5 Speen Street • Framingham, MA 01701 USA • Phone 508.872.8200 • Fax 508.935.4015 www.idc.com

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SGI

Pushing the Boundaries of the Known with a Passion for Exploration and a Talent for Solutions

An IDC White Paper
Sponsored by SGI

Analysts: Christopher Willard, Ph.D., and Karen Goldfarb

Table of Contents

"When the doors of perception are cleansed, things will appear to man as they truly are, infinite." Aldous Huxley

Imagination, ingenuity, and passion are just some of the requirements of the scientific breakthroughs that alter the way we see our world. Galileo, Darwin, and Einstein all had the courage to question the accepted to bring about the unexpected insight that radically changed our concept of reality.

In its quest to fuel both the greatest scientific breakthroughs of the twentieth and twenty-first centuries, SGI has a 20-year track record of meeting the needs of the scientific community. Harnessing its technical ingenuity to the most brilliant minds, the SGI solution allows scientists to focus on the work ahead.

Scientific superstars, such as Stephen Hawking, who is on a quest to unlock the mysteries of the universe through his COSMOS project; Nobel Prize winner John Pople, who seeks a greater understanding of the behavior of molecules; or the Los Alamos National Laboratory scientists, who use advanced computational methods to simulate nuclear explosions, are among those finding answers in the SGI solution. Whether they are mapping the brain, probing the origins of the universe, or seeking a cure for cancer, researchers all over the world are using SGI's unique technical qualities — strong scalable platforms, NUMA architecture, and high-resolution graphics — to solve the core scientific issues of our time.

As a company, SGI's philosophy has always been to focus on clients' needs, creating technology to keep up with scientific innovations. SGI President Bob Bishop articulates the company's strategy this way: "The entire mission of our company is to provide all the underlying power for all the greatest scientific breakthroughs of the twenty-first century … We are a company that's willing to make the long-term commitments it takes to make these breakthroughs happen."

This white paper explores SGI's 20-year success rate in the sciences; the factors catalyzing researchers' choice to use SGI technology, and SGI's commitment to innovation and scientific discovery.

A SHORT HISTORY OF SGI

In the beginning was the chip…

Jim Clark, the founder of SGI, brought an insouciant irreverence to the task of creating computers. The Geometry Engine, his brainchild, was a computer chip that was able to process 3D images in real time, allowing scientists and engineers to model their designs on a computer screen, eliminating thousands of lines of code and saving researchers months, or even years, of work.

His vision took hold. In 1982, Clark, then an associate professor of computer science at Stanford, along with a bunch of bright, energetic students, formed Silicon Graphics.

It was the beginning of a wild ride, one that has had a visible impact on science, engineering, medicine — and even the way the world watches movies. In Hollywood, nearly every movie in the past 10 years that has either won or been nominated for an Academy Award for special effects has used SGI technology.

But along with George Lucas and Steven Spielberg, whose acclaimed films owe much of their thrills and chills to SGI, scientists were beginning to discover the possibilities of the 3D image.

"From the very beginning," says John Mashey, SGI's chief scientist from 1992 to 2000, "SGI's reason for existence was to do real-time 3D graphics. That was the thing. There was a thing called the Geometry Engine that had been built at Stanford, and SGI was built on successors to that."

Virtual World

What Clark and his team of inventors were trying to do, Mashey explains, was to make a real-time interactive model that actually looked like the real world. Up until 1980, that wasn't possible. "What you would see on the screen would not be something that looked real," says Mashey. "You would see a single color that would look like a wire frame — you'd see a line where the edge of something was. But you wouldn't see anything that looked remotely real. It was the best you could do with computers at the time."

That all changed when SGI came on the scene. "The dream Jim Clark and his graduate students had was by using silicon chips, you could accelerate the computation to show you the reality. It isn't just to show you something real, that's rigid — just sitting there. You could actually interact with it. You could see it in real time," Mashey says.

SGI entered the technical workstation market in 1985 and introduced its first RISC-based model in 1987. In 1992, it acquired MIPS Computer Systems and was able to successfully merge technology, ideas, and scientists.

During the mid- to late 1980s, Silicon Valley was a hotbed of technological innovation, driven by people who, while often working in separate companies, created a wealth of opportunities and ventures for each other. Mashey, at that time, was working at MIPS Computer Systems, where he was one of the early designers of its innovative microprocessor.

Soul of a New Machine

The MIPS chip is a member of a generic class called reduced instruction set computer (RISC) microprocessors. "This was a major trend during the 1980s," Mashey says. "What they did was essentially knock out of the general computer market all of the older chips except Intel. MIPS was one used by a number of companies, including SGI. And so, this was the important thing for SGI because it gave them a highly competitive microprocessor to use."

Competitors began offering similar technology, but SGI established itself as a distinct presence by honing its offerings to meet the needs of scientists and engineers, allowing them to pursue their research through 3D visualization and virtual reality technology — and to do so quickly.

"You can always make wonderful images if you have an infinite amount of time," Mashey observes. "The problem is doing it in real time. Probably the heart of what SGI has done over the years is to be able to do bigger problems in real time with humans interacting with it. That encapsulates what SGI has done. The strength of SGI has always been in the wonderful things it helped customers do. Where I got so much fun from my time there was working with customers, helping them solve problems. And they were hard problems whose answers mattered."

These customers might be big personalities working on big problems, ranging from cosmic questions on the nature of the universe to questions on the nature of the human being. They might involve questions of national defense, the testing of nuclear weapons, the search for alternate sources of fuel, or a search for a way to save lives, as pharmaceutical companies discovered more efficient ways to target genes for drug research and development.

The U.S. military was one of the first to take advantage of SGI's unique graphics visualization and simulation technology, signing on in 1987 to do graphics simulation of weapons trajectories. Shortly after that time, scientists conducting advanced research in many different fields discovered the technology as well.

A Unique Vision

The goal was always real-time visualization, but with that aim came the need for many technological tasks. More, bigger, faster has been the rallying cry of most scientists describing their need for computational power and storage space. In a series of steps, SGI began refining and improving its original ideas, bringing down costs while maximizing results.

"From the beginning, SGI had a unique vision in terms of the way its systems were constructed," says Dr. Eng Lim Goh, SGI's chief technology officer. "Every other computer vendor builds their computer systems in essentially three parts — the compute engine, the data engine, and the visualization engine.

"For 20 years, SGI's core competency has been to bind these three different pieces very tightly together," says Goh. "That has been our strength for 20 years, and we will continue to maintain this strength — the tight binding of the three computer pieces."

For example, Goh says, "if you take a case of CPUs sitting on a piece of memory — and then a mixed bunch of computer processors sitting on another bunch of memory — what we do is, we bind these two groups of CPUs very tightly together to the extent that the two separate pieces of memory are seen as one single piece by the applications.

"This is the reason why we are the only company that can build a shared memory system — all the way up to 512 processors — that is a monolithic, shared, single memory system. Nobody else in the industry can do this — especially in that size," he says. "The largest the competition builds is under 100 processors. So you can see we are five times bigger."

SGI's second major achievement is its heritage in computer graphics. "We have brought real-time 3D computer graphics forward in the past 20 years to the extent that they are a commodity today. There are quite a few people imitating us," Goh says. "However, we are differentiated by working on high-fidelity visualization. While the commodity world has copied us and built real-time 3D graphics systems for gaming, we have continued to focus on high-fidelity, high-end scientific visualization."

Paths to Understanding

Scientific visualization is the ability to display multiple dimensions on a screen in a form that is meaningful to a scientist or an engineer. By allowing researchers to display objects on a screen, or see them in three dimensions in a virtual reality room, new insights follow.

"We believe visualization can play a major role in the gaining of that insight for generated data," Goh says. "And the amount of data they will generate will grow. But for scientists trying to make sense out of this growing amount of output data from high performance computing, the highest bandwidth system from the outside world to their mind is the eyes," he says. "And that's why we believe visualization will play an increasingly important role as computing power grows."

Goh, who has been with SGI since 1989, says that while there have been many advances in computing power, some things have stayed steady. "One thing that has been the same is that we consistently churn out innovations," he observes. "This has been our strength. We continue to see that. Our key motivation is to increase the productivity of scientists, engineers, and creative professionals, by giving them better, higher performance and easier-to-use simulations and visualization tools."

Making them user friendly to scientists is important, he says, because "researchers don't want to focus on computer issues. Their focus is on the research. SGI focuses on creating tools that do the work."

BREAKTHROUGHS, LEAPS OF FAITH, AND COSMIC DISCOVERIES

One question that has animated visualization in its relationship to science is: What would happen if? Researchers have their own versions of this question, and their own ways of responding. Supercomputers and visualization have revolutionized scientists' capacity to analyze and understand mass volumes of data. Doing the work required to find an answer to these inquiries might have taken years — or might never have been undertaken before. But with virtual reality, visualization tools and high-end computational power, scientists can see now in ways never before possible.

