how several NCSA researchers are using computerized visualization to enhance their research capability.



Computational chemist Harrell Sellers viewing a simulated Pd(111) molecule: "I think of the computer as a damn nice microscope that lets you see what the atoms are doing. It gives you insights you can't get any other way."

Tornado man

When he came to Urbana-Champaign in 1967 with a BS in mathematics from Wheaton (IL) College, Robert Wilhelmson, 45, had no idea he would make a career out of studying thunderstorms. "I just wanted to do an applications problem that would run on a big computer," he recalls.

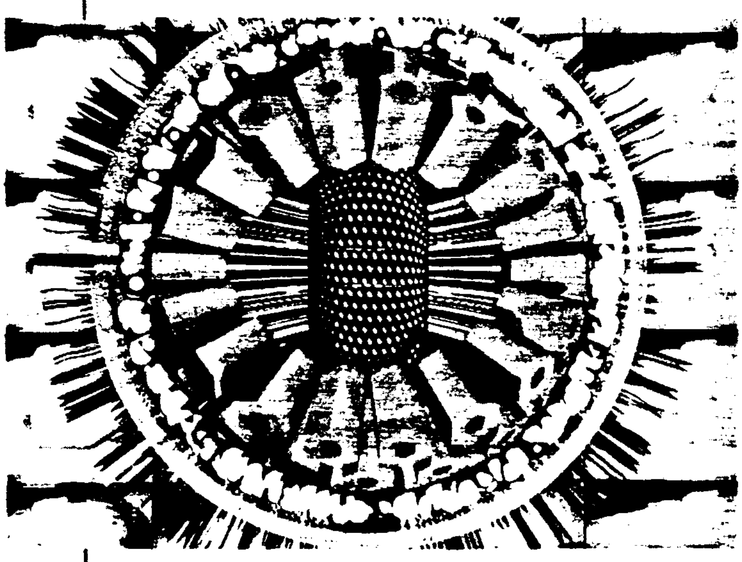
"Big" in those days was the ILLIAC IV parallel computer being constructed on the campus. The problem happened to be in atmospheric sciences. "I had no inherent interest in storms, but I could appreciate the mathematics," says Wilhelmson.

"For my PhD thesis [in computer science], I wrote one of the first models that solved the problem of storms in three dimensions," says Wilhelmson, now a professor of metereology at Illinois. Before that time, computers did not have the power to integrate partial differential equations, so researchers were stuck at the 2-D level.

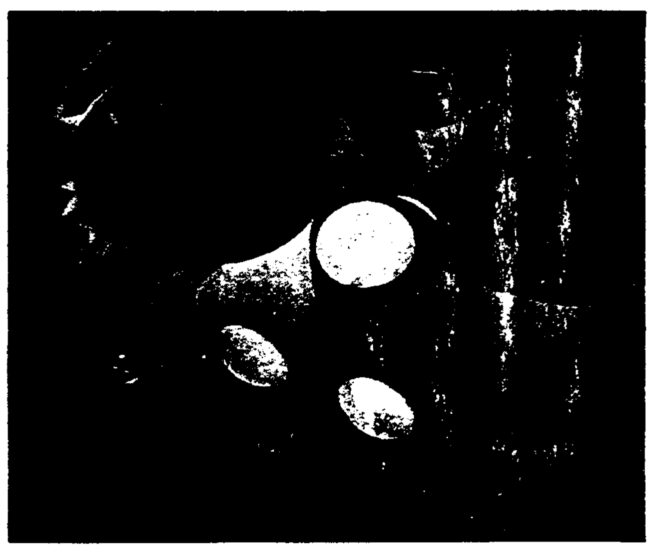
In the 1970s, Wilhelmson and Joseph Klemp of the National Center for Atmospheric Research, Boulder, CO, enhanced the model (using a CDC 7600) to simulate the behavior of storms that produce high winds and tornadoes. But at a horizontal scale of 2 km, "we were able to get only the general behavior, not the details within the storm," Wilhelmson says.

A breakthrough came in 1980. Wilhelmson, Klemp, and Peter Ray (now of Florida State Univ., Gainesville) performed a simulation that directly compared the model to observed data from a real tornado. "We were able to get actual measurements in three axes, both real data and model data, at 1-km horizontal resolution," he says.

Moving to a Cray 1 in 1980, Wilhelmson worked with Kelvin Drogemeier of Univ. of Oklahoma, Norman, comparing numerical simulations on storm outflows ("the cold air you feel



Herpes simplex virus, by artist Ellen Sandor, (Art)ⁿ Lab, Chicago. The computer-generated image, called a "phscologram," is three-dimensional in the original.



