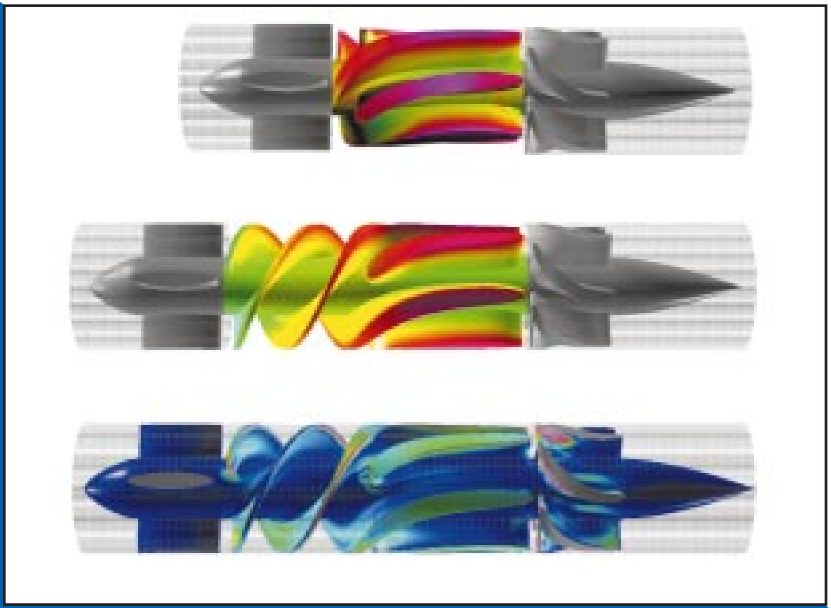
gridpoints

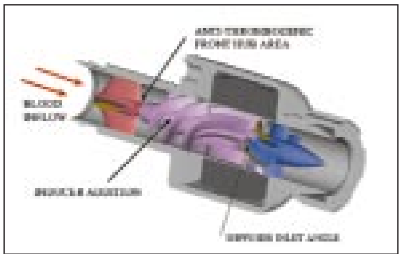
Spring 2000

The Quarterly Publication of the Numerical Aerospace Simulation Systems Division



NAS researchers use CFD technology to improve DeBakey Ventricular Assist Device
Page 4

Features



Page 4

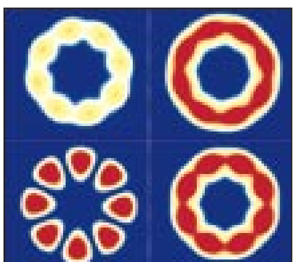
Space Shuttle Engine and CFD Technology Improve Heart Device

Using CFD technology, NAS researchers make major design changes on the DeBakey heart device, enabling its human implantation.
Holly A. Amundson

Computational Astrobiology Center Uses NAS Computing Resources to Explore Life

NASA's new center studies life and habitability on other planets using NAS's high performance computing technology.
Holly A. Amundson

Page 8



Page 12

VCSEL Lasers: Tiny Lasers, Huge Potential

Semiconductor lasers are the key to increasing information transport, processing, and storage.
Cun-Zheng Ning

NAS Division's 1999 Achievements and Awards

NAS's high performance computational resources brought a number of new technologies to fruition during the last year of the decade.
Nicholas A. Veronico

Page 17

On The Cover:

These diagrams are computational representations of blood flowing through the DeBakey Ventricular Assist Device. The top two represent pressure data in both the baseline and modified device design. The bottom shows areas of varying shear stress levels in the new mechanism. For more information, see CFD Technology Applied to Life-Saving Heart Device, on page 4. (Datasets courtesy of Cetin Kiris)

gridpoints

Vol. 1, No. 2 • Spring 2000

Executive Editors: Bill Feiereisen, John Ziebarth

Editor: Nicholas A. Veronico

Writers: Holly A. Amundson, Cun-Zheng Ning

Graphic Designer: Eunah Choi

Illustrator: Gail Felchle

Photographer: Michael Boswell

Contact the Editor:
Nicholas A. Veronico
Gridpoints
M/S 258-6
Moffett Field, CA
94035-1000
Tel. (650) 604-3046
Fax (650) 604-4377
nveronico@mail.arc.nasa.gov

The staff of *Gridpoints* would like to thank the following people for their assistance in preparing this publication:

Dallas Anderson, Dick Anderson, Joel Antipuesto, Rupak Biswas, Michael Boswell, Alan Cassell, Chinley Chang, Samson Cheung, Bob Ciotti, Christine Cortez, James Donald, Jill Dunbar, Chris Gong, T.R. Govindan, Ana Grady, Dick Gunderson, John Hardman, Chris Henze, Vee Hirsch, Mary Hultquist, Tony Keefe, Cetin Kiris, Chris Kleiber, Dochan Kwak, Tammy Leal, George Makatura, Meyya Meyappan, Cun-Zheng Ning, Bill Nitzberg, Todd Novak, Andrew Pohorille, Marcia Redmond, Julie Reynolds, Gregory Schmidt, Jack Szostak, Ryan Spaulding, Valerie Steele, Jim Taft, Bill Thigpen, Richard Thompson, Michael Wilson, Mindy Wilson

Gridpoints is a quarterly publication of the Numerical Aerospace Simulation Systems Division at NASA Ames Research Center. The division's staff includes government employees and contractors from Cray Research Inc., SGI, Advanced Management Technology Inc., Computer Science Corp., and Raytheon Company.

Visit us on the web at:
http://www.nas.nasa.gov/Gridpoints

From The Division Chief

The Spring issue of *Gridpoints* features a cross-section of the work taking place in the NAS Systems Division. Over the last year, we've worked to bring about important changes within the division, including a broadened mission and a new organization, the start of the Information Power Grid project for distributed high performance computing, the installation of the new 512-processor SGI Origin 2800 system — the largest single-image system in existence today — and the replacement of the NAS mass storage system, to name a few. These changes have enabled the division to support NASA's high performance computing community, and conduct research projects that will have far-reaching benefits.

One such project, which will positively affect people around the world, is the work done by Cetin Kiris and Dochan Kwak, in NAS's Research Branch. Using computational fluid dynamics technology and the NAS Facility's high performance computers, these two scientists greatly improved the performance of the DeBakey Ventricular Assist Device, a small heart pump designed to sustain patients awaiting heart transplants.

Part of the NAS mission is to lead the country in the research and development of high performance computers. Toward that end, Cun-Zheng Ning, on the quantum optoelectronics project team, has been studying the properties of Vertical Cavity Surface-Emitting Lasers, or VCSELs. Ning's VCSEL modeling will help NASA researchers understand how these lasers behave, and will ultimately lead to the development of optical interconnects for future petaflop-scale desktop computers, multi-gigabit ethernets, and applications for future spacecraft.

In addition, the NAS division staff will become a major resource for the newly established NASA Computational Center for Astrobiology (NCCA), located at Ames Research Center. In support of NCCA, NAS will develop advanced computational algorithims and parallelized computer codes to model protein and DNA sequences. And, NAS visualization tools will enable NCCA scientists to interactively view and manipulate their data in 3-D. Our staff is preparing to support a variety of new computational research projects from NCCA, and the results of these efforts will be presented in future issues of *Gridpoints*.

For those of you who can't wait for the next issue, I invite you to preview stories featured on the front page of our new website (which launched in late March) at http://www.nas.nasa.gov. You'll also find the latest division news, information on current research, technical papers and reports published by NAS staff, and much more.

As always, I welcome your feedback.

Bill Feiereisen
wfeiereisen@mail.arc.nasa.gov

NAS Mission

To lead the country in the research and development of high performance computing for NASA Programs and Missions by being the first to develop, implement, and integrate new high performance computing technologies into useful production systems.

To provide NASA and its customers with the most powerful, reliable, and usable production high performance computing systems in the country.

News From NAS

New 512-processor Origin Used for X-plane Analysis

Collaborative efforts between the NAS Systems Division and SGI to build a high-performance, 512-processor computer has paid off in a big way. The Origin 2800, *Lomax*, has helped scientists make monumental accomplishments in their research. In late January, *Lomax* demonstrated an advance in integrated aerospace design capabilities by running CFD datasets of the NASA/Boeing X-37 in a very short turnaround time. The X-37 is

A team of researchers from Langley Research Center employed computation fluid dynamics on NAS's 512-processor Origin 2800 to simulate thermodynamic conditions of the X-37's re-entry through the atmosphere. (NASA) an experimental launch vehicle that flies through the low density, upper atmosphere at speeds in excess of Mach 20 (14,340 miles per hour). This hypervelocity environment produces complex CFD effects and chemical reactions in the air surrounding the plane — CFD includes physics that cannot be duplicated in a traditional wind tunnel.

Researchers Richard Thompson and Frank Greene from the Aerothermodynamics Branch at NASA Langley Research Center used *Lomax* to investigate the X-37's aerothermodynamics and hypervelocity conditions upon re-entry into the atmosphere. The project required exclusive use of *Lomax* for 120 hours, running up to 480 processors during testing. Thompson estimates that, "*Lomax* is faster by a factor of 15 or more when compared to a CRAY C90 computer running the same application." Not only did the 512 save significant time on analysis of the x-plane, it produced a high degree of accuracy in the results. "The computing horsepower afforded by NAS and *Lomax* on this project enabled us to bring high-fidelity CFD into the design phase at a critical point, avoiding costly delays and redesigns later in the program." gp

The NAS Systems Division's visualization lab furnishes remote and local users with visualization equipment and technology to enhance the understanding of computational simulations and experimental data. On the right is the Responsive Workbench where a Collaborative Virtual Mechanosynthesis (CVMS) user manipulates 3-D simulations viewed by an audience on the presentation screen at left. (Michael Boswell)

Collaborative Visualization Tool Brings New Perspective to Atoms

In February, researchers Chris Henze and Bryan Green in the NAS data analysis group established an application for distributive, collaborative, remote computational steering of atoms, Collaborative Virtual Mechanosynthesis (CVMS). CVMS is a new, state-of the-art application enabling interaction with atomic structures. "It's like playing virtual tug-of-war," jokes Henze.

"The collaborative VMS will be a valuable educational tool, as well as an excellent design tool," says Green. Utilizing CVMS for teaching chemistry will enable students to explore the geometry of molecules, and "live" atomic structures. Using Fakespace Inc.'s Responsive Workbench, teachers will have the ability to manipulate a 3-D image of a molecule while students wearing polarized glasses watch the interaction on a large screen.