As Arthur C. Clarke, the visionary author, wrote in 1962: "Any sufficiently advanced technology is indistinguishable from magic." Visualization has helped scientists achieve things they may have never imagined before and in fields as diverse as medicine, chemistry, cosmology, defense, oil and gas exploration — and even archaeology. Here then, are some results of SGI's commitment — and of this new perception.

MEDICINE

At the Montreal Neurological Institute, UCLA's Laboratory of Neuroimaging (LONI), as well as other medical centers around the world, neurologists are using advanced computational tools to create an atlas of the brain. Across oceans and continents, while preparing for a delicate, dangerous procedure, doctors perfect the surgical techniques they will use to separate twins. And everywhere, medical technicians are using MRI and CT imaging tools to diagnose illnesses.

The risks of invasive surgery, the delicate tasks of administering an anesthetic, the complex process of planning for an operation — all are aided by the revolutionary techniques that are fusing the highest levels of computer graphics and medicine to allow doctors to observe patients' bodies virtually. And by doing so — this new technology is revolutionizing healthcare in the twenty-first century.

Mapping the Brain: Scientists Chart a Brave New World

"The brain is the soul's fragile dwelling place." William Shakespeare

It used to be considered a wilderness, an unknown territory whose mysterious boundaries would remain forever undiscovered, but now high-end computational tools are helping scientists find a way to chart the human brain, as they visualize their way through this once mysterious place. By doing so, they are learning to see, in a new way, the manifestations of emotion, memory, and all the developmental leaps along the way.

And while, it seems, no two brains are alike, scientists are working to establish some fixed points: a grid with points of longitude and latitude, a series of parameters that will make up a kind of encyclopedia, an atlas of human development. This now, is a brave new world, infinite in possibilities, whose contours have yet to be fixed.

"It is very true that no two brains are alike," says Dr. Alan Evans, the Welsh-born researcher who heads the Montreal Neurological Institute's Brain Imaging Center (BIC). "But it's also true that most brains have some similarities. What we always try to do is find what is normal and what is the range of normal. And that's the only way you can characterize what is abnormal. It's all about making connections between blips."

Those blips show up when researchers using MRIs and other imaging tools take pictures of a subject's blood flow in the brain after performing certain tasks such as looking at images or remembering number sequences. Other tasks might involve an emotional recollection.

Worldwide Endeavor

Montreal Neurological Institute's BIC is at the center of a worldwide effort to codify this knowledge. With a grant from the National Institutes of Health, it is part of a larger study that spans continents, known as the Human Brain Project, to gather data on children's brain development.

SGI technology is a key component in this international effort to create this atlas of the brain. BIC researchers have been using its computational tools since 1984.

"Our whole world, these days, requires massive amounts of computation because we can collect so much data — but it's useless if we can't process it intelligently," says Evans.

"We have to develop lots of software algorithms for image processing, statistical analysis, and all of this has to happen fast — because we're collecting data off subjects all the time. So we never have enough computer power, and we never have enough storage space. We always want more because we're a research institute. So if we've got enough — then we're not researching," Evans says. "We've got to be pushing boundaries all the time."

The SGI Origin 3800 server, one of many high-level computational tools the BIC is using, "has allowed us not only to do things faster but also to conceive of things that we could never have conceived of before — you couldn't even think of it before all of this because it would have taken forever to run … it would have been always impossible," according to Evans.

Mapping the Universe; Mapping the Brain

In 1992, the BIC, along with the University of Texas and UCLA, created a consortium to explore these issues. The endeavor has expanded to become the International Consortium for Brain Mapping, and it involves researchers all over the world. Their dream of creating a computational brain atlas is very different from the mapping used in traditional brain research.

"Typical neuroanatomical atlases are usually made up of 100 pages of slices showing a single human brain that has been photographed many times from a variety of different angles from top to bottom, right to left, and front to back," Evans explains. "It's all very qualitative — you're just looking at pictures .... But the kind of atlas now envisioned is quite different and will have enormous consequences for neurological research.

"The idea here was we would collect hundreds of brain sets in adults, to begin with, to start building a computational atlas — a statistical atlas of brain anatomy," Evans says. "This whole new idea of mapping is very much like mapping the geography of the world. Everybody has to use a common coordinate system. But rather than saying latitude and longitude as we would on the surface of the world — you can talk about fixed points, such as x, y, and z — and everyone knows exactly what you are referring to. This new language produces a common quantitative framework."

Small Signals; Huge Results

"When you do these experiments," Evans says, "the signal you are picking up is so small that you can't see it in one subject, so the same experiment might be done in maybe 10 or 20 subjects — and then the scientist can average the results.

"Think of it like a shoebox, you take my brain and put it in a standard shoebox. We rotate it, translate it, and scale it so it fits into a standard shoebox," explains Evans. "But if we then did the experiment on you, we would take a 3D image of your brain, rotate it, scale it, translate it, and overlay it into the same space as mine. You do that 20 times, and at every 3D location, you have the change in blood flow in each of those 20 subjects — so you identify what is the average change — and that's where you begin to pick up very small signals because they appear always in the same place."

This shoebox idea is relatively simple, he says, but has large implications. Now people all over the world will be able to do the same experiment, and they will check exactly in x, y, and z coordinates, he says.

Evans admits that at first, traditional brain researchers were a bit resistant to the benefits of large-scale computing. "But in the last decade there's been quite a change — there's been a recognition that this is the way science is going," he says. "You can't divorce science now from huge computing solutions."

SGI and Brain Research: "A Natural Partnership"

Evans says SGI has been a formidable partner, right from the very beginning. "I think we chose SGI because when we really started getting intensive in our 3D analysis and computer processing during the late 1980s, SGI was the only company which we really felt understood 3D quantitative analysis. We first of all got 3D graphics workstations from SGI. As time has gone on — our needs for pure number crunching have gone up and up and up. And it was just a very happy coincidence for us that at the same time, SGI recognized the need to get into high-end computer servers — or what we used to call the supercomputer.

"So their [SGI's] move from 3D visualization to large-scale supercomputer systems paralleled our needs. SGI has been a natural partner for our scientific evolution," Evans says.

The Reality Monster and Brain Research

Like his colleague at the Montreal Neurological Institute, Dr. Arthur Toga of UCLA's Laboratory of Neuroimaging (LONI) is involved in this immense undertaking — creating a computerized Baedeker of the brain.

At LONI, he is conducting research and investigations into brain structure and function, using a variety of neuroimaging strategies, including magnetic resonance imaging, positron emission tomography, and optical intrinsic signals, to generate 3D images that will increase understanding of the human brain. A group of scientists, researchers, and doctors compile all this data using advanced computational tools provided by SGI. The tools perform all of the tough stuff — computational analysis, storage, and 3D visualization.

"When I began (researching) in the late 1970s, we couldn't do this at all," Toga says. "It was just completely impossible — you couldn't conceive of anything like this. So what's been fun is as the complexity of the questions we have been asking has increased, the capability of the technology has kept pace — or even leapfrogged ahead. In a notoriously competitive profession, it has created a new camaraderie.

"These projects require that you bring a number of subspecialties [computer science, mathematics, physics, anatomy, neurophysiology] together in an integrated, multidisciplinary way that you would never have thought of 15 years ago," he says. "You have to work together .... It's really been a kind of revolution."

Among his stable of Onyx2 processors and desk site systems is SGI's Reality Monster. The system is capable of analyzing the immense amounts of data that will be needed to create this new computerized atlas of the brain. Currently, according to Toga, the system supports 50TB of online storage.

Toga's team works with very large data sets. The challenge is manipulating large 3D displays in which each point in the display can have many bytes associated with it. These complex data sets make texture mapping and visualization difficult. "Most machines, even if you have fairly potent graphics cards … can not handle this," says Toga. "But the Reality machine provides us with a way to examine the data and interact with it as we try to devise and find new ways to measure and look at [brain maps]. I don't know of any other machine that is able to display that amount of data."

The goal of all this research, Toga says, is to try to understand normal brain development. By doing so, perhaps, he says, scientists will be able to pinpoint the abnormal. "If we could find a signature that describes the brain of a particular population — one could say then, for example, what does the brain of early onset Alzheimer's disease look like? This technology could help us do that before behavioral consequences of the disease [appear], and that would provide us with a decision-making tool as to whether to administer some drug treatment," explains Toga.

The populations studied by the LONI team include the aging as well as people with brain tumors, schizophrenia, fetal alcohol syndrome, and other neurological anomalies. Despite the variety of populations studied, the research premise remains the same: to develop a map of the brain.