Glyphosate molecule (Roundup herbicide) model by T.J. O'Donnell, using his Gramps program on a Stardent Titan workstation. Yellow shows area of tight H_2O binding.

when a storm comes through, caused by the air rushing toward the ground") to lab data on density currents, to get down to more detailed features.

They also looked at lines of storms and the interaction between storms at a coarser resolution. Due to the limits of their computational power, however, the researchers could not combine the detailed and coarse data into one model. They had to go back and forth between the data sets.

The early 1980s brought Wilhelmson's first crude attempt at visualizing his research. He produced a film in which the cloud was represented by a wire frame. For a scientific meeting in 1981, Peter Ray built a crude 3-D model of a single storm, gluing paper arrows representing the outflow vectors to a huge sheet of cardboard. "You could walk around it, but it was static, one instant in the life of a storm," Wilhelmson recalls.

In the mid-1980s, Wilhelmson and Drogemeier created a video that employed new techniques for visualizing fluid flow and compared the model to laboratory results. But it was not until 1987, with the help of NCSA visualization expert Donna Cox, that Wilhelmson was able to render a cloud and watch it evolve over time. Since then, his video has become a classic of the genre.

The simulated storm is made up of 300,000 cubes, each described by nine

'Building' organs on the computer

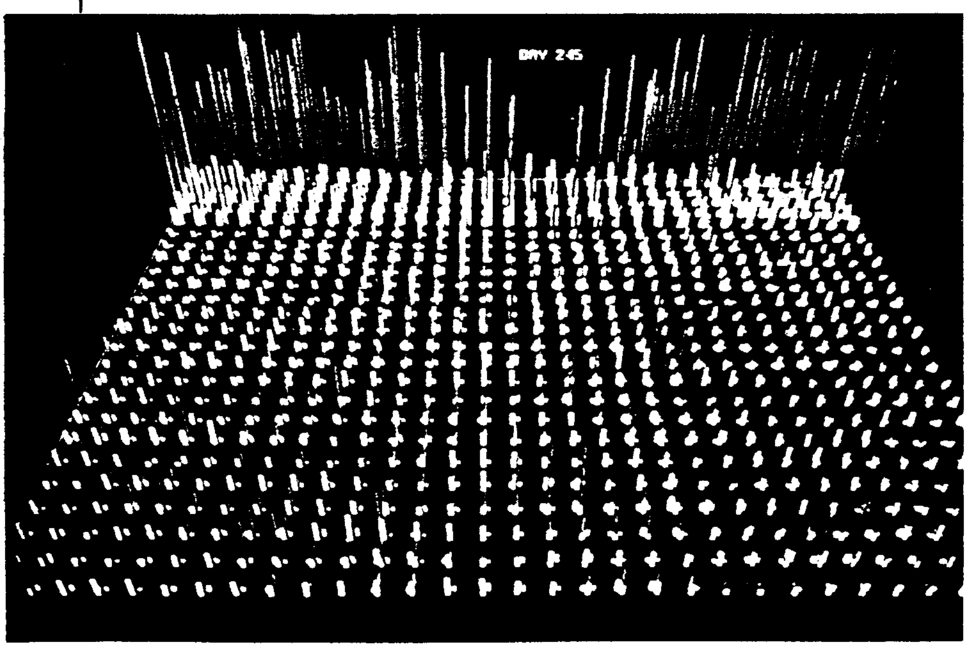
CANCER RESEARCHER Philip Iannaccone is intrigued by this question: Rather than deducing after the fact how cells propagate into organs, could we use computer visualizations to determine *prospectively* how organs develop from a few cells? If so, what might we learn about the formation of cancerous cells?

Iannaccone, 42, a pathologist at Northwestern Univ. Cancer Center, Chicago, has been studying mosaic patterns in the organs of genetically raised chimeric rats since 1980. "The mosaic patterns are generated by patterns of cell division, and we wanted to know the dynamics that give rise to these patterns," he says.

With Leland Berkwits of DuPont, he performed computer simulations using colored balls to represent cells, to see how they would form into patterns under various rules. Comparing these images to slides of chimeric rats' livers, the team discovered "very complicated, highly variegated patterns" similar to those in the rat liver slides.