"This visualization tool can be used to rehearse assembly processes for future nanotechnology projects," explains Henze. Taking advantage of CVMS to assemble a molecule prevents the user from building a structure that would not survive in nature — the application will only permit a design where atoms bond correctly to one another. CVMS currently operates on a single server to run molecular simulations. Multiple clients can view the simulation at physically remote locations from the server, moving atoms from their own viewpoints — independent of other clients.

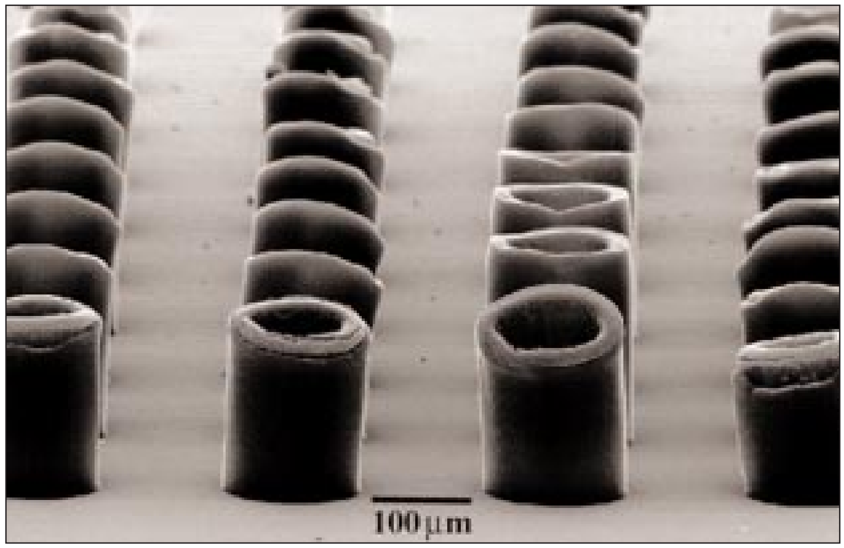
The Responsive Workbench is equipped with a stereo visor and wand enabling the operator to orient and manipulate the model. The images are not created from precalculated datasets, but are generated as the simulation runs — the user introduces new forces that are incorporated into the calculations. "The haptic device is force-sensitive, allowing the user to feel the sense of attraction or repulsion of bonds being created or broken. I was amazed by the realism of feeling the forces between the bonds of the atoms," Green says.

Usually, the server for CVMS runs from an SGI Onyx workstation. The client also uses an Onyx workstation located in the NAS visualization lab. Having run the application on the 512-processor SGI Origin 2800, *Lomax*, in the past, the team can see a potential for the program to take advantage of all 512 processors. "Eventually, the 512 will be useful for supporting nanotube and other simulations with tens of thousands of atoms at a time," Henze explains.

To date, the CVMS application has solely run the Brenner Potential code, working with only carbon and hydrogen atom simulations. In the future, Henze and Green would like to write code to model other types of atoms, especially biomolecules. Specifically, they plan to incorporate the Amber code, or one of its derivatives, to run biomolecular simulations and protein folding with the CVMS on *Lomax*. Eventually, the NAS team would like to generalize the application even further — extending current molecular dynamics computations to include electronic structure calculations. Achieving this goal will require running on multiple servers simultaneously. "CVMS is turning into a hub for the investigation of molecules," states Henze. "The application has the potential for becoming a really great problem-solving environment. Adding the capability for electronic structure calculations may be a good first step in that direction," Green adds. gp

NAS's Nanotube Technology Used to Develop Biomedical Devices

Recently, NASA Ames' Integrated Product Team (IPT) on devices and nanotechnology was awarded a grant from the National Cancer Institute to develop a biosensor technology enabling the early detection of cancer cells. The project draws on knowledge and technology from 35 researchers center-wide, including the nanotechnology and modeling team at NAS, and will focus specifically on leukemia research.



NASA's Integrated Product Team on devices and nanotechnology has recently discovered a way to control the growth of carbon nanotubes. Here, nanotubes are grown in a vertically aligned fashion. The sensor used for detection of cancer cells must be attached to a perfectly straight nanotube to ensure an accurate diagnosis of cancer. (Integrated Product Team)

David Loftus, cancer specialist at Stanford Medical Center, is collaborating with the IPT by contributing medical knowledge to the project. Previous nanotechnology research by NAS scientists Jie Han and Deepak Srivastava form the foundation for this project.

The IPT plans to develop a tiny biosensor that will enable an instantaneous biopsy — inserting a probe at the end of a nanotube into bone marrow via a catheter to search for cancerous cells. Current diagnostic procedures are painful — marrow is extracted from the spine, and it can take 10 days to two weeks to receive biopsy results.

Nanotechnology involves the creation of functional materials, devices, and systems through control of matter on a very small scale — on the order of a billionth of a meter. IPT project manager Meyya Meyyappan says, "Nanotechnology applies very well to cancer detection and diagnostics." The carbon nanotube is a very versatile material, and can be used for structural applications, being very strong and light. They are also excellent for electrical applications, such as this project, which includes an electronic detection system.

"Before nanotubes could be grown in the lab, the team had to have an understanding of the properties and uses of the nanotube. Using computer models has helped bring us to this understanding," explains Meyyappan. IPT member Alan Cassell adds, "The theory and a lot of the idea generation have come from NAS." Specifically, NAS researcher Jie Han, technical lead for the project, was the first to explore the possibility of nanotechnology being used for the early detection of cancer.

The team has recently developed a procedure to control the electrical and structural properties of nanotubes grown for this project. They have also determined a method for attaching a probe molecule to the tip of the carbon nanotube, enabling an almost instantaneous detection of cancer cells.

Once nanotubes are grown and bonded with a probe molecule, they are studied using an atomic force microscope (AFM) to understand the interaction between the sensor and the cancerous cell. IPT researchers will investigate the sensor by modeling the interaction of a DNA sequence using an AFM. The team is counting on NAS's visualization capabilities to provide a clear picture of the probe molecule's structure and how it can be joined with nanotubes. gp

Space Shuttle Engine and CFD Technology Improve Heart Device

Using CFD technology, NAS researchers make major design changes on the DeBakey heart device, enabling its human implantation.

Inspired by a life-saving heart transplant in 1984, NASA Johnson Space Center engineer David Saucier began designing a heart assist device with the guidance of his surgeons, Dr. Michael E. DeBakey and Dr. George P. Noon from Baylor College of Medicine, Houston. The DeBakey Ventricular Assist Device (VAD) is a miniaturized heart pump designed to increase blood circulation in heart failure patients. Through the collaborative efforts of MicroMed Technology Inc., the NAS Systems Division at Ames Research Center, and NASA Johnson Space Center, the DeBakey VAD has evolved from Saucier's initial design work on an axial flow pump.

Early versions of the DeBakey VAD caused thrombus formation (blood clotting) and excessive hemolysis (red blood cell damage). NAS scientists Cetin Kiris and Dochan Kwak employed NASA Space Shuttle main engine technology, NAS computational fluid dynamics (CFD) modeling capabilities, and NAS high performance computing technology to improve the heart device's performance. "Dochan and I are extremely proud of our collaboration and have high hopes that this work will improve many lives," says Kiris.

In the past, Kwak, Kiris, and NAS colleague Stuart Rogers, developed the INS3D computer code that was applied to rocket propulsion research. This same code was used to improve the DeBakey pump. Kwak explains, "When designing a VAD you have to look at stagnant and high shear regions. Red blood cell damage was too high and blood was clotting around the bearing area in the original device, and it would stop rotating. We were tasked with solving these problems using CFD."

Before NAS researchers became involved in the project, Kiris says, the DeBakey device lasted no more than two days when implanted in animals. In collaboration with MicroMed Technology CEO Dallas Anderson and chief engineer Robert Benkowski, Kiris and Kwak made modifications that have enabled the device to perform for more than 100 days. The longest successful trial period to date in a human was 123 days, after which a donor heart was transplanted. The team's ultimate goal is to make the VAD an alternative to heart transplant surgery.

Approximately 20 million people worldwide suffer annually from heart failure, a quarter of them in America alone. In the United States, an alarmingly low 2,500 donor hearts are available each year. The DeBakey VAD prolongs life until a suitable transplant heart is available, and is used to boost

	baseline design	new design
hemolysis index	0.02	0.002
thrombus formation	yes	no
test run time	2 days	120 + days

Performance of the newly designed VAD improved drastically following the implementation of modifications suggested by NAS researchers. Thrombus formation (blood clotting) was eliminated, the hemolysis index (cell damage) was reduced significantly, and the test run time was extended. This dataset incorporates the clinical results from Baylor College of Medicine and MicroMed Technology Inc.

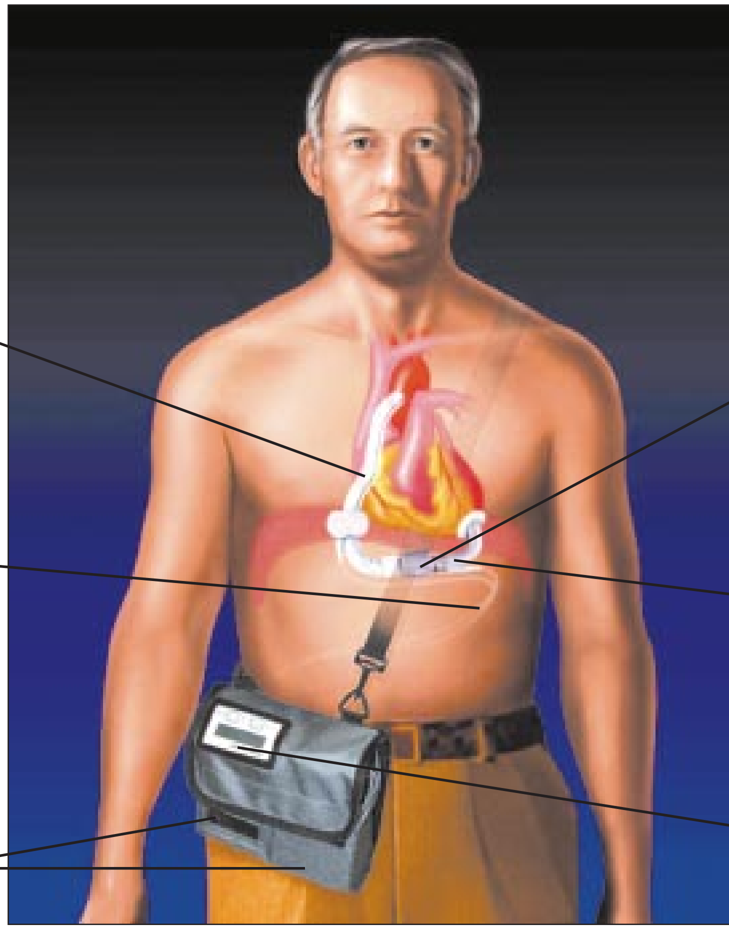


Figure 1. The lightweight and fully implantable DeBakey Ventricular Assist Device gives patients mobility and freedom. The internal battery has a two-hour life, enabling patients to take a shower or swim. (MicroMed Technology)

blood flow in patients suffering from hemodynamic deterioration; that is, loss of blood pressure and lowered cardiac output. Successful European trials of the device suggest its ability to provide long-term ventricular assistance.