Illuminating the Body: The Center for Human Simulation

Dr. Victor Spitzer, the director of the Center for Human Simulation at the University of Colorado, is a man with a mission: to illuminate the human body and, on a virtual level, to create a living entity.

Envisioning an era in which medical researchers would need to expand their resources with both print and digital images, the National Library of Medicine (NLM), in 1986, began exploring the idea of creating a biomedical images library. In 1991, the NLM chose the University of Colorado as the site to develop models of the human body. The goal was to create three-dimensional, anatomically detailed representations of the male and female bodies. The Visible Man, created in 1993, and the Visible Woman, created in 1994, are manifestations of that goal.

"The rationale and goals for the project are to provide data to researchers so they could build models of the human body. The reasons to do so range all the way from medicine to entertainment," says Spitzer. According to the NLM, the male data set contains 1,971 digital axial anatomical images obtained at 1.0mm intervals, which accounts for 15GB of data. The female data set contains 5,189 digital anatomical images obtained at 0.33mm intervals, accounting for 39GB of data.

Virtual Life

Spitzer is working to further extend digital imagery by developing methods to study these models as if they were alive. "It's about the "cyberfication" — the virtual "realityness" — of the human body," he says. "It's about maleness and femaleness. And it's about visualizing, graphically, the human body as it really is — not just visualizing the body as it is today but bringing this body back to life, in cyberspace."

"We have a frozen body that has been sectioned at every millimeter for the man and every third of a millimeter for the woman," Spitzer explains. "How do you bring it back to life? The first thing you do is make it move — make the arms move, make the legs move. Then you start to bring it back to physiological life. You do that by making the heart move — beat like it realistically should — making blood flow in the vessels; making the vessels move like they should because blood is flowing through them."

It's a project very much akin to brain mapping, Spitzer says. "Ultimately, this will be a computational resource that researchers can look at from all over the world and [into which they can] deposit information. It will be an area to publish things in. For example, if you want to find out about the gallbladder, you can just go to this visual interface. So, ultimately, it will be like a good computational book," he says.

"All this is a compute problem," says Spitzer. "And the compute problems grow as I start dreaming about making this man come to life. … Bringing him to life means bringing in all the expertise of the pulmonary people to make sure his lungs move correctly and the kidney people to make sure his urine flows properly. All that data needs to be brought together into one data set to make him do things synergistically." However, Spitzer notes, "there's not enough computer power out there yet to make his whole body move realistically — nor is there enough knowledge to make it move realistically."

The center uses two SGI machines: a 64-processor Onyx and an 8-processor Origin. "Originally we chose SGI for its graphics capabilities," Spitzer says. Now, the company relies on SGI for its speed. "It's a combination of things," he says. "It's a platform you can depend on for moving data around quickly. The SGI [machines] provide the ability to analyze data."

Medical Students Will Benefit

Eventually, Spitzer believes, a virtual representation of the body will be as good as, if not better than, the cadavers normally used for teaching medical and nursing students about anatomy. "Most healthcare workers don't get access to cadavers; now you will be able to provide a virtual one to teach the anatomy of the living person," he says.

Spitzer predicts that the Next-Generation Visible Human will have a higher-resolution, better body, with better means of illustration. It will also focus on specific areas of anatomy, such as the thorax, head, neck, and knee. The simulations, which will allow medical and nursing students to see and explore the effect of medical procedures in real time, are similar to those used with pilots for flight training.

Surprisingly, entertainment was cited as another reason for the creation of the Visible Human Project. "People love to see the inside of someone else's body," says Spitzer. "People are infatuated by their own bodies — it doesn't have to be in a grotesque kind of way." As film producers strive for more realistic effects, they need better models of the dynamics of the human body. "Hollywood loves human forms," says Spitzer. "There has been tremendous progress since 1990 in people being able to copy human forms [for digital effects]."

Other Notable Achievements

With the help of an SGI-powered Dextroscope, a neurosurgical planning system developed by Volume Interactions, doctors in Singapore were able to separate conjoined Siamese twins. The Dextroscope transforms multiple 2D images into stereographic 3D graphics, enabling doctors to plan complex surgeries in advance. Using the system, surgeons rehearsed for the grueling 97-hour operation, which took place in April 2001. The preplanning to separate the Nepalese girls took place on two continents over a period of six months.

At Stanford University, vascular surgeons can view different surgical options as they use powerful SGI supercomputers to calculate a patient's blood flow. The results, embedded in the patient's 3D MRI data, allow doctors to customize each operation. Medtronic, Nucletron, and Electra are among the surgical system manufacturers using SGI technology.

Research scientists at the Ohio Supercomputer Center, using SGI 3D technology, have created a unique method of training doctors to administer an epidural analgesia, a form of anesthesia often needed during childbirth and some surgeries. The delicate procedure, which requires an exact placement of the needle, can be dangerous and difficult. However, with SGI technology and funding from the Department of Defense, the center has created a virtual system that allows anesthesiologists to "practice" using 3D models. This ability to practice first leads to increased proficiency during actual procedures.

BIOCOMPUTATIONAL CHEMISTRY: WATCHING MOLECULES DANCE

Understanding the structure of molecules and gaining insight into how a protein fits into a cell are crucial for researchers trying to understand how disease progresses. High-end computers are helping scientists by simulating and visualizing the lives of cells.

With advanced computational techniques made possible by SGI servers, researchers are able to implement new algorithms that use X-ray crystallography and nuclear magnetic resonance (NMR) data to model and simulate 3D structures of protein molecules.

At the State University of New York in Buffalo, scientists are working on new techniques for molecular structure determination. Using an Origin 2000 server, combined with the vividly titled computational method known as Shake-and-Bake (SnB), Dr. Russ Miller is working to solve complex molecular structures. With the SnB algorithm, along with the parallel processing capabilities of the Origin 2000, he is finding new ways to attack the scientific phase problems of X-ray crystallography. "On my first power-up test of the Origin 2000 system, I conducted a trial run of Shake-and-Bake. In 90 seconds, I was able to analyze structures that used to take hours," Miller says. "Consequently, it is now feasible to determine the structure of proteins heretofore too large or time-consuming to undertake. This is the kind of computational power that will lead to the development of more effective drugs."

For example, Vancomycin — a powerful antibiotic — is often used as a last resort for gravely ill people. But emergent strains of bacteria resistant to the drug have risked making it ineffective. Miller is looking at modifications of Vancomycin's structure. "If the structure of the antibiotic is understood, then it can be modified," he says.

At Northwestern University, John Pople, the internationally acclaimed chemist who won the Nobel Prize in 1998 for his work in applying computational methods for understanding and predicting molecular structure, has used SGI solutions throughout his career.

Pople, who shared the award with physics professor Walter Kohn, was praised by the Nobel committee "for developing computational methods making possible the theoretical study of molecules, their properties, and how they act together in chemical reactions. These methods are based in the fundamental laws of quantum mechanics." The British scientist made his computational techniques accessible to researchers by designing the groundbreaking GAUSSIAN computer program — now used by chemists, universities, and companies all over the world.

During an interview published shortly after winning the award, the chemist said he saw no end to the possibilities of technology and chemistry: "We've now reached a point where theoretical chemists can begin to make reliable predictions about the properties of molecules without actually having to carry on experiments." He noted that during his lifetime, the efficiency of computers "… has gone up by eight power of ten — that's a factor of 100 million — in the last 20 years or so."

Quantum Chemistry

In Industry, Technology Helps Scientists Leap Ahead

Solving the fundamental mathematical equations that model the structure of chemicals based on the locations of their electrons is at the core of research in quantum chemistry. Using these complex equations effectively, however, was problematic prior to advances in supercomputer power.

For scientists working in the chemical industry, understanding the behavior of catalysts or radioactive wastes has been a pressing concern. At Dupont, scientists are using quantum chemistry models to help design better catalysts. Catalysts are chemicals or materials that trigger and enhance chemical reactions, and they are used in more than 60% of today's chemical products and 90% of chemical processes. Working in partnership with SGI and Molecular Simulations Inc. (MSI), Dupont scientists are creating new approaches to catalysis.

"The problems we are trying to solve are very much state-of-the-art — how chemicals react on novel catalyst surfaces," says Dr. Steve Lustig of DuPont Central Research in Wilmington, Delaware. "Historically, we've made a lot of progress understanding how molecules react with catalysts that are dissolved in solutions. Reactions that occur on catalyst surfaces can present much larger, more complex problems."

Simulating reactions using MSI's CASTEP program on two SGI Origin 2000 servers is one of the ways they are studying this problem. "Quantum chemistry is being used to solve the electronic structure of molecules reacting on catalyst surfaces," Lustig says. "This is very computationally intensive. High-performance computing is really necessary."