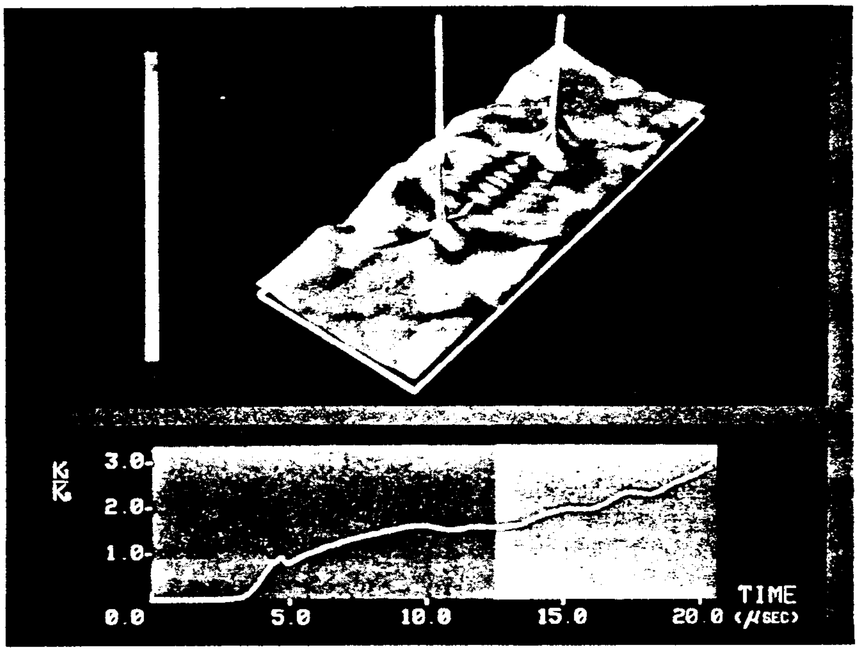
Iannaccone says visualization has helped them see that the relative *proportion* of various cells is crucial to the development of mosaic patterns in organs, while cell *movement* is not so important. They also found that the patterns are fractals.

"The point of the research is that very simple but highly iterative rules can lead to very complex patterns," says Iannaccone. "This suggests that organ development itself may be patterned by very simple but highly iterative rules."



Entymologist David Onstad (above) works with a simulated distribution of healthy (green, at left) and diseased (red) European corn borers. Blue indicates healthy larvae in diapause, or hybernation; yellow, diseased larvae in diapause. Says Onstad: "I didn't want only the astrophysicists to be using the supercomputers."

'Every frame of that video has a teraflop of data, a million million bits,' says EVL's Tom DeFanti.



***Robert Haber's simulation** of wave patterns in a brittle material being cracked at a speed of 1 km/sec. Color indicates strain energy density; dark blue is lowest. Vertical position represents the square root of kinetic energy density. Bottom graph shows stress intensity factor at the crack tip vs. time.*

equations, written in finite difference form, representing the behavior of water and ice in the atmosphere and the physics of compressible gas flow.

Add 3-D space and time (the equations are calculated for every six seconds in the storm's life) and you have an enormous number-crunching problem. "In essence, you're trying to view things in 13 dimensions, from a purely mathematical view," Wilhelmson says. NCSA's $12 million Cray X-MP/48 takes five hours to crank out a complete thunderstorm simulation.

Despite their success with storm visualization, Wilhelmson and his colleagues have been confounded in their attempts to simulate a tornado. "We've redesigned the model to get very high resolution in the surface boundary layer [the area near the ground where vigorous updrafts occur in the tornado's rotation]," he says. "It's important to capture the data near the surface, at very high resolution—50 to 75 m—and in a way that accurately depicts the physics," he says.

The NCSA researchers recently revised the model to allow for "nesting"—in effect, putting finer and finer resolutions of the model "inside" itself, while maintaining the interactions among the more coarsely resolved models.

Wilhelmson feels confident that they will solve the surface boundary layer problem and produce a scientifically valid visualization of a tornado before year's end.

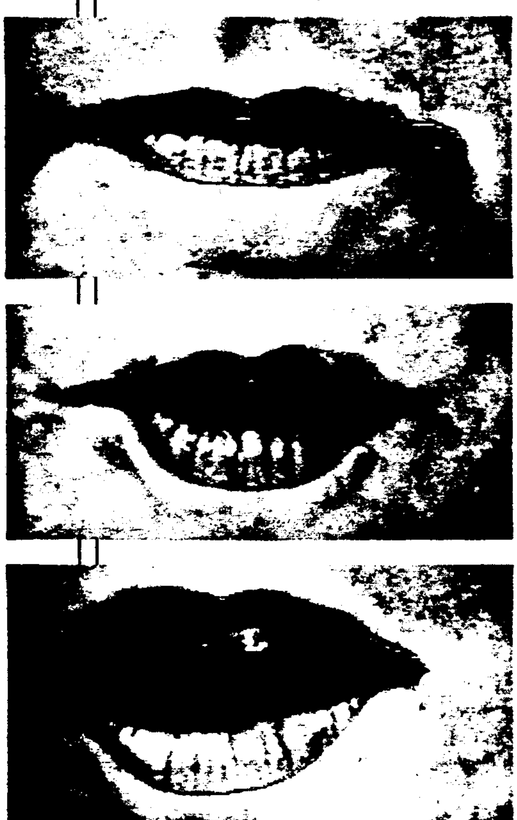
Forecasters then will be able to match the data on their screens with this model and identify those storms that are potentially damaging and kill almost 100 people a year, he says.