The DeBakey VAD is an improvement over existing VADs because of its compact size, low power requirements for operation, and lower cost. Approximately one-tenth the size of any other heart device currently on the market, the DeBakey VAD weighs less than 4 ounces and is the size of two AA batteries — small enough to fit inside a child's chest — and requiring only eight watts of power to operate (see Figure 1).

Collaboration between Baylor College, NASA, and MicroMed Technology is producing a more affordable device. The current retail price for a typical heart assist unit is $75,000. Designers at MicroMed project that the DeBakey VAD can be manufactured at a substantially lower cost. To date, 24 patients have received the device, and the number is expected to more than double by the end of this year.

NAS Design Improves Device Performance

Kiris and Kwak modeled blood flow through the device using the same CFD flow solver algorithm used to analyze the fuel turbopump for the Space Shuttle's main engines. The fuel pump turns at 12,000 to 15,000 revolutions per minute (rpm), compared to the VAD's impeller blades that rotate at approximately 10,000 rpm. The impeller circulates blood at a flow rate of five liters per minute. CFD technology used in the Space Shuttle's main engine design and the VAD improvements are similar; any advancements or new discoveries in one can be applied to the other. The VAD experiments provide a testbed for adapting main engine technology to a very small device. The miniature size and delicate operating conditions of the VAD make measuring the blood flow in the device difficult without CFD analysis. "With CFD, we could immediately pinpoint what components of the device caused undesirable blood flow patterns," Kwak says.

Using CFD and data from previous animal trials, the NAS team performed simulations of blood flow in a cow. Clinical

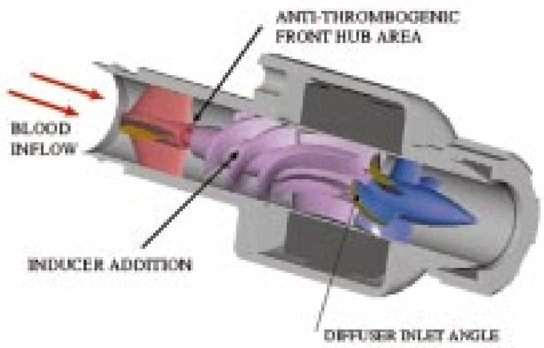


Figure 2. Using CFD analysis, NAS researchers Dochan Kwak and Cetin Kiris found that major design modifications to the DeBakey Ventricular Assist Device were necessary. The result of these changes: overall efficiency of the device was increased by 22 percent. (MicroMed Technology)

trials conducted on cattle blood confirmed that the CFD analysis showed similar flow data results. "Having the ability to use CFD for flow simulations can reduce animal testing," explains Kwak.

The NAS research team investigated seven different designs, altering cavity shapes, blade curvature, and impeller tip size. They then suggested three major design modifications to solve the problems of cell damage resulting from exposure to high shear stress and interrupted regions of blood flow in the DeBakey VAD (see Figure 2).

"The first improvement was the addition of an inducer that spins with the impeller, drawing the blood in and out of the device," explains Kiris. "Additionally, the inducer provides enough pressure rise, which eliminated back flow in the impeller hub region. The front edge of the blades were slanted forward, allowing blood to flow at the correct angle with the impeller, thereby increasing the efficiency of flow through the device (see Figure 3)."

Second, CFD results suggested that the original design of the device caused clotting in the front bearing area where the blood passes over the flow straightener and meets the impeller blades. By expanding the hub area's width, the team increased blood circulation, eliminating stagnant sections where clotting was known to occur. Additionally, they tapered the hub surface, accelerating blood flow, creating good "wall washing."

Finally, the NAS scientists examined the exiting flow angle of the blood and repositioned the diffuser angle. Says Kiris: "Changing the diffuser blade angle aligns it with the blood flowing through the device (see Figure 4), creating a smoother transition of blood over surfaces, and reducing shear stress, which causes cell damage." Clinical tests conducted by MicroMed Technology and Baylor College have confirmed the improvement in performance — hemolysis was decreased tenfold (see table, page 4).

Working Together to Save Lives

Collaboration between NAS, Johnson Space Center, Baylor College, and MicroMed, lead to a patent specifically for the new design modifications made on the DeBakey VAD. "NASA Administrator Daniel Goldin's support has been very important to the success of the project, as Dr. DeBakey's support has been important to the success of MicroMed Technology," says CEO Anderson. In 1999, the device was recognized by the U.S. Space Federation's Space Technology Hall of Fame as an application of space technology that will benefit humankind.

Before the DeBakey VAD can save lives in the U.S., the Food and Drug Administration (FDA) must approve its use in humans. Once the unit has received FDA approval and passes clinical trials, Anderson projects that a long-term version of the device may save 60,000 lives a year. "The successful implementation of the DeBakey VAD will be a monumental accomplishment in the history of medical technology," says Anderson.

The work NAS researchers accomplished on the device is a good demonstration of the adaptability of CFD technology to other applications. "There is a definite need for more high performance computing technology — on a larger scale, to allow researchers to develop a long-term VAD that

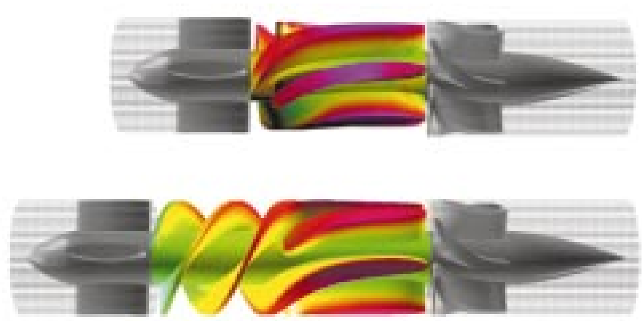


Figure 3. Visual comparision of the original VAD, top, and the unit after modifications by NAS researchers, lower. Adding an inducer to the DeBakey device eliminates the dangerous back flow of blood by increasing pressure and making flow more continuous. The device is subjected to the highest pressure around the blade tips, shown in magenta. (Cetin Kiris)

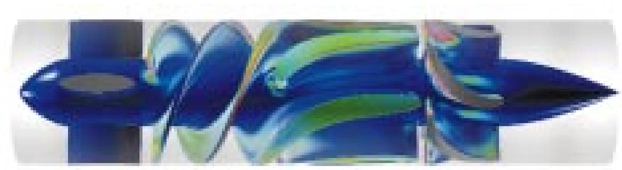
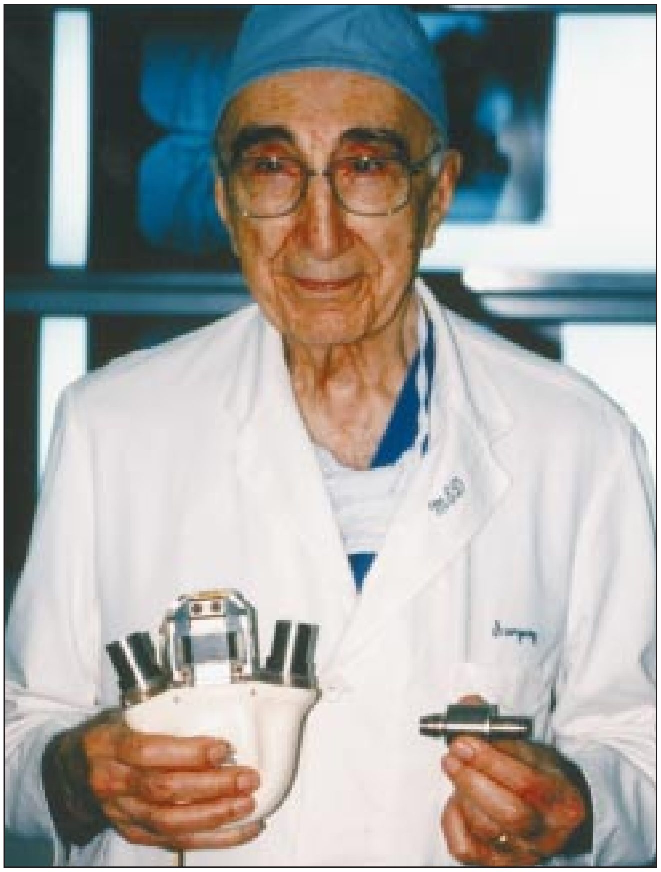


Figure 4. Measuring blood flow patterns over the surface of the diffuser using CFD analysis points out areas of high and low shear stress. The blue areas denote low stress; magenta regions represent areas of turbulent blood flow. The tiny area of high shear stress shows a lower amount of red blood cell damage. (Cetin Kiris)



Dr. Michael Ellis DeBakey, 90, is a renowned cardiovascular surgeon, teacher, and medical expert. A pioneer in the field of heart transplantation, he has been practicing at the Methodist Hospital, Houston, for more than 45 years.

will adapt to changes in the body's need for blood flow. In the future, we'd like to develop controls for the DeBakey VAD that will slow the pump when a patient sleeps, and increase blood flow when a person walks or climbs stairs," explains Kwak. "The methods of CFD analysis used on the DeBakey heart device can be applied to other biomedical devices in the future." gp

—Holly A. Amundson

For More on the DeBakey VAD:

- Visit MicroMed Technology's website at: http://www.micromedtech.com
- Additional background information on the DeBakey VAD is available at: http://www.methodisthealth.com/debakey/VAD.htm
- NASA's collaborative efforts with the DeBakey Ventricular Assist Device project are available for review online at: http://www.ttechnology.com/articles/nov_98/nasa_baylor.html

DeBakey VAD Development Timeline

Ventricular assist devices have saved lives since the 1950s. Michael E. DeBakey was the first doctor to successfully implant a partial artificial heart in a patient. He has been working on the design of heart devices for more than 30 years, and has performed surgery on more than 60,000 people in the Houston area alone.