Drug Research

Visualizing Genes: Virtual Reality and Drug Research at Johnson & Johnson

Inside the Cave at the Academic Computing Services Amsterdam (SARA), a research facility in the Netherlands that allows scientists to observe data virtually in 3D, Dr. Peter J. van der Spek, leader of Janssen Pharmaceutica's bioinformatics team, may find himself moving through images of the human genome. In the darkened space, he can project genes, chromosomes, and cells on the Cave's three walls and floor. It is a place where researchers can rotate, walk through, and observe huge amounts of data generated by genomic, chemical, and medical research.

What Van der Spek sees in the cave will help him make decisions about which genes to target for drug intervention, which choices might be dead ends, and which choices might be "eureka" experiences for his team's quest to cure or treat diseases. Visualization and the use of virtual reality are crucial elements of drug research and development at Janssen Pharmaceutica, a division of Johnson & Johnson (J&J) Pharmaceutical Research & Development.

SARA, one of the most advanced computing and networking centers in the world, houses, among other technologies, the Dutch national supercomputer, an SGI Origin 3000 series server that supports scientists who conduct fundamental and applied scientific research. The virtual reality and 3D visualizations generated on the Origin are used for data mining in genomics. Visualization essentially allows the scientists to extract more information in a shorter time frame than would be possible with a more conventional approach.

Research Strategy Gives Scientists Competitive Edge

Van der Spek, along with his research team, makes the journey to SARA from Belgium to observe data gleaned from earlier research. "What we try and do is make some simulations there by making use of their very heavy infrastructure," Van der Spek explains. "So we do some simulations and then bring the data back to our company. We basically buy calculation time over there and make use of their cave." He describes the cave as a "classroom where you put stereo glasses on with your colleagues. You walk into the room and see the data all around you. This is very fascinating. That's virtual reality technology."

A former cancer researcher who has worked in the field of bioinformatics for the past 10 years, Van der Spek joined J&J three years ago, where he became director of the bioinformatics research team. He is also the main sponsor of the bioinformatics project connected with SARA. Currently, his activities focus on drug research and molecular pharmacology, including DNA chip analysis.

At J&J, he says, all bioinformatics platforms run on SGI. He describes the visualization technology as a "very serious investment for our company" and a way to hone its competitive edge. The search for novel intervention points that may lead to pharmaceutical development is one of the catalysts for the use of this kind of technology.

"We have to find novel intervention points," Van der Spek says, referring to which genes will be targeted in terms of drug development. "Therefore, we deal with a lot of public and proprietary data. We try to be more competitive than other companies. With my research team here, we have set up certain strategies to mine [data] as efficiently as possible through this kind of data. And so, we have developed certain routines. We were the first to implement virtual reality technology with bioinformatics approaches."

Study of Cells Reaps Rewards

Van der Spek and his colleagues don 3D glasses to observe complex cellular processes. "Every cell is basically a small chemical factory in which lots of different processes are going on at the same time," the researcher observes. "In every cell there are lots of small molecules. These molecules are being changed by enzymes and the proteins. What we try and do is actually interfere slightly on these chemical reactions with our drugs, of course. And that's how most drugs work. They just act on balances of small molecules present in different cell types.

"We try to understand these biochemical processes by looking at what compounds and what enzymes are present in cells," he says. "We know for many cells which genes are active — and so we know which proteins are there and which enzymes are there. So we know which molecules can actually be converted in those cells. What we look at is different types of genomic data. We explore known relationships — and unknown, novel ones. We look at the data and try to explore new correlations that are actually in the data, which have not yet been observed by other scientists."

The technology is also used in diagnostics, clinical trials, predisposition, and gene variation. Therapeutic areas using this kind of technology for drug research include oncology, virology, neurology, immunology, and gastroenterology, as well as the study of metabolic disorders.

Research Possibilities Enlarged by Technology

This 3D cell analysis approach has paid off enormously. "The most exciting thing about this whole project," Van der Spek says, "is that this cave and virtual reality technology allow us to look at really vast amounts of data, which with conventional approaches and software are not possible."

While many pharmaceutical companies are using visualization technology for research, they are usually doing it on visualization platforms on PCs. This is restricting, he says, because of the limited amount of data it is possible to visualize.

SGI's technology and expertise have been a crucial factor in helping the company develop its drug research strategy, Van der Spek says. While the SARA facility is used for virtual reality viewing, the data analysis and research are done back home in the lab in Belgium. The laboratory uses two Origin 3000 machines. He calls the Origin "a very rich machine, with 64 processors in there, possessing quite some crunching capabilities."

Transforming Data into Knowledge

The core focus of researchers at J&J is to identify novel targets and intervention points that have pharmaceutical functions. "Everything in bioinformatics nowadays has to do with going from data to knowledge," Van der Spek says. "So if you integrate your data in the proper way, you actually gain knowledge."

Van der Spek says he likes to offer his students the following advice: If you want to understand genes, listen to an orchestra. "Because in an orchestra, it is different instruments, which at the same time make music," he says. "At the same time, if you look at genes in a cell, there are lots of different genes at the same time present. It's all at the same time, but it's the changes over time which make you recognize that this time, this orchestra is playing this music.

"That's why we look at how gene expression changes over time. If you have just one time point, you don't know what you are looking at. But it's of course like the music. These subtle things which change make you recognize the music. For us it is the subtle group of genes which changes — it's actually related to the process of what you're looking at," he says. "With virtual reality technology, it is possible to track all of this."

Prioritizing Research

There have been many significant discoveries so far. "There have been identified, several new intervention points which are being broached full out in different therapeutic areas," Van der Spek says. "These have been very clear applications in the areas of cancers; there are clear applications in areas of central nervous system. These tools allow us to monitor disease progression."

Of course, blocking progression is also a form of treatment, he says. "So, if we find markers that are indicative for disease progression, that of course is very important. That makes you understand the whole process — what might be delaying, at the molecular level — the transition — for instance, from a benign to a malignant tumor," he says.

Visualization enables researchers to prioritize. "We want to work on the most promising targets," Van der Spek explains. "Almost all pharmaceutical companies have enough targets — they have so many targets, that actually their problem is to pick the most promising ones. That's another reason we moved toward this virtual reality technology. It's actually helping the process of prioritization of the most promising targets."

Drug Research and High Computing: A Mutual Embrace

During the 1980s and 1990s, pharmaceutical companies, looking to design drugs more efficiently, turned to advanced computational methods. Along with the virtual reality approach used at Janssen Pharmaceutica, several organizations have used and are using SGI's technology to help visualize and mine the data involved in chemical and molecular processes, thereby saving time, money, and energy. Most important, this work will ultimately save lives as scientists more quickly hone in on the genes to target in drug research.

In an international, collaborative effort, researchers are working together to join forces to gain a greater understanding of the human genome. At Merck, automated systems reach out in the night, visiting Internet sites to gather information on genomic sequences conducted by other research centers around the world. "It all happens automatically, with no human intervention required," says Dr. Rick Blevins, director of bioinformatics. "We're getting protein and DNA sequences from datacenters around the world and bringing it back for internal massaging and mining."

The human factor takes over then, as approximately 1,000 Merck scientists dip into the data with an internally developed data mining platform that allows them to comb through the Oracle8 databases running on SGI Origin servers through a Web interface. "We have about 70 processors worldwide, and our SGI Origin servers are always talking to each other," he says. "When you're dealing with such large databases, it's essential to be able to read quickly from the disc. The 80MBps throughput we're getting makes it easy for researchers in any facility to have fast access. As a result, researchers have the data they need to speed their time to insight."

Too Much of a Good Thing ...

But all these new innovations can create a lot of data — sometimes too much. As Mae West once said: "Too much of a good thing can be wonderful." But data overload can result. Roche Pharmaceuticals is developing a unique approach to the issue. "We're approaching enterprise datacenter magnitudes within each business area," says Bob Guthrie, research director of discovery informatics at Roche. "Because of that, we need to take an enterprise approach to support issues such as data backup, data restore, and data storage management," he says.

One way the company is approaching these issues is to create a central database that enables access for Roche researchers globally. "SGI has provided a lot of assistance in developing our strategies," he says. "Our needs are growing rapidly. We are adding lots of storage and servers and ultimately will have a storage area network to link our storage environment to the computer-intensive, data-crunching side of the business."

BIOINFORMATICS

Bioinformatics focuses on the structure of biological information and biological systems, merging data gathered through the study of the human genome with the tools of mathematics and computer science.

The Human Genome Project

"I sing the body electric ..." Walt Whitman

There are 3 billion letters, experts say, in the alphabet of life. With the combined efforts of scientists from Japan, the United States, and Europe, along with the help of advanced technology, researchers published the so-called Genetic Book of Life in February 2001.