Studying insect epidemics

While insect population growth might not seem to lend itself to computer simulation, visualization has become an ideal research tool for entymologist David Onstad.

For the past five years, Onstad, 33, has been studying the European corn borer, a familiar pest that damages corn by burrowing into the stalk. "The problem has been around for 70 years, so we have plenty of data," says Onstad, whose PhD is from Cornell Univ., Ithaca, NY.

Arriving in Urbana-Champaign in 1985, Onstad began developing a



'Snakes' and computers

THESE LIP PATTERNS are outlined in "snakes." Snakes are active contour models that lock onto nearby image edges and track their motion, says a researcher who uses them.

"We want to make computers 'see' or 'feel' the contour of an image, the same way computers can see or feel text," says Andrew Witkin, 38, associate professor of computer science and robotics at Carnegie Mellon Univ., Pittsburgh.

"The idea of snakes is to lock onto and track over time the shape and motion of edges and other linelike features, which are important because they capture a lot of the information in a picture," says Witkin.

His research has been conducted with Michael Kass (now of Apple Computer) and Demetri Terzopoulos (now of Univ. of Toronto).

Ultimately, research into such "interactive modeling" could lead to improvements in computer-aided speech therapy and to computers having the ability to literally read your lips and perform your commands, says Witkin.

With visualization, says entymologist David Onstad, 'I can see how masses of insects interact.'

model to simulate the life cycle of the corn borer and its susceptibility to *Nosema pyrausta*, a single-cell microsporidium.

His model tracks seven factors: space in two dimensions, time, and four variables related to the corn borer and the microsporidium. Each computation in the video requires solving 160,000 equations in time steps of a tenth of a day over 25 years. With Cox's aid, he has produced a video that traces 50 generations of insects in an 800-plant cornfield.

"Even though the astrophysicists use more CPU hours than I do, per computation I'm using just as much," says Onstad. Each simulation requires 100 min of CPU time.

Onstad believes that being able to visualize the massive data in his project has helped him understand the real life-and-death process that goes on in Midwestern corn fields.

"We can see the dynamics of the overall changes in population, how quickly the epidemic progresses in the insect population, how it is spreading throughout the cornfield from insect to insect," he says. "It takes only two minutes to vary the temporal and spatial dynamics for a whole season, and I can flash hundreds of those before my eyes on the workstation and get an idea of how masses of insects interact, how diseased insects interact with healthy insects."

All cracked up

Visualization also is being used at the university's engineering department, where Robert Haber, Hyun Koh, and Hae-Sung Lee are studying how cracks grow at high speeds—15-millionths of a second—in brittle materials, such as GaAs.

Ten years ago, Haber, now 37, was completing his civil engineering PhD at Cornell. "I did some crude work on a VAX, figuring out the shape of fabric structures, such as you see in the roof of the Pontiac [MI] Silverdome," he recalls.

In the course of that study Haber came across another problem: Could you determine if the fabric would rip if you stretched it over a cable?

To solve the problem, he created the "floating grid." It works this way: to solve problems of *solid* mechanics, engineers often use a Lagrangian frame; here, the grid over which the required laws of physics are expressed is "fixed" to the material being studied. To solve problems of *fluid* mechanics, engineers use an Eulerian frame; here, the grid is fixed in space and the material flows across it.

Haber combined the two approaches, anchoring the grid around the material being investigated but moving the grid at the point of fracture, where the particles are most dynamic, so that the grid follows the crack tip.

For the past five years, Haber and his colleagues have been trying to visualize how crack propagation works. Originally, each simulation took five days of CPU time. "The second iteration started to show us three important areas—the stress intensity factor, strain energy density, and kinetic energy density—which we would never have understood without the visualization," says Haber.

Since last summer, the researchers have been running the simulation in real time by mounting it on an Alliant minisupercomputer, using vectorization and multiprocessing.