1984: NASA Johnson Space Center's David Saucier begins initial design work on an axial flow pump ventricular assist device with the help of Dr. DeBakey.

1988: NASA Johnson Space Center and Baylor College of Medicine sign a memorandum of understanding to develop the DeBakey VAD.

1992: NASA begins funding the project after Johnson Space Center (JSC) Director George Abbey expresses interest in Saucier's work.

1993: A contract is initiated between JSC and Baylor College. NAS research scientists Dochan Kwak and Cetin Kiris visit JSC to study the device. NAS is asked to develop CFD procedures to analyze blood flow through the device and apply the results to design and performance improvements.

1994: Kwak and Kiris begin work on design analysis of the heart device using the CRAY C90 high performance computer housed at the NAS Facility.

1996: Full design rights are granted to MicroMed Technology Inc., a company dedicated to producing and promoting the heart pump.

1998: On November 13, the first six DeBakey VADs are implanted in European patients by Roland Hetzer and DeBakey at the German Heart Institute of Berlin. One of the patients, 56 year old Josef Pristov, is able to return home and spend Christmas with his wife after a month's stay at the clinic for recovery and monitoring.

1999: Additional funding is allocated for the project in August by NASA Ames Research Center. A patent for the device is awarded on September 7, for the three major design changes to the device as a result of the CFD analysis done by Kiris and Kwak. NASA Ames is listed as a co-inventor of the device with Johnson Space Center, MicroMed, and Baylor College of Medicine.

Computational Astrobiology Center Uses NAS Computing Resources to Explore Life

NASA's new center studies life and habitability on other planets using NAS's high performance computing technology.

How did life begin and evolve on Earth? Does life exist elsewhere in our galaxy? What future do humans have on other planets? We have pondered these questions for ages. At Ames Research Center, the NASA Center for Computational Astrobiology (NCCA), established in November 1999, is using high performance computing resources at the NAS Facility to uncover new clues for understanding the origins, evolution, and future of life. "The center requires a multidisciplinary approach," explains NCCA Acting Director Andrew Pohorille. "Drawing on the expertise of nearly 40 researchers located throughout Ames, NCCA merges information technology and various life sciences to solve biological problems with high performance computing resources," he says.

NCCA is tasked with developing models for the origin of cellular life, to determine its sources and identify organic molecules in space and on planets beyond Earth, to analyze the evolution of microbial and simple multicellular systems, and to develop theoretical techniques for identifying signatures of existing or extinct life beyond Earth. "To achieve NCCA's research goals, our scientists use

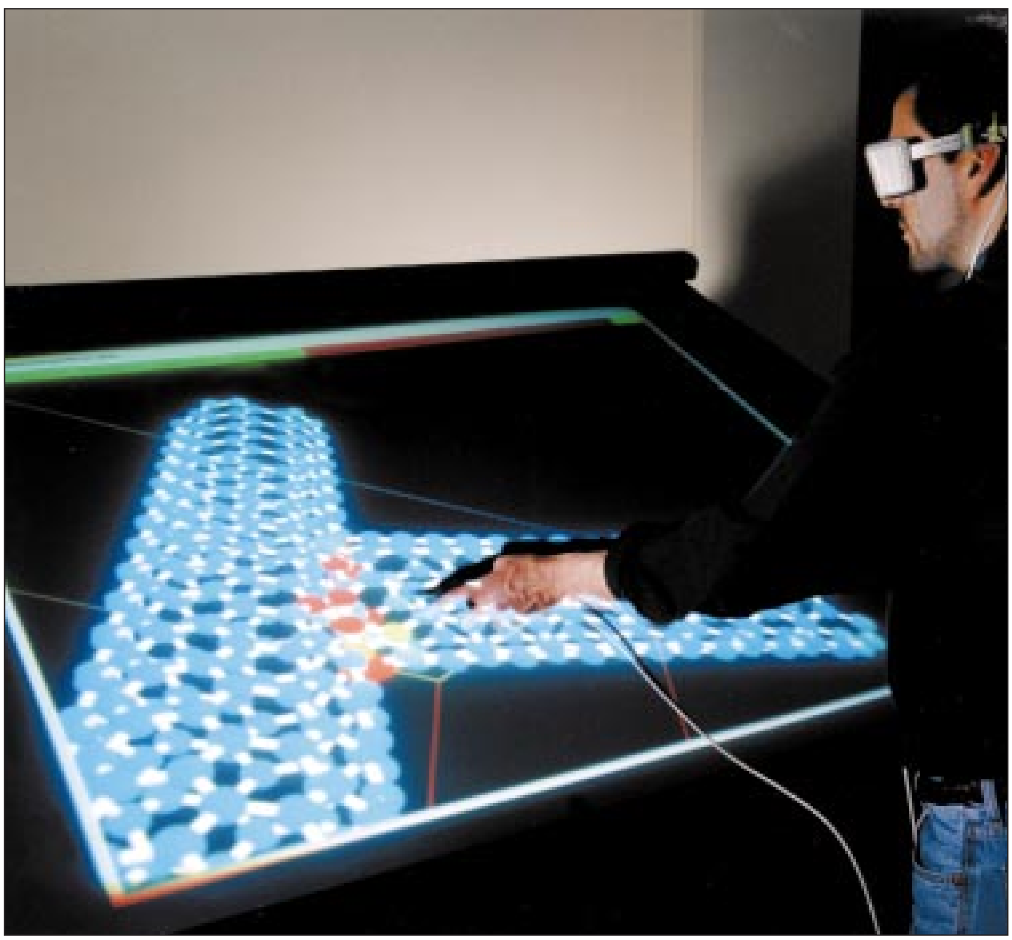


Figure 1. The Responsive Workbench, manufactured by Fakespace Inc., is a valuable visualization tool for researchers. Here, NAS researcher Chris Henze manipulates a simulated graphite T-junction, enabling him to study the molecular structure from any angle imaginable. (Tom Trower)

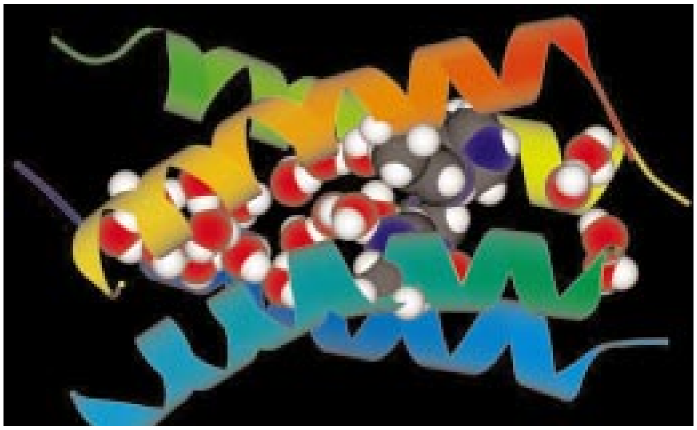
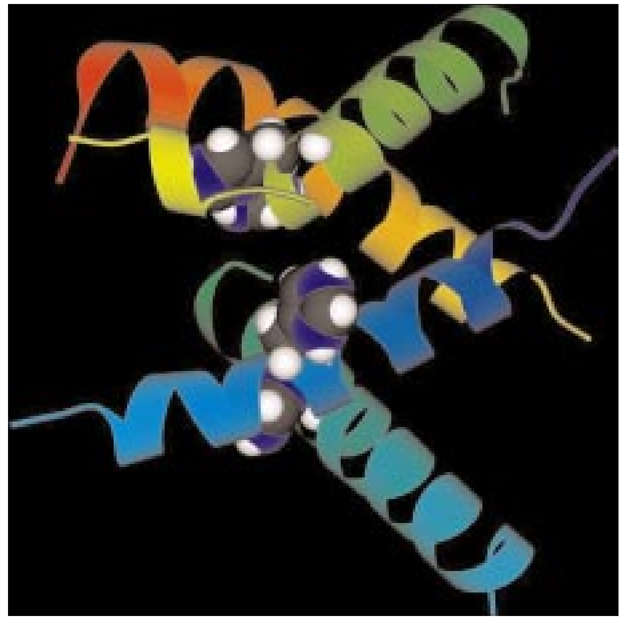


Figure 2. The M_2 protein is an ion channel protein that has the ability to transfer protons across cell walls. This application demonstrates the ability of NAS high performance computers to support simulations that will help researchers better understand the function of proteins and bio-molecules through visualization.
(Courtesy of Michael A. Wilson)



the NAS Facility's high performance computing resources and draw upon its expertise in the parallelization of computer codes, the use of complex algorithms, and its suite of visualization tools," explains Pohorille. "Working with Chris Henze and Bryan Green from NAS's data analysis group, we are striving for real-time 3-D visualizations of our molecular simulations using VMS — Virtual Mechanosynthesis — software that allows researchers to interact with and study the behavior of a molecule in three dimensions" (See Figure 1, opposite).

Additionally, NCCA is working with NAS scientists Nagi Mansour, Karim Shariff, Jim Taft, and Alan Wray to develop a highly parallelized molecular dynamics code for *Lomax*, the 512-processor SGI Origin 2800. The Origin system provides NCCA with a larger, faster computing resource capable of supporting applications, requiring lengthy simulation times, such as M_2 proteins (see Figure 2).

Exploration Through Computation

Computational astrobiology applications are still relatively new to NAS. Astrobiologists are beginning to apply nearly two decades of world-class experience NAS researchers have acquired in computational physics and fluid dynamics to the simulation of biological processes. "Computational astrobiology can be looked at the same way as CFD — once the importance of simulations in astrobiology have been demonstrated, the need for greater compute power and resources at NAS will result," says NAS senior scientist T.R. Govindan.

Current computer technology has the ability to support biological simulations on the molecular level for about one microsecond. However, most biological processes extend about one millisecond of time, an order 1,000 times longer than current computer capabilities. Simulating protein folding is a prime example of an application requiring tremendous computer resources. "The problem is, simulations involve repetitive calculations of Newtonian equations of the motion of atoms, which can only be carried out for certain periods of time. We are at least three orders of magnitude away from our goal," says Pohorille.