Scientists are now faced with a new challenge — how to determine the function of each of the 30,000 to 40,000 genes that make up human DNA and of the hundreds of thousands of proteins those genes produce.

At Kyoto University Institute for Chemical Research (ICR) in Japan, scientists built a new scalar system for genomic research that opened in January 2002. The new supercomputer — a massively parallel 800-CPU supercomputer system supplied by SGI Japan — will help researchers analyze data based on molecular networks relating to the human genome project. It also runs an assortment of computational chemistry software. ICR also uses an Origin 2000 server and an Onyx graphics supercomputer.

SGI Japan also provides support for the GenomeNet system, which is run by the Bioinformatics Center, allowing genome researchers around the world to access its data 24 hours a day, every day of the year.

During the same week that the genome researchers announced their landmark discovery, Stanford University acquired an SGI Origin 3800 as part of its BIO-X program, which seeks to support interdisciplinary research in biomedicine and biotechnology.

Charles Taylor, assistant professor of surgery and mechanical engineering, praised the close collaboration the university has been able to achieve with SGI and with the emerging field of biocomputation, which uses advanced computational analysis to solve difficult problems in genetics, protein analysis, surgical planning, and other biosciences.

"The Origin 3800 marks the beginning of a new Stanford-SGI partnership in biomedical supercomputing," Taylor says. "It's now the biggest supercomputer at Stanford and one of the largest at any university dedicated exclusively to biocomputation."

WEATHER AND CLIMATE MODELING

Do You Think It Is Going to Rain? Climate Modeling at NOAA

Meteorologist Ron Stouffer's passion has always been for weather — all kinds. When he was younger, friends called him the "Weather Nut." Now, as one of the chief scientists at the National Oceanic and Atmospheric Administration's (NOAA) Geophysical Fluid Dynamics Laboratory, he focuses on climate changes, especially global warming.

Stouffer has won numerous awards and published more than 50 papers on climate and climate change. "Climate modeling," he says, "is the main tool used throughout the world for climate research. It couldn't be done without all this technology."

Stouffer works with an SGI Origin 3000 at NOAA's Geophysical Fluid Dynamics Laboratory in Princeton, New Jersey. The system is used to simulate deserts, oceans, and winds; predict when the next hurricane will strike; and study the long-term effects of global warming.

The lab has created "a computer program that represents the physics of the atmosphere and the ocean," according to Stouffer. Aspects such as the equations that govern the motion of the atmosphere, as well as the way heat moves inside the atmosphere and the ocean, are coded into the model. The model is run, and the results are compared to what one sees in the real world.

"And then, you can start, in some sense, playing games with it, things that you can't do to the real world," he says. "You can change things; see what happens. One of the things that people changed many years ago to see what would happen was the amount of greenhouse gases in the atmosphere. And that's how global warming research began."

During the early days, computationally — the whole planet was represented by a mere nine or ten grid boxes. At that time, around 1967, a simple equation might have taken hours to run through a computer. However, as high-performance computers have increased in power, they have enabled more complex modeling. "Now, they have literally hundreds of thousands — if not millions — of grid points in them," he says. "And it is possible to simulate climate over time — even as long as hundreds of thousands of model years."

Turning on the Sun

Much of Stouffer's time is devoted to studying the greenhouse effect, which some attribute to various human and industrial activities, that has resulted in an excess of carbon dioxide in the atmosphere and a depletion of the ozone layer. "People are putting what I call greenhouse gases — carbon dioxides, various fluorocarbons, ozone, which is a greenhouse gas — into the atmosphere," he says.

"Anytime you burn anything, any kind of fire — the by-products are carbon dioxide and water. And carbon dioxide has a very long lifetime in the atmosphere," explains Stouffer. "So, due to human activities, the carbon dioxide is gradually increasing. The reason the verbiage 'greenhouse' is used is that people have likened what happens in the environment to what happens inside a greenhouse.

"These gases are transparent to sunshine so that the sunshine keeps coming into the planet, unchanged," he says. "But as in the greenhouse, you have a pane of glass that blocks the heat from getting out. So the greenhouse heats up on a sunny day. These gases are acting to do a similar thing, in that they are inhibiting the heat that would naturally escape from the earth, and that's causing the earth to warm."

As a scientist, Stouffer uses visualization and modeling to understand the phenomena. An experiment using an Origin 3000 might look like this: "What we do is we first build a model in which greenhouse gases aren't changing. After that, the first thing would be to assess the realism of that model. And then, once we are satisfied with the realism of that model, this is now our control climate where things aren't changing," explains Stouffer. "Then we run experiments where we change the greenhouse gases, or we change conditions — if we're doing past climates, like in the past 100 years — we can put volcanoes in because various volcanoes have gone off in the past. And they affect climate. And as it turns out, the amount of sunshine reaching the earth has changed over the past 100 years, so we can put that in.

"And so, you let the equations govern how the earth responds in this computer simulation. And then what you can do is compare — say for the past 100 years — the model climate to what happens in the real world and make assessments of the effect of humans on climate," says Stouffer.

OIL AND GAS EXPLORATION

The Search for Energy Sources: The SGI Solution

During a recent SGI-sponsored energy summit held at the University of Texas in Houston, former U.S. Secretary of Energy Bill Richardson spoke about the need to develop new energy sources and how visualization technology has been revolutionizing the industry.

"As Secretary of Energy, I know firsthand the importance of science and technology in our energy future, having seen examples of how high-tech decision-making tools, like robotic oil rigs, have transformed the industry," Richardson said during the March 2002 conference. "This remarkable commitment to continuous technological improvement has helped the industry reliably meet the energy needs of appreciative nations around the globe," he said.

Virtual reality technology and 3D visualization, made possible by advanced computational tools, allow more efficient, environmentally friendly oil and gas exploration. Major oil companies, such as BP Amoco, Arco, Exxon, and Statoil, have all implemented these new technologies.

New Technology Creates Seismic Changes in Industry

At the University of Colorado's BP Center for Visualization, scientists and engineers are using these new technologies to help refine and streamline this process. Dr. Geoffrey Dorn, who oversees all research at the center, says he has always used advanced technology in all of his scientific research, including 3D seismic interpretation, research in reservoir modeling, and drilling engineering.

Large-scale collaborative visualization has become a crucial component of the oil and gas industries, Dorn says. "What we found in the oil and gas industry is that the use of large-scale visualization greatly improves the efficiency of the work you are doing, the accuracy, the completeness. It also improves the collaboration between people of different disciplines," he says.

Using virtual reality technology vastly increases efficiency, reducing costs, because it reduces the amount of time needed to plan drilling operations, Dorn says. "The experience we have had in the oil and gas industry is that using this large-scale visualization typically helps you achieve those kinds of efficiency improvements. You can typically compress months down to a few weeks."

SGI Plays Role in Industry

Dorn sees SGI playing a significant role in the industry: "One of the big issues that came out of the energy summit that ties the energy industry and SGI together is the tremendous volume of data the oil industry generates — the amount of processing we need to do to take all that data and process it into the 3D seismic volumes that we use for interpretation. SGI not only does high-end graphics, but they have some very good computational servers."

SGI's remote visual technologies are also useful, he says, "because a typical major oil and gas company will have a technical center in one city — say Houston — and then they will have operating offices scattered around the world. A much more effective way of doing that, as we do today, is to have visualization centers in all of their offices. They can link together in real time and make use of their experts at their technology center as virtual experts around the world."

Immersive visualization, which is the technique most oil companies use, involves a virtual reality room (or "cave"), in which data is projected in stereo on three walls and the floor. The system tracks the viewer's head and hand positions and projects the data as if the viewer were moving inside the simulated image.

"[Specific applications] depend on the problem you're working on," Dorn explains. "You might be displaying 3D seismic data and interpreting that for the geological structures or fluid content — or trying to identify reservoirs for drilling and exploration. Or you might be going in with a 3D model of a known reservoir and existing development well pattern that you've already drilled — and going in to try and drill additional wells to try and develop the reservoir."

DEFENSE

As terrorism becomes an increasing threat, the high-tech industry is playing an important role in supporting new strategies to create a cohesive policy of defense and homeland security. SGI technology is used in such areas as public health and safety, the protection of critical infrastructure, transportation security and efficiency, border security, disaster planning and recovery, law enforcement, and weapon system simulation.

Nuclear Weapons Testing at Los Alamos

Maintaining the United States' stockpile of nuclear weapons remains a crucial element of national defense. Los Alamos National Laboratory (LANL), along with Sandia and Lawrence Livermore National Laboratory, has been given that mission. Since October 1992, this task has had to be accomplished through methods that do not involve underground nuclear testing. In addition, the United States decided to halt nuclear weapons production, creating requirements for reliable testing and maintenance of the country's remaining stockpile of nuclear weapons.

