



Success Story

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Associate Director
DBI

SGI® Visualization Technology Accelerates Research at the University of Delaware

In the new Visualization Studio of the Delaware Biotechnology Institute (DBI) at the University of Delaware, a graduate class of eight students wearing stereo glasses is seated before a 100-square-foot screen in a black room. They are interacting with a room-sized display of a three-dimensional protein. As the professor manipulates the molecule, the students ask for changes in orientation, discuss the protein's structure, build on each other's observations, and point out bonding sites. With this 3D visualization, powered by an SGI® Onyx® 3200 supercomputer, they will achieve more in minutes than they could achieve in many hours of independent work at their individual workstations.

DBI: A New Interdisciplinary Research Facility

The 72,000-square-foot Delaware Biotechnology Institute (www.dbi.udel.edu), is part of a statewide partnership of government, academia, and industry to establish Delaware as a center of life sciences within the East Coast biotech corridor that stretches from Boston to North Carolina's Research Triangle Park. The state, the university, and DBI are two years into an ambitious, six-year \$120 million plan that will create a statewide network of people and facilities focusing on interdisciplinary research, education, and economic development.

Research and education at the multidisciplinary institute is focused on agriculture, human health, marine ecosystems, and biomaterials. Faculty, students, and professionals are skilled in molecular biology, genomics, proteomics, structural biology, and computational biology. The institute's facility and its 40 scientific laboratories are designed to accommodate 170 faculty and student researchers. Located in the Delaware Technology Park, adjacent to the university campus, DBI also serves as an incubator for start-up companies centered on life sciences.





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"The Delaware Biotechnology Institute, a research facility designed for scientists by scientists, serves as a reminder and a very real symbol of a partnership between the state of Delaware, higher education institutions, and the private sector," Dr. David P. Roselle, president of the University of Delaware, says. "This facility demonstrates, better than any words could do, the promise and the benefit that can come to us all when these three entities work together. We are especially pleased to be working with SGI, a company with an international reputation for its leading-edge technologies."

SGI: Adding the Power of Immersive Visualization

DBI's state-of-the-art instrumentation, featuring mass spectroscopy, custom microarrays, structural biology, sequencing, bioimaging, and bioinformatics, is grouped in core instrumentation centers run by highly qualified professionals. A major facility in the bioinformatics core center is the immersive, interactive, 3D environment in the institute's new Visualization Studio. SGI Professional Services managed this SGI® Reality Center™ installation project, which includes a 15x8-foot FakeSpace rear-

projection screen. A six-processor Onyx 3200 visualization supercomputer with two graphics pipes drives a pair of Mirage 2000 projectors to deliver an edge-blended image with a total resolution of approximately 2500x1024 pixels.

"The Visualization Studio will make our researchers more productive," says Dr. Karl V. Steiner, associate director of DBI. "Our brains are powerful interpretive engines, but we can help them greatly by presenting data visually. By using visualization tools, scientists will be able to discern critical information much more rapidly. That's why I believe that visualization needs to become a major part of life sciences research."

Protein Folding and Remote Collaborative Immersion

Prof. Yong Duan of the University's Department of Chemistry and Biochemistry uses visualization tools to study peptide-folding processes in amino acids. Duan's folding simulations, which depict events that take just a few nanoseconds in the real world, may require a computer run of five days or more on a single-processor

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Graduate Student,
DBI

computer. Duan pauses regularly during the simulation to capture the current status of the configuration of the folding peptide. He then combines these captured positions into a movie that will be displayed in the near future in immersive stereo on the SGI® Onyx® family system. Starting from a straight-chain conformation, Duan is simulating all-atom models in continuum solvent. Much of the rapid initiation of the folding process takes place within one nanosecond, while unfolding of intermediate states, which constitutes the rate-limiting step, takes about 10 nanoseconds, followed by the formation of helix-turn-helix and the completion of the folding. It is striking and highly informative to watch the 16-amino-acid straight-chain molecule fold, contort, and gradually assume a helix formation.

A few blocks away on campus, Dr. Guang Gao, professor of Electrical and Computer Engineering and director of DBI's Center for Bioinformatics, is developing remote collaboration techniques that will allow two immersive facilities to share visualizations simultaneously over high-speed communications lines. In Gao's SGI Reality Center facility, the output of a 2-CPU SGI Onyx family system is displayed on a 4-by-6-foot FakeSpace® screen. This smaller system, which has been in place for two years, actually helped jump-start DBI's 3D simulation programs. Gao is now using it for preliminary studies of technology that will enable a scientist and a surgeon, for example, to plan an operation jointly by interacting with the same medical images from separate immersive environments. SGI® OpenGL Vizserver™ software will play a key role in this development.