NCCA's need for increased computing power is already being addressed with the development of the Information Power Grid (IPG) — a collaborative project in the NAS Systems Division (See *Gridpoints*, Winter 1999, page 20). The IPG will be a high performance computing infrastructure linking remotely located computers and storage devices to run complex computations. "Distributed computing will be an excellent approach to solving many problems in astrobiology," states Pohorille. In the future, the IPG can provide the distributed computing power necessary to execute such computations as molecular simulations. Protein modeling can be adapted to the new computing environment by reformulating algorithms. Pohorille believes that, "when the IPG is operational and accessible, it will be a valuable tool for NCCA in modeling quantum chemical simulations of organic molecules in interstellar media."

A focus area of study within astrobiology, says Pohorille, is bioinformatics — the computational analysis of protein and DNA sequences. A typical protein module is comprised of 30 to 80 amino acids. During evolution, amino acids in proteins are added, deleted, or replaced by other proteins. These changes accumulate over time so that it becomes increasingly difficult to discover similarities between proteins performing similar functions in very different organisms. Using a supercomputer enables researchers to rapidly identify matches among billions of protein sequences. Computational analysis allows researchers to identify functions, categorize structures, and determine origins of different proteins. "Information gathered from the computational

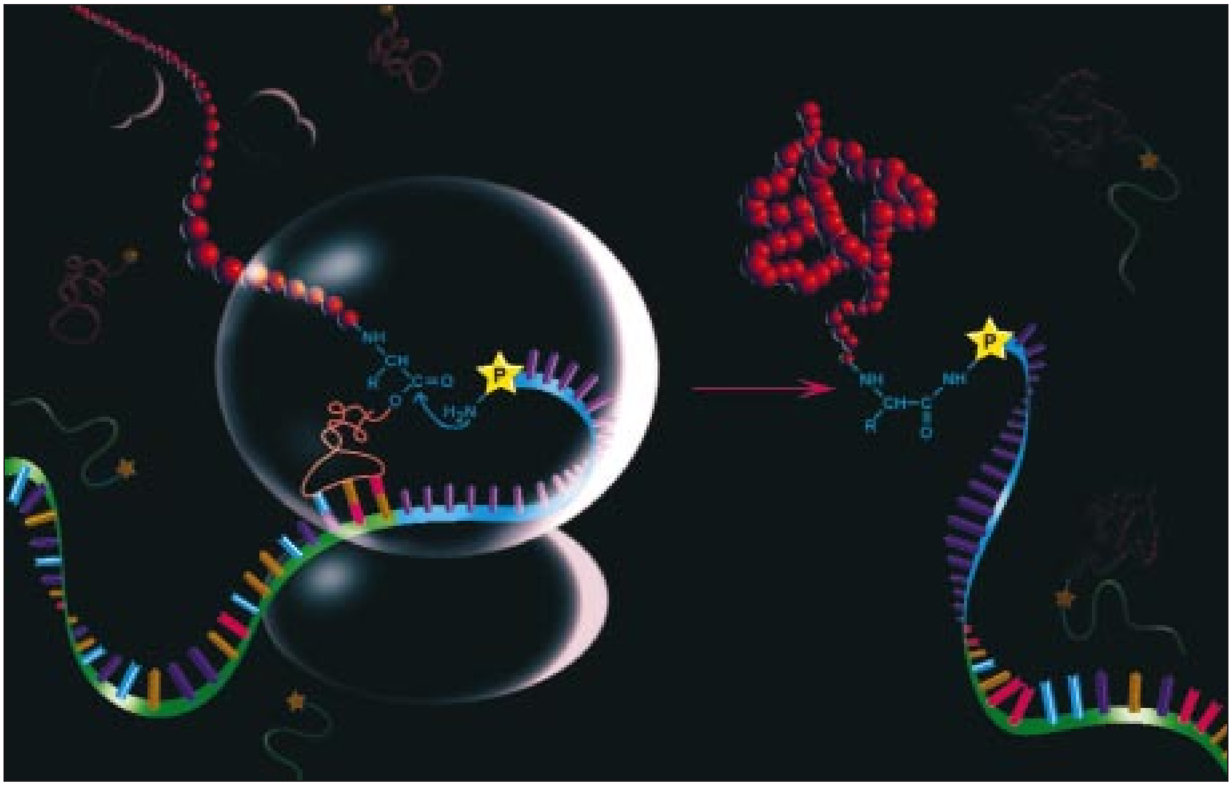


Figure 3. *In vitro* (artificial) selection and augmentation are extremely valuable tools for protein classification. Here, the protein is undergoing a continuous cycle of *in vitro* selection and growth to help identify the structure from an extensive library of known protein configurations. The "P" represents puromycin, an antibiotic that functions by repressing the translation of a bond forming organic compounds. This repression helps define the original protein structure and the carrier of the genetic information — important to the formation of proteins, making the protein readily identifiable. This process, recently developed by researchers at Harvard Medical School, may be used to prepare new protein libraries for future research.

(Artwork by Pauline Lim — Reprinted from Journal of Molecular Biology, Volume No. 297, Issue 2, Glen Cho, Anthony D. Keefe, Rihe Liu, David S. Wilson, and Jack W. Szostak, Constructing High Complexity Synthetic Libraries of Long ORFs Using in Vitro selection, pp. 309-319, Mar 2000, by permission of the publisher, Academic Press.)

approach allows us to reconstruct the evolutionary history of living organisms on Earth, and connect them with the evolution of the biosphere, thereby leading to a deeper understanding of the process of evolution," says Pohorille.

The field of computational astrobiology has both a philosophical and practical side. The philosophical aspect is represented by an overwhelming curiosity about life's beginnings. The evolution of life is not clearly understood, and there are large gaps in the knowledge base of the transformation from organic molecules to fully evolved monocellular organisms.

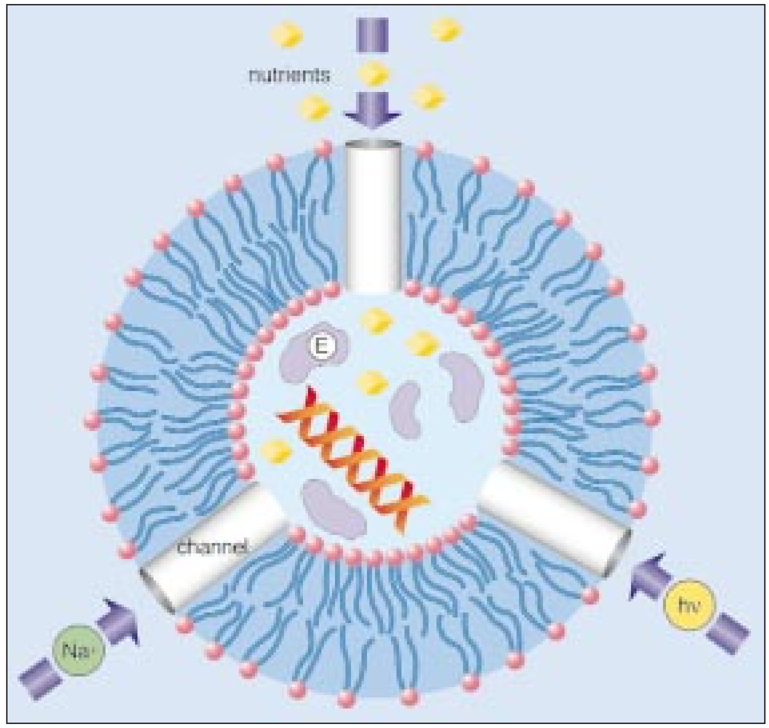
NCCA's mission, according to Pohorille, is to learn as much as possible about these gaps in the evolution of life, beginning with the earliest known cells, called protocells (see Figure 4, opposite). Protocells are primitive cells maintaining several essential life functions. The molecules forming the protocell originated from a pre-biological environment; that is the biosphere on Earth between 4.2 and 3.8 billion years ago when there was almost a complete lack of oxygen in the atmosphere. Researchers are attempting to piece together how these molecules self-organized into a cellular structure and how they functioned, by studying computer simulations. Scientists hope to gain knowledge of how these cells process energy from the environment and transport nutrients through cell membranes.

The practical side of computational astrobiology is represented in the pharmaceutical industry with new drugs (rational drug design), and in human gene studies with the discovery of previously unknown evolutionary relationships. One of NCCA's research partners, Harvard Medical School, has created a method to evolve novel functional proteins that may have existed since the beginning of life, while others may have biotechnological or medical applications (see Figure 3). Modeling these very primitive cells may help uncover some clues to the mystery of evolution. NCCA is examining Harvard's model to explain the theory and functionality of the protein.

Roadmap to Success

In June 1999, NASA scientists and administrators met to define funding requirements, goals, and objectives for

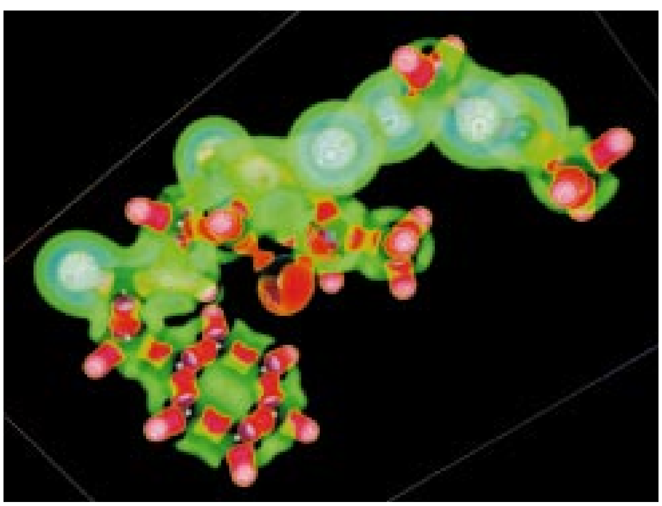
Figure 4. Protocells are the origin of cellular life. This image depicts the basic functions of a protocell; yellow represents the capture and utilization of environmental energy, blue represents the transport of nutrients, and green represents the transport of ions.
(NASA Exobiology Program)



NCCA. Ames Center Director Henry McDonald presented NCCA with a grant from the Director's Discretionary Fund to launch the center. Subsequently, NASA Administrator Daniel Goldin has made the study of astrobiology a budget priority for the space agency.

As the leading site for computational astrobiology, NCCA will advocate new research and technology as well as software recommendations, recruit teams of astrobiologists and information scientists, and guide future NASA astrobiology mission planning activities. Seminars and workshops will be an active way for NCCA to develop world-wide collaborations among researchers and promote computational astrobiology to other sciences.