Testing Moratorium Creates Need for Simulation

Under the Stockpile Stewardship Program, the Accelerated Strategic Computing Initiative (ASCI) was implemented in 1995 to carry out U.S. policy goals to replace earlier means of testing and creating requirements for new levels of computational capability.

Computer simulations allow scientists to understand weapons capabilities and their problems as well as enable them to keep testing the reliability and health of the country's nuclear arsenal. Before the moratorium on testing, simulation was used more as a guide to give scientists ideas of what to expect from a particular weapon. Simulation also helped reduce the number of actual nuclear tests required.

Los Alamos, in partnership with SGI, purchased the Blue Mountain machine in November 1998. The system, which helped ASCI successfully meet the ASCI 1999 and the ASCI 2000 milestones, is used to model and simulate a wide variety of phenomena, including astrophysics research.

Dr. Bernhard Wilde, a Los Alamos fellow who heads the laboratory's thermonuclear applications group, says that with the changes in policy came changes in the way his team handled the testing of the nuclear stockpile, creating the need for new codes and new styles of experimentation.

"Our fundamental purpose is that every year we have to certify that the [nuclear] stockpile works as it's supposed to work," Wilde says. "That is our number 1 purpose at the laboratory — to do that certification. And we do that for every weapons system. In order to accomplish that, in the past, we used to do nuclear tests and we used to run codes. And the codes, in general, did quite well, but they weren't perfect. So we used the codes as a guide to help us design a nuclear test.

"A code is a simulation tool that has a tremendous amount of physics in it — all of the physics — or almost all of the physics that's required to simulate a nuclear explosion," Wilde explains.

New Codes, New Dimensions

Under the program, scientists at Los Alamos developed codes that have additional physics in them. This work involved more of a 3D approach.

Validating the new codes and designs has become one of the tasks given to the Blue Mountain machine. "We use these simulation capabilities to create new models for the weapons systems," Wilde says. "In the past, almost all of our design and analysis work was done in 1D and 2D. So the other big thing, in addition to the additional physics and code, we are able to do is 3D analysis. So, now we have all these complex codes, and they have a lot of physics in them. And these codes have to be validated, and the way they are validated is through test problems.

"So what we're trying to do," he explains, "is develop new models with the newer codes such that we will have a capability that when a problem comes along with a weapon … we can use this newer and better model that has more physics on it and can be done in 3D to find an answer as to whether or not the problem that was found in the surveillance of the nuclear weapon when it was taken apart was a big thing or not — whether it can be corrected easily or whether we have to rebuild all these weapons."

In addition to nuclear testing, Los Alamos has a role in a variety of different areas: countering proliferation and terrorism, preventing proliferation of weapons of mass destruction, and building defense technologies.

Toward some of these goals, Wilde says above-ground experiments are also conducted on non-nuclear weapons stock with the help of computer simulation. These experiments might involve research on the performance quality of lasers, power pulse systems, gas guns, and high-explosive systems. "That's done for real, but we predict the results of these experiments with these new simulation tools," says Wilde.

Inside an Explosion: New Technology Takes You There

The searing light and heat created by an explosion of a nuclear bomb does not occur during a simulation. And there is none of the devastating environmental damage that underground nuclear testing might cause. "The simulations are on a computer, so they don't physically shake the earth," Wilde says.

However, this kind of research may create another kind of explosion — one of insight. "There is a feeling of excitement in the understanding that running these simulations can create," he says. "And what the implications then are for the certification of the stockpile. And then what the implications are for essentially keeping this deterrent alive. There is certainly national pride in certifying these weapons. There aren't many people who do that — there's only a handful of people in the world who do."

Wilde describes using the 3D visualization cave to observe the results of a simulation: "[Upon entering the room], the simulation will be all around you. It will be possible then for a scientist to rotate, manipulate, and focus in on the data being studied. Temperature changes will be represented through color.

"You can step the simulation forward in time or zero in on a physical ravine, and you can actually walk physically inside the simulation. You won't feel an explosion — but you will see a simulated flash, and, depending on what you're looking at, you can look at all sorts of physical variables, the density; the temperatures, the pressures, etc. It's like watching a movie — but you're inside of it," he says.

Often, one problem to be studied will require many visualizations, entering a variety of different conditions, Wilde says. "We don't just run one simulation — we run hundreds and thousands of simulations in order to study how that particular event would evolve. So we input these parameters, and we give the problem set up to the code essentially, and the code crunches the numbers. Visual studies are run at varying resolutions, from coarse to fine — to see what can be learned," explains Wilde.

Simulations Used for Different Phenomena

Scientists at LANL also use remote visualization techniques to collaborate with other research organizations, including Lawrence Livermore; Sandia, the Naval Research Laboratory in Washington, D.C.; the atomic weapons establishment in Britain; the Omega Laser Laboratory at the University of Rochester; as well as scientists at the University of Arizona and the University of Michigan.

"In addition to studying physics related to nuclear weapons," Wilde notes, "it also gives us the opportunity to study some very basic physics for astrophysical phenomena." These studies range from simulation of supernova explosions to historic asteroid impacts.

CREATIVE COLLABORATIONS

Creativity and Collaboration Make Good Science at the University of Utah

Imagining solutions to real-life problems is the philosophy that guides the University of Utah's Scientific and Computing Institute. From tracking the spread of pollution from an industrial plant to the design of chemical plants and factories, scientists and researchers at the institute are using advanced computational tools to create new solutions in medicine, industry, and engineering. A multidisciplinary effort has created a place of creativity and collaboration and cross fertilization of fields, where research in one area nourishes and catalyzes knowledge and invention in others.

Dr. Chris Johnson, the institute's director since 1992, says its eclectic approach has involved several research initiatives using SGI: "Some [initiatives] have been involved with scientific visualization, some with problem-solving environments for scientific computing, for inverse and imaging problems, and large-scale parallel computing."

The institute has a large number of collaborators across the country using its software applications. Among them are Harvard University, MIT, Caltech; Brown University, as well as national laboratories, such as Los Alamos and Lawrence Livermore.

"What usually is the case is they [the research facilities] have a different problem they want to solve — they work with us to solve that particular problem using our expertise and our large-scale visualization tools," says Johnson.

Anatomy Becomes Destiny

One invention that began its life because of visualization and simulation is an implantable defibrillator that came out of the institute's work.

"The idea was — what if we were to devise a small, implantable electrode that we could place in a body — a patient — via catheter that would go off automatically at the onset of a cardiac fibrillation," Johnson says, recalling the process of its creation.

"Basically, with a small amount of voltage, it would shock the heart before it went into this massive ventriculation," he explains. "That was the idea. However, you can't just go and experiment on live patients. That's where computer simulation steps in."

Different bodily tissues possess different rates of electrical conductivity; for example, blood is 50 times more conductive than bone. Johnson and his team create geometric models of patients derived from their MRI scans to test the material properties of electrical conductivity.

After putting in all of these different material properties, the team still faced design issues in terms of what the sizes and shapes of the defibrillation electrodes should be, Johnson says. The following questions needed to be answered: Where should they be located? How much voltage should they give up? When should they go off to be the most effective?

All of those questions were answered by simulation and modeling. "We basically created this computer model and put in all these material properties of the conductivities of the tissue," says Johnson. "We then were able to simulate the voltage and current from these defibrillators themselves, so then we could design different sizes and shapes of the defibrillators internally, place them in different places, simulate their effect on the body, calculate the amount of current which reaches the heart, and then visualize the models and the results of these simulations."

From that invention, came others. Researchers from an oil and gas company came and saw it, saw the simulations of blood flow, and wanted to apply it to seismic research. The software created at the institute has also been used to collaborate on a chemical plant design. It's even been used to simulate the spread of pollution from a smokestack in Europe.

Everything All at Once

Without SGI, Johnson says, none of this would have been possible. "It was a real tight link between large-scale computing and large-scale visualization," he explains. "Before we got machines on the level of Origins, we would have to run all of our simulations on one machine — then move all the data over to our SGI and visualize it."

Johnson says SGI's move into more powerful machines that had faster, multiple CPUs was a turning point for the institute's research. "When they first started to make faster CPUs and put them in parallel with each other, and they already had fast graphics and then, they linked those together in a single computer. This is what really made the difference for us," he says. The institute started out with the Power Challenge and the Power Onyx back in the mid-1990s, and then moved on to the Origin 2000. "That was when they came out with the Infinite Reality Graphics System," he explains.

"It's very scalable," Johnson says. "That's where SGI's niche is right now. They have this tight link between simulation and visualization — and the ability to scale very well on simulation and visualization to large-size problems."

STARS

Cosmology

Was there a first event — a big bang — that led to a causal chain of events that created the universe? And if so, what caused it? Professor Stephen Hawking, along with his colleagues at the University of Cambridge, are using an SGI Origin 3800 in their COSMOS project to try and find out.