Visualization Accelerates Bioinformatics

The explosion of data generated by genomics research poses an enormous challenge for investigators, who must use computational biology techniques to search enormous databases. DBI, along with other biotech-based institutions and companies, has turned to predictive modeling and computer simulation to accelerate the process.

“Many investigators are using readily available tools like BLAST to solve comparative genomics questions,” Gao says. “Over the next decade or two we will be looking for other ways to predict how genes function. And that is where visualization can play a dramatic role.” To that end, Praveen Thiagarajan, a DBI graduate student in Electrical and Computer Engineering, used SGI® OpenGL Volumizer™ to write CAVEVOL, which enables scientists to display stereo models of microscopic cross-sections and other volumetric data in the Visualization Studio.

Under the advisement of Professor Gao, Thiagarajan also developed PATTVision, a new approach to the visual data mining of biosequence data. PATTVision gives researchers a visualization framework for discovering and comparing amino acid sequence patterns. “There are a good number of pattern alignment tools for comparing patterns in genomic data,” says Steiner. “Most of them use 2D methods or color to highlight what a certain gene may be coding for. What PATTVision does, I believe for the first time, is to take



genomic analysis to the third dimension and allow us to detect Meta-Patterns for sequence homology analysis.” Using SGI Reality Center visualization power to travel along a PATTVision output is like flying over a big-city skyline with low buildings and skyscrapers in coded colors. Meta-Patterns, a new concept, helps define and compare patterns within sequences, bringing out similarities and differences among members of protein-sequence families.

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Biological Images: 3D In Vivo

Although SGI Professional Services installed the Visualization Studio only in April 2002, it is already integrated into a number of unique initiatives. In the institute's Bioimaging Center, essentially a state-of-the-art microscopy lab, scientists are using the center's multiphoton confocal microscope to capture images from a vascular corrosion cast of the kidney glomerulus [a capillary cluster that forms part of the kidney's blood-filtering system]. The microscope uses one of its three lasers to produce 250-nanometer-thick optical slices to create a 3D image, which can represent up to several millimeters of tissue depth. This capability enables University of Delaware investigators to examine living tissue samples repeatedly over time in three dimensions. The images can be piped to the SGI Onyx 3200 system over DBI's internal Gigabit Ethernet network.

“These glomerulus images were among the first samples we sent to the Visualization Studio,” says Dr. Kirk Czymmek, director of the DBI Bioimaging Center. “The effect was powerful. We started by microscopically imaging a half-inch diameter rat kidney. In the studio we then displayed a six-foot stereo version of the image that we can interactively manipulate and explore in three dimensions. Research is already under way to extend this approach to in-vivo imaging of living cells and tissues in 3D and over time—an extremely powerful tool to better understand dynamic cellular processes.”

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The Future: Education and Haptic Interfaces

“When we configured the Visualization Studio,” says Steiner, “we decided not to make it a CAVE environment, which would involve at least three walls and effectively limit occupancy to three people, since they would throw shadows on the display walls and get in each other’s way. We wanted a facility that was both a research room and an education and training tool. We planned to seat 8 to 10 people comfortably. And we also wanted to be able to use the room for presentations, to share some of the exciting new research results with visitors to the institute.”

DBI is now working towards a program that will enable the institute to collaborate with hospitals on the use of its SGI visualization technology for training and education. DBI plans to develop and implement 3D visualization tools that display nondestructive imaging data from computer tomography, x-ray, ultrasound, and other sources for the training of interns. Initially, the focus may be on anatomy training. Other applications, such as the use of the immersive environment for the interactive planning of surgery, are bound to follow.

Haptic feedback will be the next step in immersive visualization using SGI technology. A group in the University of Delaware’s Department of Electrical and Computer Engineering, led by Professor Ken Barner, already uses two robot arms that are linked to the smaller SGI visualization facility. These robots provide tactile feedback based on the interaction with virtual objects. They will stop further movement of your hand or the 3D mouse as if you had made contacts with a real object, not a virtual one. “We are interested in taking this work further, developing algorithms that will simulate contact with soft tissue,” says Barner. “It’s still early, but we’re already working with several investigators on this topic.” And SGI technology will play a critical part in it.



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