NCCA has established a budget of nearly $2 million for fiscal year 2001, and will seek funding from a number of sources including NASA's Astrobiology Integration Office (AIO). Pohorille projects that the center could potentially have a NASA Research Announcement (NRA) established by the end of 2001. "An NRA will help specify NCCA's issues, attracting people to contribute their work to help meet the center's goals," Pohorille explains. He also states that an advisory board for the new program is being established to provide a source of external oversight and advice. AIO lead Gregory Schmidt believes that, "we are at the beginning of a wonderful new opportunity to create the tools that will allow us to model everything from the constituent molecules of life to global biospheres. I believe that NASA could, and should, take the leadership role in computational astrobiology. To do it right we should continue making investments in this tremendously exciting new area."



The molecule Penamecillin was simulated by NAS researcher Chris Henze to study its biological activities using special visualization rendering techniques developed at the NAS Facility. The figure was produced to highlight regions of electron accumulation (red to white shading) and electron depletion (green to blue). This molecule has a strong hydrogen bond that attaches to the surface of bacteria, helping eliminate it from the human body.
(Chris Henze)

Collaboration is the key to success for the new center. "Various researchers will come together toward one program, and different fields of study will now have a common goal," says Pohorille. "Through this collaborative research project, and the use of high performance computers, will come a new understanding of biological and evolutionary processes." gp

—Holly A. Amundson

Learn More About Computational Astrobiology

- Visit the NASA Center for Computational Astrobiology homepage at: http://cca.arc.nasa.gov/

- For astrobiology-related events and news, visit: http://astrobiology.arc.nasa.gov/index.cfm

VCSEL Lasers: Tiny Lasers, Huge Potential

Semicondutor lasers are the key to increasing information transport, processing, and storage.

By Cun-Zheng Ning

In the 1960s, lasers were the weapon of choice for many science-fiction movie villains. Today, 40 years later, lasers are a part of everyday life — from barcode scanners at supermarket check-out counters, to CD player reader-writers, and optical interconnects in fiber communication networks. Scientists are now looking toward the future, when tiny micron-sized lasers will form the foundation of petaflops-class computers. One of the first steps in developing an optical interconnect for future high performance computers has been acccomplished by researchers from NASA Ames Research Center's Quantum Optoelectronics Project in the Numerical Aerospace Simulation (NAS) Systems Division.

"Although the petaflop computer is still 20 years in the future, VCSEL (Vertical-Cavity Surface-Emitting Laser) modeling and simulation achieved by NAS and the Quantum Optoelectronics Project (QOP) will one day make the desktop petaflop computer a reality," says Meyya Meyyappan, device and nanotechnology IPT project manager. The goal of the group is to acquire a capability similar to that of computational fluid dynamics for the national optoelectronics industry. Meyyappan believes that, "In the near term, VCSEL research will impact all consumers through the improvement of many high tech devices."

History may confirm Meyyappan's prediction, for during the past 15 years, improvements in personal computer technology have been transferred to numerous consumer products including smaller, higher-powered cell phones, lap tops, and palm-sized organizers. VCSEL technology has started down the same path: companies like Xerox are already looking at VCSELs to improve future generations of high-speed color printers, and Hewlett-Packard is

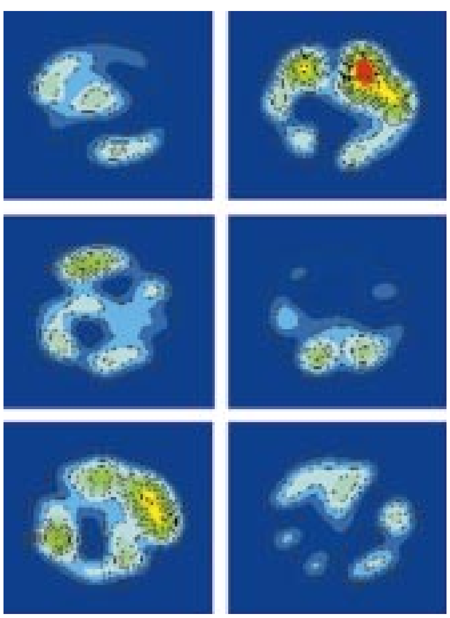


Figure 1: Graphic depiction of a gain guided VCSEL of 20 microns in diameter modulated at 12 GHz displaying the near-field intensity profile, averaged over 20 picoseconds — the pattern changes from one frame to the next. These changes significantly degrade the quality of the interconnect; thus for high speed, large aperture VCSELs, a fully space-time resolved simulation is critical in predicting and designing bandwidth.

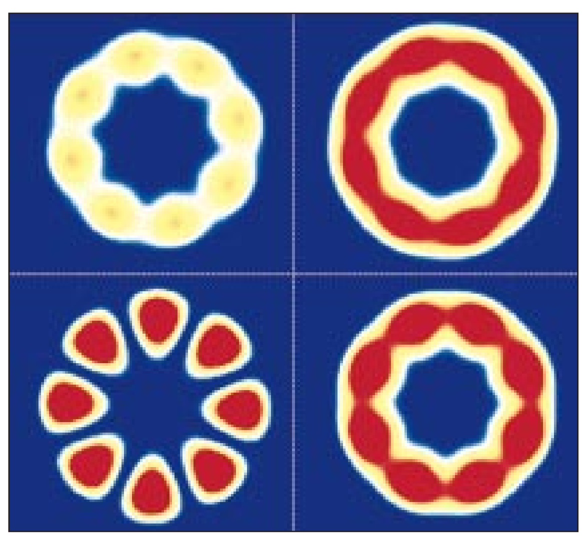


Figure 2: Snapshots of the laser intensity distribution at the VCSEL output facet for the case of a ring contact.

What Are VCSELs?

Lasers come in a variety of shapes and sizes — from the Lawrence Livermore National Laboratories Petawatt laser that has a peak output of a quadrillion watts and is the size of a building, to semiconductor lasers that have output power as small as a few milliwatts. VCSELs, or Vertical-Cavity Surface-Emitting Lasers, represent the most advanced semiconductor lasers at the frontier of today's research efforts.

Regarded as the "transistors" of optoelectronics, VCSELs differ from traditional edge-emitting lasers (EELs) that have dominated semiconductor lasers for almost 30 years. Figure 3 represents the difference between these two types of lasers. VCSELs are the smallest coherent light sources and the most efficient light converters, with an efficiency of around 50 percent from electrical to optical power. Vertical-Cavity means the cavities of these lasers are vertical in relation to the semiconductor wafer. Surface-Emitting means that the light comes out from the surface of the wafer.

VCSELs are typically as small as a few microns both in diameter and length, and offer many potential advantages over EELs: For example, they can be easily tested at wafer-level without costly processing; and fabrication in quantities of tens of thousands per wafer is feasible — as shown in Figure 5 (see page 14). Due to their special configuration, VCSELs have a circular beam output with a very small beam divergence, as opposed to the elliptical beam cross section of EELs. Such circular beams with little astigmatism make them ideal for both free-space coupling to other optical elements and to be effectively launched into optical fibers. In addition, VCSELs have a very low threshold current down to below a milliampere and high bandwidth under modulation. These unique properties combine to make VCSELs ideal for optical interconnect applications.

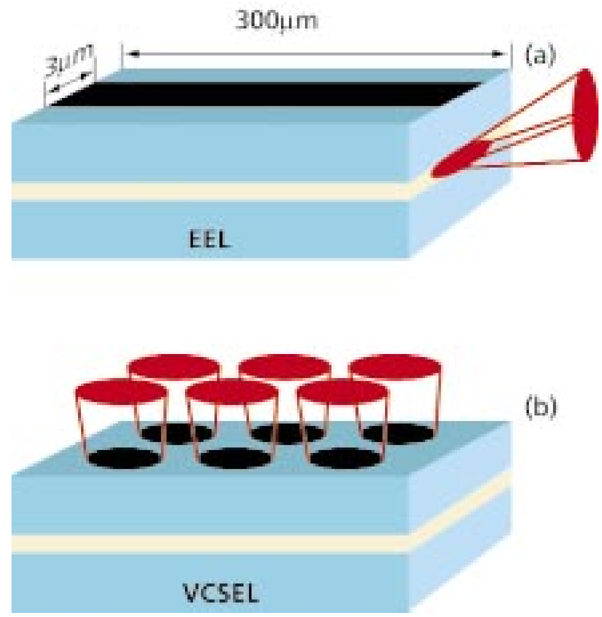


Figure 3: Comparison of a more traditional edge-emitting diode laser (EEL), top, and VCSELs (bottom). Note the EEl laser light comes from the edge of a semicondutor wafer with an astigmatic diverging beam of an elliptical cross section. VCSEL light comes from the wafer surface with a much smaller divergence angle and circular beam cross section. The black areas in both models represent the electrical contacts that define the laser's active regions.

developing VCSEL technology in its next generation multi-gigabit ethernet. Within NASA, optoelectronic devices such as detectors, sensors, and laser-based altimeters and interferometers are already critical elements of space exploration.

As space travel becomes increasingly reliant on information technology (IT), more optoelectronic devices will be employed in future missions. The modeling and simulation tools developed at NAS will directly benefit the design of smaller, higher speed, more radiation resistant, and less power-consuming devices and systems for NASA.

First Step: Modeling and Simulation

Understanding how VCSELs behave enables computer-aided design and optimization of quantum structures before incurring the cost of actual semiconductor wafer growth (see Figure 4, page 14). NASA scientists, in collaboration with Weng Chow of Sandia National Laboratory, Stephan Koch of Philipps-Universitat Marburg, Germany, and Jerry Moloney of the University of Arizona, have developed comprehensive capabilities for simulating microscopic physics within a VCSEL, which forms the basis for VCSEL simulation.

Knowledge gained from this project enables future design and engineering of VCSELs on the basis of first-principle theory, large-scale modeling, and computer simulation. Additionally, today's VCSEL research provides input for the next level of modeling and simulation when predicting and designing future VCSEL-based systems (see Figure 7, page 15).