About 10 to 20 billion years ago, according to the Big Bang theory, a much hotter, denser universe suddenly expanded in all directions, releasing powerful bursts of radiation and matter. That explosion allegedly left the whole universe covered in what scientists call cosmic microwave background (CMB) radiation. Because of its uniformity, physicists believe that this CMB is a remnant from the Big Bang. At Cambridge, Hawking and his team will be exploring this cosmic microwave background as a way of testing the theory.

During a January 2002 press conference to announce a five-year deal that will create the largest cosmology supercomputer in the United Kingdom, Hawking provided scientists, who had also gathered there for an SGI-sponsored symposium in honor of his 60th birthday, with the following explanation:

"A key research area of our consortium is the scientific exploration of the cosmic microwave background, the relic radiation left over from the Big Bang fireball, usually just called the CMB. The COSMOS supercomputer is the main platform on which we are developing techniques to analyze data from the world's most ambitious CMB experiment — the Planck Surveyor satellite, which is due for launch in 2007. This analysis is very computationally challenging, but it will give us unprecedented new information about the origin and present state of our universe.

"Cosmology is a rapidly advancing and highly competitive field, driven by new observational results. The COSMOS supercomputer has allowed us to turn our ideas very rapidly into concrete predictions, ensuring that U.K. cosmologists continue to make leading international contributions. On the shared-memory SGI Origin 3800 server, we can easily scale up our workstation codes to tackle really big problems, without all becoming computer jocks. We get time to think about the universe, not just about programming. We have benefited from leading-edge shared memory technology from SGI ever since our first Origin family computer arrived in 1997, and we plan to continue to do so."

Scientists working on the COSMOS project will be using data taken from the COBE satellite, launched in 1989 by NASA, which was searching for evidence of the Big Bang and the structure of the universe.

"The COBE satellite images were the first to show that on top of the smooth CMB, you began to see these small ripples," says Dr. Paul Shellard, director of the COSMOS project. "These primordial ripples, or perturbations, evolved into the structure of the universe — galaxies, stars, etc. Hawking and his team will be trying to find out just what caused these ripples."

Mapping the Sky: As the Universe Expands, One Scientist Tracks

Scientist Edwin Hubble, who in 1920, using a 100in. telescope from Mount Wilson, analyzed the light from other galaxies and discovered that almost all of them are moving away from us at a velocity that is proportional to their distance from the earth. From this discovery, he concluded that the universe is expanding — a concept that revolutionized scientific thought in the twentieth century and changed the way people thought about the origins of the universe.

Recent theories, however, suggest that not only is the universe expanding — it's accelerating outward as well. "Apparently, the universe is not just flying apart. It's actually flying apart at an ever-increasing rate — it's accelerating — it's speeding up," says astronomer Brent Tully from his research laboratory at the University of Hawaii.

"Dark matter and dark energy are the big characters in this long-playing tug of war," says Tully. "No one seems to know exactly what dark matter is. We know that the influence of dark matter's gravity is trying to pull things together. Dark energy is pushing space apart. For billions of years, dark matter has dominated and caused the creation of galaxies and stars and everything we know. But in the last few billion years, dark energy seems to make up most of the universe and has something to do with gravity. Dark energy, the propulsive force, seems to have emerged only in the last few billion years. Dark energy has become ascendant." Tully calls them "two mysteries, one on top of the other."

Making a Chart of the Sky

Meanwhile, Tully maps the universe with an SGI O2 desktop machine. So far, he's charted 30,000 galaxies, and he will add to that number. "Always expanding," Tully says. "No one knows how big the universe really is — but the general school of thought now is that it's infinite."

Tully says lately he's been sticking to the neighborhood: "I have studied the details of the local supercluster … down to the local group. I've been involved in sorting out the neighborhoods around where we live. The downtown core is the Virgo cluster, which is about 50 million light years away. We are in the suburbs of the Virgo cluster."

Tully is currently most focused on learning about the universe's structure — what lies between its filaments, suns, planets, and empty spaces. With its high-resolution graphics capabilities, the O2 helps him to see — and to visualize a greater understanding.

While mapping, he says, "I can see this 3D scene — which is this distribution of nearby galaxies. It's a scene which I can rotate — and look at from different perspectives. I can fly through it. By wearing 3D crystal glasses, I can have the screen project an image which is viewable in a 3D sense. So I can actually begin to view and appreciate the structure that is involved."

A World Once Hidden, Now Revealed

Scientifically, there have been huge payoffs. "The sheer complexity of the universe has been made apparent by visualization," Tully says, describing a moment of clarity made possible by technology. It happened, he says, while he was looking at images in the cave at the University of Illinois — an environment in which images are projected onto three walls and the floor.

"You wear these liquid crystal glasses — so the two eyes are seeing different polarizations," he says. "It gives you a sense of 3D. While I was looking at my data set — the local supercluster — it really felt like I was a big giant striding across the universe with eyes the size of a galaxy. I was seeing this whole-scale change.

"You see that there's this structure — the structure of the universe — and it became more of a living thing," he says. "It was like being able to visualize a once unseen world."

Communing with Stars

Tully says it was show business that helped him see the possibilities of the technology. "Hollywood had a big leg up on us, in the sense that lots of people were doing very well with visualization," he explains. "In science we weren't doing nearly as well …. Really, it was just a lack of resources. The tools were there, the need was there, but somehow we just lacked resources ... to do proper visualization …. And that's when I got interested in what SGI had to offer."

While Tully's primary purpose in doing this work is for research, the mapping has great educational possibilities. "It's not very useful if it's not communicated," he says. "So this really is my learning and communication device."

In terms of its resources and expertise, Tully says SGI has been a great inspiration. "SGI continues to be a leader in this business of visualization," he says. "I find it tremendously valuable to be able to call upon these resources — both in the computers and software and in the knowledge of people associated with visualization. I don't want to become an expert in visualization — so I really appreciate having the hardware and access to people who are experts."

What Makes Scientific Computing Distinctive?

We believe that scientific and technical computing make up a unique segment of the overall computing market. As the case studies demonstrate, scientific computing (and technical computing in general) has many unique requirements for computing systems, including:

- **Continual demand for increases in computing power.** Once you solve the problem, it's no longer interesting. Models become more detailed and complex over time, which in turn leads to requirements for more computing power.
- **Ability to manage large data sets.** A side effect of more complex models is large data sets. Scientific computing systems must be able to both support large data sets during simulation runs and manage these data sets over the long term, staging files to secondary and archival storage when not in use.
- **High-performance I/O.** Data movement is often the rate-limiting step in technical applications; thus, technical systems must be able to stream data from peripheral storage to memory to processors and back again.
- **Large memories.** The ability to maintain applications data in memory supports faster solutions by reducing dependence on the performance of peripheral storage systems.
- **Visualization requirements.** Large models and data sets create requirements to present results in a form that can be easily understood and manipulated by scientists. Visualization essentially provides a mechanism to match the performance of the computer with the performance of the human mind.

In addition to generating demanding requirements for computer systems, scientific computing fills an important role as a proving ground for technology innovations. New algorithms, computations methods, architectural approaches, operational concepts, and so on often find their genesis in scientific computing, to be adopted over time by other segments of the technical market.

Opportunities and Challenges for Computer Vendors

The distinctive aspects of scientific computing present computer vendors, such as SGI, with a mixed bag of opportunities and challenges.

Opportunities

Long-term opportunities for computer systems vendors in the scientific computing market include:

- **Insatiable requirements for performance.** The overall effort to understand the nature and dynamics of all aspects of the physical universe is most likely an unattainable goal. (Fortunately, partial results have proved to be very useful.) Thus, scientific computing markets can generate requirements of computing performance that can keep up with or exceed gains generated by Moore's Law improvements in system components and/or architectural innovations. These requirements for performance should help maintain market stability over the long term.

- **Relatively stable market.** Scientific computing markets tend to be less affected by economic instabilities due to a combination of long-term government support for educational and national research organizations, national security requirements, and economic drivers for new technologies.
- **New market entry point.** The combination of science and computing can generate new market opportunities for the computing industry by leveraging computing technology to help solve otherwise intractable problems. As the potential for the biosciences market indicates, the ability to solve new classes of problems creates new research and industrial opportunities, which in turn require greater computing resources.

Challenges

Scientific computing has proved to be a very demanding, fast-paced arena in which to do business. The challenges the vendors must address if they choose to play in this market include:

- **Keeping pace.** The major challenge for computer vendors is to keep up with scientific user requirements. As science moves forward so do demands for more powerful and often more specialized systems. This fast pace can cause a conflict for computer vendors that need to develop systems to meet the broadly diversified requirements of both technical and commercial users.
- **Competitive anomalies.** The excitement generated by scientific computing can be viewed as providing computer vendors with visibility, marketing, and public relations benefits. Thus, vendors may compete in the market with reduced expectations for monetary return. In addition, scientists have been known on occasion to develop their own in-house computing solutions, ranging from clusters to specialty computers; in this case, computer vendors can find themselves in competition with their customers.