With Cox's help, they also have developed a visual device called "tensor glyphs"—pie-shaped 3-D images, which represent the 3-D state of stress.

The research on brittle fractures could have applications in aircraft, aerospace, civil and naval engineering, metal pipelines, and electronics, notably GaAs applications. "You want to control the cracking when you break the wafers into chips," says Haber.

Yet another promising area of research involves visualizations of "creep" in ductile materials, such as plastic pipe. "We've been working on that for two or three years, and it's tougher than we thought it would be," says Haber. But any success could have enormous impact in, for example, the gas pipeline industry.

Visual enchantment

Those with experience in scientific visualization warn that it can be seductive.

"The danger is that the graphics can be very enticing," says Kodak's Larry Ray. "You want the visualization to support your research. Don't get trapped into thinking you're [filmmaker] George Lucas. It can be a very powerful tool, but it can also be a major time sink."

Entymologist David Onstad concurs: "You're always going to have more data than you can visualize, so

Visualizing artificial worlds

SCIENTIFIC VISUALIZATION is taking some researchers right out of this world—and into new realms of "virtual reality" or "CyberSpace."

At NASA Ames Research Center, Moffett Field, CA, a team headed by research scientist Scott Fisher has created the Virtual Environment Interactive Workstation (VIEW).

Outfitted with stereoscopic goggles and sensor-fitted gloves, researchers can use the VIEW system to interact with objects inside simulated environments, such as a model of the space station.

The technology could permit NASA engineers on Earth to manipulate robots in space, perhaps allowing them to build an orbiting space station without leaving the ground.

Already, NASA engineers have used the technology to "step inside" a simulation of the vortex stream produced by the high-pressure fuel flow within the space shuttle's engine.

Some researchers don't seem interested in how computers interact with people, says MIT's Alex Pentland.

you have to make decisions about which data sets to visualize."

Still others see the "fancy image" school of visualization as missing the point.

"Computer scientists have been interested in building bigger, faster machines but not in how the machines interact with people," says Alex Pentland of MIT's Media Lab. "A computer can't recognize a bolt or how to put a bolt in a hole. We're not even talking about artificial intelligence but about the ability of the computer to operate at the level of your dog: 'Here's a slipper, fetch it,' " says Pentland.

Kodak's Larry Ray echoes the view of a number of researchers who say they would trade some quality in the images for speed and power. He also believes that more research in computer visualization is needed.

"We can now take a system and go from a simulation down to the visualization, but we haven't completed the loop," he says. "We haven't got it where we have the simulation and are able to change the parameters and iterate the initial geometry yet."

Ray sees hardware improvements affecting how researchers work. "We have to disconnect this process from the Cray," he says. "We now have devices close to the computational speed of a Cray, and more cost-effective. When you get 20 Mflops on a chip, you'll blow most anything away. When you can get that power down to the individual level, your productivity will be expanded immeasurably."

Software improvements, such as those being developed in NCSA's RIVERS program (Research on Interactive Visualization Environments), also are crucial. "We don't want to be working in batch modes," says NCSA's Bob Haber. "That's not the way scientists work. We're up at three in the morning, sort of on fishing trips, and we often don't know in advance what color mappings will work, or the perspective, or whatever.

"We want a hands-on approach to visualization, because we understand the science," Haber says. "We don't want to have to hand it over to someone else to visualize the data."

NCSA's Larry Smarr says that's already beginning to happen. "In the past year, we've had 2,000 users in 180 universities log on to the mainframe, but there may be 50,000 or more who are using the CDROM software," a visualization package developed by Apple Computer (in cooperation with NCSA) for use on the Macintosh II workstation.

These packages are fairly easy to work with, says Smarr. "My son, who's in third grade, is using these images to go through all the sciences," he says. "When we have tenured professors to the house for dinner, he takes them down to the basement and shows them how to do visualization."

Thus, by serving as "information intermediaries," NCSA and the other supercomputing centers could indeed bring the power of scientific visualization to every researcher's lab.

Maybe your lab will be next. **R&D**

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Reference Materials

"Glossary of Microcomputer-based Vision/Imaging Terms."
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"Glossary of Technical Terms."
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"Listing & Reference Manual" (directory of software and hardware used in imaging technology).
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"Visualization in Scientific Computing" (report) and "SIGGRAPH Video Review" (videotape).
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Scientific Virtual World Users Group

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(Developing a Usenet data base of virtual-world research.)

Scientific Events

Siggraph '90
(August 6-10, Dallas)
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1990 Super! Conference
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