The QOP team based its current simulation on Maxwell Effective Bloch Equations (MEBEs). Figure 8 (see page 16) shows how this model was constructed using microscopic physics. In this simulation, the MEBEs are solved using the finite difference method with an algorithm developed by QOP scientist Peter Goorjian. The model and the algorithm are flexible enough to handle any shapes in the active region, such as ring, rectangular, elliptical, or circular

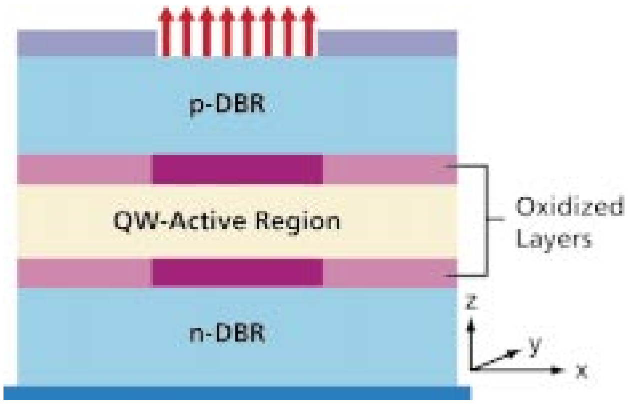


Figure 4: Schematics of a VCSEL: p-DBR and n-DBR are two stacks of semiconductor layers on both sides of the quantum well active region. Typically each stack consists of 20 to 30 pairs of semiconductor layers to achieve near-perfect reflection. The quantum well active region contains quantum wells of a few nanometers in thickness each. The total thickness of the device is a few microns.

contacts. Figure 1 (see page 12) shows representative snapshots of the near-field intensity profile in the x-y plane (compare to Figure 2) in the case of a ring contact.

Using NAS's Computing Power

Numerical simulation of VCSEL equations poses formidable challenges. Fortunately, NAS has considerable computational resources and capabilities in CFD research. These specialized resources and tools — high performance computers, computational algorithms, and methods — position NAS to perform comprehensive, large-scale simulations of optoelectronic devices.

Once the QOP team wrote the VCSEL computational code, they discovered that additional computing power, beyond a single CRAY C90, was needed. The team contacted Samson Cheung, a NAS scientific consultant who assists NASA scientists and researchers in academia and industry in getting the most from the NAS Facility's computing assets.

"When the VCSEL computational code was handed to me, it was written to run on the Cray computer," relates Cheung. "It was not a parallel code — it was coded for one CPU to make the computations in a serial manner. I ran one test computation of a VCSEL cycle, and it took .04 seconds per time step on the Cray. Considering that the VCSEL modeling project involved two million time steps to complete a single calculation — that would have taken one Cray working non-stop for 24 hours."

"I modified the code for the SGI Origin 2800, *Lomax*, essentially instructing the computer to divide the task between not one, but 16 CPUs running simultaneously. This reduced the compute time for a test equation from 4 minutes on the Cray to 10 seconds on *Lomax*. Using an SGI Origin 2000 with 16 CPUs took the calculation from a day's work down to one hour."

Cheung notes that a direct benefit of this teamwork within NAS is that the parallelization improvements have made the VCSEL computational code portable, and it can now be run on any Cray, SGI Origin 2000, or Sun Microsystems Starfire high performance computer. This portability allows industry and academia the opportunity to incorporate the QOP team's findings into other VCSEL research.

Extending NAS's current modeling and simulation capability, the team is now studying thermal effects and electronic transport across multilayer structures. The quantum optoelectronics team is working on a model that couples different temperatures to the rest of the laser model, so that a comprehensive, yet computationally manageable VCSEL model can be developed.

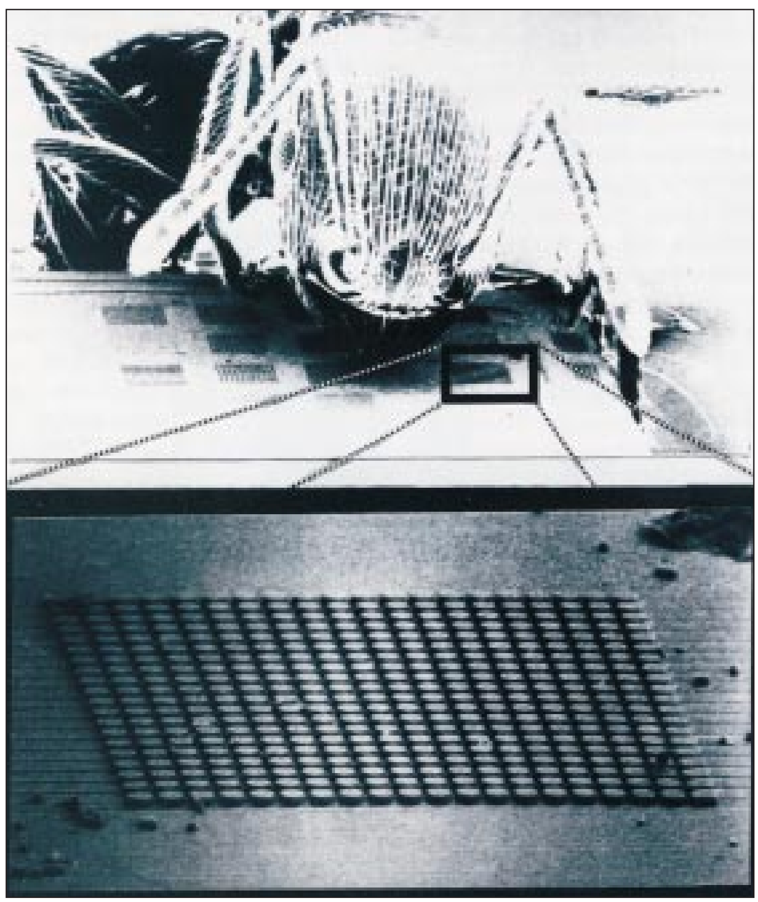


Figure 5: Magnified thousands of times, an ant peers down at a VCSEL array. A single array has been enlarged and shows that each array is composed of nearly 400 VCSELs. (A. Scherer, from Harbison and Nahory, "Lasers, Harnessing the Atom's Light," *Scientific American,* 1998)

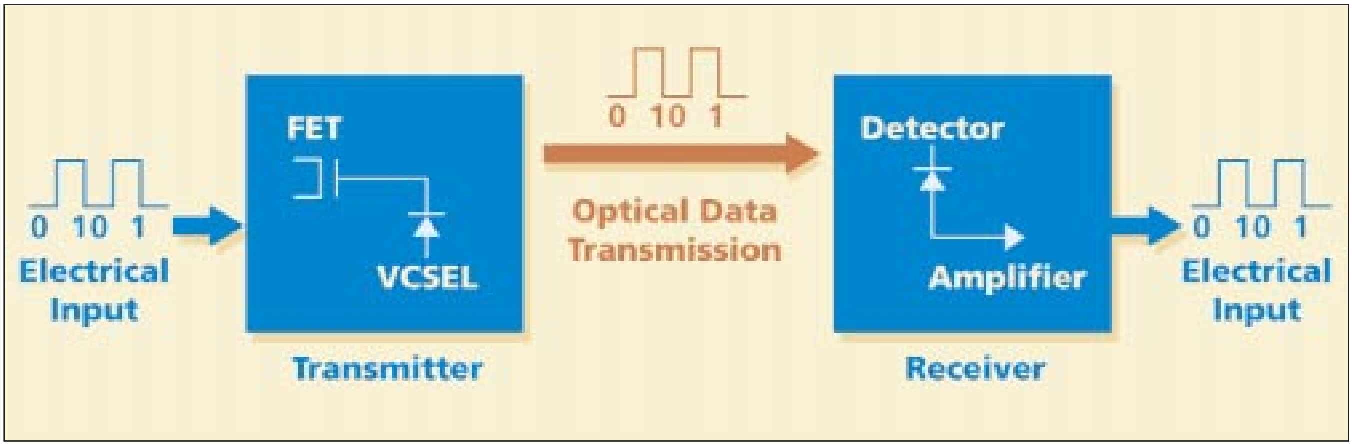


Figure 6: VCSEL-FETs (Field Effect Transistors) are integrated device-based optical interconnects. The input electrical signal is converted to optical signal through the VCSEL-FET cell. The optical signal can be transmitted through optical fiber (as in telecom or datacom) or in free-space (as inside a computer).

Molding Tomorrow's IT

Many future IT applications, such as high-speed switching or data transmitting in local area networks, will rely upon optical interconnects based on VCSELs (see Figure 6). The advantage of such interconnects over Edge Emitting Lasers (EELs) is that VCSELs can be easily integrated with traditional electronic devices such as field effect transistors, or by wafer bonding technology with a complementary metal-oxide-silicon (CMOS) circuit, to form smart-pixel arrays.

Smart-pixel arrays with hundreds of VCSELs have been demonstrated with a single channel speed of up to 1 gigahertz (GHz) per second, resulting in a total throughput of up to 100 gigabits (Gb) per second. Using smart-pixel arrays will allow integration of laser driver circuits, photo detectors, and CMOS circuits — all within a very compact area — and will eventually lead to very large-scale integration of photonics and optoelectronics integrated circuits.

While Moore's law states that computer chip power doubles every 18 months, a similar law for optical communication declares that bandwidth doubles at least every year. To maintain such a rate of increase in bandwidth, both per-channel speed and the number of channels must be increased. Current mainstream transmitters for optical communication are based on either light emitting diodes (LEDs) or high-speed EELs. Although LEDs have advantages of easy packaging and low cost, they have lower modulation speed. EELs have high modulation rates, but are difficult to build with high-density, two-dimensional arrays. VCSELs combine the advantages of both. The same VCSEL-based smart-pixel arrays are used for telecom and datacom, both in high-speed switching networks and as high-speed, parallel transmitters or transceivers. As the 1.3 and 1.5 micron meter VCSELs become mature and competitive, VCSELs will play an important role in the telecom industry.

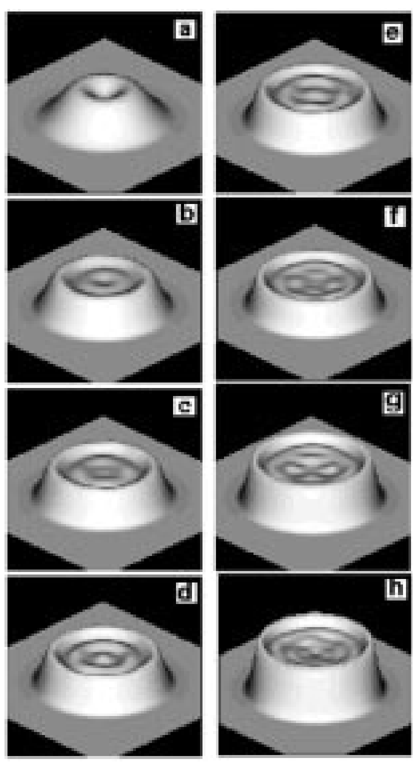


Figure 7: Near-field intensity profiles for an index-guided VCSEL of 15 microns in diameter, averaged over 1.38 nanoseconds, for a series of increasing pumping levels from left to right. As indicated, the individual patterns look much more regular after the average, and resemble the "modes" typically measured in a large aperture VCSEL. The time evolution of these "modes" on shorter time scales, are, however, much more irregular and complex than those shown in Figure 1.