Meeting the Challenges

From its inception and throughout its history, SGI has developed computing systems designed to meet the requirements of scientists and engineers. It has identified its mission as follows:

"Be the world leader in high-performance computing, complex data management, and visualization; develop and deliver products, services, and solutions that enable technical and creative customers to gain strategic and competitive advantages."

The company is very tightly focused on providing computing solutions to scientific and other research and development organizations. We believe that SGI's focus, combined with its experience in the scientific computing markets, positions the company to remain a strong competitor in the technical computing area.

CONCLUSION

One of the oldest and best definitions of supercomputing is the use of computational methods to support and advance scientific inquiry. In this sense, scientists use high-performance computers for tasks ranging from simulating physical phenomenon prior to experimentations to develop a better understanding of factors involved in the phenomenon, to analyzing events that are not subject to direct experimentation, to testing hypotheses and theories through modeling and simulation, to managing very large databases and visualizing the results of research.

IDC believes the cases presented in this paper demonstrate the effectiveness of SGI's computational and visualization solutions across a very broad spectrum of scientific applications and environments. SGI is also one of the few companies in today's market dedicated to developing and fielding hardware and software systems solutions designed specifically to meet the needs of the technical computing market.

IDC Worldwide Offices

CORPORATE HEADQUARTERS

IDC
5 Speen Street
Framingham, MA 01701
United States
508.872.8200

NORTH AMERICA

IDC Canada
36 Toronto Street, Suite 950
Toronto, Ontario M5C 2C5 Canada
416.369.0033

IDC California (Irvine)
18831 Von Karmen Avenue
Suite 200
Irvine, CA 92612
949.250.1960

IDC California (Mountain View)
2131 Landings Drive
Mountain View, CA 94043
650.691.0500

IDC New Jersey
75 Broad Street, 2nd Floor
Red Bank, NJ 07701
732.842.0791

IDC New York
2 Park Avenue
Suite 1505
New York, NY 10016
212.726.0900

IDC Texas
100 Congress Avenue
Suite 2000
Austin, TX 78701
512.469.6333

IDC Virginia
8304 Professional Hill Drive
Fairfax, VA 22031
703.280.5161

EUROPE

IDC Austria
c/o Loisel, Spiel, Zach Consulting
Mayerhofgasse 6
Vienna A-1040, Austria
43.1.50.50.900

IDC Benelux (Belgium)
Boulevard Saint Michel 47
1040 Brussels, Belgium
32.2.737.76.02

IDC Denmark
Omøgade 8
Postbox 2609
2100 Copenhagen, Denmark
45.39.16.2222

IDC Finland
Jarrumiehenkatu2
FIN- 00520 Helsinki
Finland
358.9.8770.466

IDC France
Immeuble La Fayette 2
Place des Vosges Cedex 65
92051 Paris la Defense 5, France
33.1.49.04.8000

IDC Germany
Nibelungenplatz 3, 11th Floor
60318 Frankfurt, Germany
49.69.90.50.20

IDC Italy
Viale Monza, 14
20127 Milan, Italy
39.02.28457.1

IDC Netherlands
A. Fokkerweg 1
Amsterdam1059 CM, Netherlands
31.20.6692.721

IDC Portugal
c/o Ponto de Convergancia SA
Av. Antonio Serpa 36 - 9th Floor
1050-027 Lisbon, Portugal
351.21.796.5487

IDC Spain
Fortuny 18, Planta 5
28010 — Madrid
Spain
34.91.787.2150

IDC Sweden
Box 1096
Kistagangen 21
S-164 25 Kista, Sweden
46.8.751.0415

IDC U.K.
British Standards House
389 Chiswick High Road
London W4 4AE United Kingdom
44.208.987.7100

LATIN AMERICA

IDC Latin America
Regional Headquarters
8200 NW 41 Street, Suite 300
Miami, FL 33166
305.267.2616

IDC Argentina
Trends Consulting
Rivadavia 413, Piso 4, Oficina 6
C1002AAC, Buenos Aires, Argentina
54.11.4343.8899

IDC Brazil
Alameda Ribeirao Preto, 130
Conjunto 41
Sao Paulo, SP CEP: 01331-000 Brazil
55.11. 3371.0000

International Data Corp. Chile
Luis Thayer Ojeda 166 Piso 13
Providencia
Santiago, 9, Chile
56.2.334.1826

IDC Colombia
Carerra 40 105A-12
Bogota, Colombia
571.533.2326

IDC Mexico
Select-IDC
Av. Nuevo Leon No. 54 Desp. 501
Col. Hipodromo Condesa
C.P. 06100, Mexico
525.256.1426

IDC Venezuela
Calle Guaicaipuro
Torre Alianza, 6 Piso, 6D
El Rosal
Caracas, Venezuela
58.2.951.1109

CENTRAL AND EASTERN EUROPE

IDC CEMA
Central and Eastern
European Headquarters
Male Namesti 13
110 00 Praha 1
Czech Republic
420.2.2142.3140

IDC Croatia
Srednjaci 8
1000 Zagreb
Croatia
385.1.3040050

IDC Hungary
Nador utca 23
5th Floor
H-1051 Budapest. Hungary
36.1.473.2370

IDC Poland
Czapli 31A
02-781 Warszawa, Poland
48.22.7540518

IDC Russia
Suites 341-342
Orlikov Pereulok 5
Moscow, Russia 107996
7.095.975.0042

MIDDLE EAST AND AFRICA

IDC Middle East
1001 Al Ettihad Building
Port Saeed
P.O. Box 41856
Dubai, United Arab Emirates
971.4.295.2668

IDC Israel
4 Gershon Street
Tel Aviv 67017, Israel
972.3.561.1660

IDC South Africa
Building 9, Pebble Beach
Fourways Golf Park
Roos Street
Fourways, Gauteng
South Africa
27.11.540.8000

IDC Turkey
Tevfik Erdonmez Sok. 2/1 Gul
Apt. Kat 9D
46 Esentepe 80280
Istanbul, Turkey
90.212.275.0995

ASIA/PACIFIC

IDC Singapore
Asia/Pacific Headquarters
80 Anson Road
#38-00 IBM Towers
Singapore 079907
65.6226.0330

IDC Australia
Level 3, 157 Walker Street
North Sydney, NSW 2060
Australia
61.2.9922.5300

IDC China
Room 611, Beijing Times Square
88 West Chang'an Avenue
Beijing 100031
People's Republic of China
86.10.8391.3610

IDC Hong Kong
12/F, St. John's Building
33 Garden Road
Central, Hong Kong
852.2530.3831

IDC India Limited
Cyber House
B-35, Sector 32, Institutional
Gurgaon 122002
Haryana India
91.124.6381673

IDC Indonesia
Suite 40, 17th Floor
Jakarta Stock Exchange
Tower 2, Jl. Jend. Sudirman Kav. 52-53
Jakarta 12190
6.221.515.7676

IDC Market Research (M) Sdn Bhd
Jakarta Stock Exchange Tower II
17th Floor
Jl. Jend. Sudirman Kav. 52-53
Jakarta 12190
62.21.515.7676

IDC Japan
The Itoyama Tower 10F
3-7-18 Mita, Minato-ku
Tokyo 108-0073, Japan
81.3.5440.3400

IDC Korea Ltd.
Suite 704, Korea Trade Center
159-1, Samsung-Dong
Kangnam-Ku, Seoul, Korea, 135-729
822.551.4380

IDC Market Research (M) Sdn Bhd
Suite 13-03, Level 13
Menara HLA
3, Jalan Kia Peng
50450 Kuala Lumpur, Malaysia
60.3.2163.3715

IDC New Zealand
Level 7, 246 Queen Street
Auckland, New Zealand
64.9.309.8252

IDC Philippines
703-705 SEDCCO I Bldg.
120 Rada cor. Legaspi Streets
Legaspi Village, Makati City
Philippines 1200
632. 867.2288

IDC Taiwan
Room A2, 21st Floor, Hsin Kee
Building, 460 Hsin Yin Road, Sec 4
Taipei, Taiwan
886.2.87806818

IDC Thailand
27 AR building
Soi Charoen Nakorn 14,
Charoen Nakorn Rd., Klongtonsai
Klongsan, Bangkok 10600
Thailand
66.02.439.4591.2

IDC Vietnam
Saigon Trade Centre
37 Ton Duc Thang Street
Unit 1606, District-1
Hochiminh City, Vietnam
84.8.910.1233; 5

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