The QOP team predicts that within the next few years, VCSEL-based optical interconnects will be an integral part of multi-gigabit local area networks, allowing fast communication between workstations and leading to high throughput workstation clusters. In addition, VCSEL-based switching networks, optical logical elements, amplifier, and routing devices are all being pursued to eventually create all-optical digital or analog computers. Optical

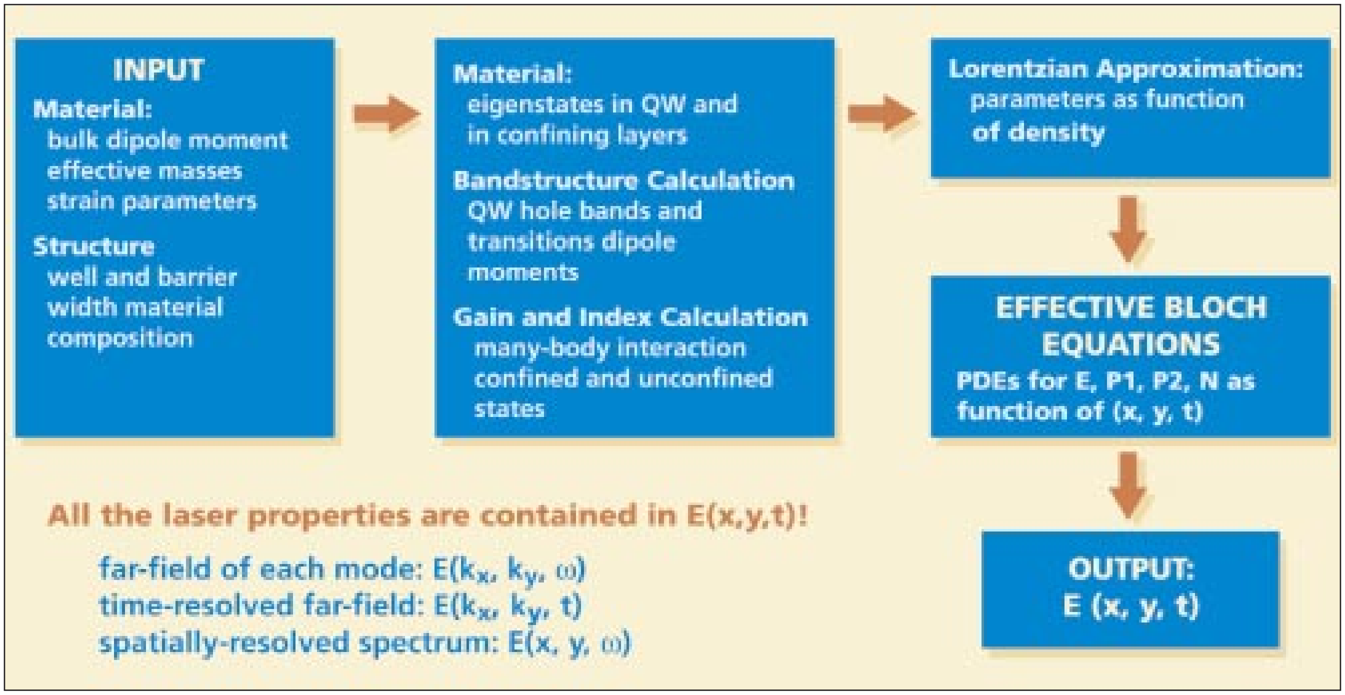


Figure 8: This flow chart details the bottom-up approach in semiconductor laser modeling and simulation as employed by Ning and his colleagues at NAS. The simulations are based upon Maxwell Effective Bloch Equations (MEBEs).The MEBEs are solved using the finite difference method with an algorithm developed by QOP scientist Peter Goorjian. The modeling simulation and the algorithm are flexible enough to handle any shapes in the active region, such as ring, rectangular, elliptical, or circular contacts.

computers promise many advantages such as high parallelism, higher speed, and three-dimensional architectures, and are still in the early stage of development.

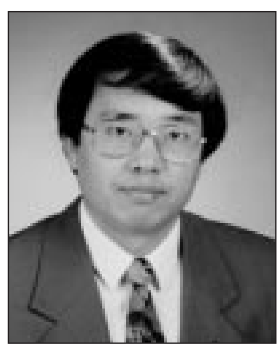
The Future

Computational optoelectronics researchers are facing the same challenges that CFD and computational electronics faced some decades ago. The worldwide optoelectronics industry is growing at a phenomenal speed, mainly fueled by the insatiable demand for high-speed networks, high-speed computing, and high-density data storage. As the industry continues to grow, and as the devices and systems become increasingly complex, the need for design and simulation tools will continue to expand. To meet this challenge, NAS scientists have taken a position of leadership in optoelectronics research by expanding the knowledge base for the development of tomorrow's quantum optoelectronics industry.

"NAS has outstanding computers, and NASA has the technology and the smart people who have solved partial differential equations using complex algorithims on a variety of platforms," says Meyyappan. "Working with other quantum optoelectronics researchers, the QOP team will make significant advancements in VCSEL technology. As scientists, we are at the right place at the right time to make great contributions to the science of quantum optoelectronics." gp

Acknowledgements

VCSEL modeling and simulation efforts are part of the Computational Quantum Optoelectronics research in the science and technology group led by T.R. Govindan. The project is part of the Devices and Nanotechnology Integrated Product Team (IPT) managed by Meyya Meyyappan. Peter Goorjian, Samson Cheung, and Jianzhong Li are also involved in VCSEL modeling and simulation.



Cun-Zheng Ning is a senior research scientist in NAS's science and technology group. He obtained his Ph.D. in theoretical physics from the Institute for Theoretical Physics and Synergetics, University of Stuttgart. Previously, he was a research assistant professor at the University of Arizona. Ning has published more than 60 papers and has presented many invited talks in Europe and the U.S. He has served as chair or technical committee member of numerous international conferences. Ning was awarded the Ames Director's Discretionary Fund in 1998 and 1999. He can be reached at: cning@nas.nasa.gov.

NAS Systems Division's 1999 Achievements and Awards

NAS's high performance computational resources brought a number of new technologies to fruition during the last year of the decade.

The NAS Systems Division's activities during 1999 reflect the diversity, drive, and determination of an organization adapting to change while making significant strides in new technologies. The division expanded its high performance computing power, which enabled numerous research projects to achieve their goals. By forming partnerships with industry, academia, and other NASA centers, the division is striving for a leadership position in the future of high performance computing.

NAS Y2K Compliance: No Incidents

Work on the year's first milestone began on January 11, 1999, when the NAS Y2K team, headed by Bill Thigpen, began a four-day test of the division's systems for compatibility with the millennium date change. This involved resetting all computers and monitoring the date rollover of the CRAY C90 and J90 computers as well as the SGI Origin cluster, the NAStore mass storage system, the Portable Batch System, and other databases, networks, and web servers. The test team successfully validated that all systems would provide trouble free operation in the new millennium. The year-long effort was concluded January 10, 2000, giving the Y2K team additional time to meet any date rollover-related computer issues.

Storage System Replaced

NAStore, the division's mass storage system, was comprised of two non-Y2K compliant Convex systems and occupied about one-third of the NAS Facility's machine room. In February, the high speed processor group, led by Alan Powers, began work to replace NAStore with two SGI Origin 2000-based systems: *S1*, an eight-processor Origin 2100 capable of storing nearly 600 gigabytes of information; and *Lou*, a 12-processor Origin 2400 system that maintains nearly three terabytes of data and is linked to a pair of RAID disks — a set of disks that are coupled to a

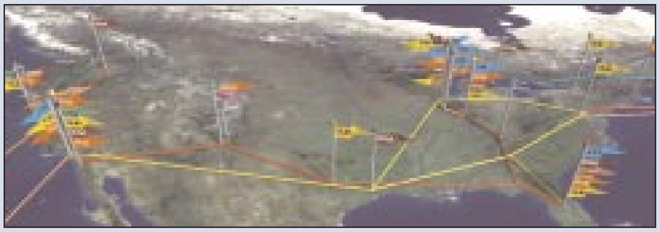
parity disk. (If one disk fails, the parity disk takes over and the data is reconstructed, eliminating down time for disk replacement and data restoration.) The efforts to prepare for and convert the NAStore system to an Origin-based platform have brought the division a faster, more reliable data storage center.

Information Power Grid Achievements

Researchers at NAS have been working in collaboration with numerous high performance computing centers to develop the Information Power Grid (IPG). The grid is a distributed, high-performance computing infrastructure that manages a group of geographically distant computers and interfaces, storage devices, and workstations. A prototype grid, launched in October, is now up and running and links the NAS Facility with NASA's Langley and Glenn Research Centers, as well as the Department of Energy's Argonne National Laboratory in Illinois, and the Information Sciences Institute (ISI) at the University of Southern California.

Grid Forum Launched

The NAS Facility and Argonne National Laboratory cohosted the first Grid Forum Workshop, held at Ames Research Center June 16-18, where more than 140 researchers from industry, academia, and government sites gathered to determine how the grid would operate, and to establish what infrastructure was needed. Using Globus, the high-performance computer interface software, computers will be able to communicate with each other, and



Grid Forum participants agreed that a user guide should be developed. Fielding input from NASA's IPG community and other grid collaborators, NAS's Pam Walatka produced the *Globus Quick Start Guide*, which includes the basics for setting up an account and running a job. Copies were distributed at SC99, and the document is available online at:

http://www.nas.nasa.gov/~walatka/QuickStart.pdf

Grid Service Software Under Development

Additional grid infrastructure development saw NAS researchers team with Argonne and the NCSA to develop the Grid Information Service. This policy-based tool will provide guidelines for user accounts, simplify a user's interface with the IPG, provide access control for grid resources, and store information on the jobs that have already been run.

512-Processor SGI Origin 2000 Debuts

NAS and SGI demonstrated the world's largest single system image supercomputer at SC99 in November. "With the SGI 2800 system, a team of engineers can evaluate the

Lomax

performance of aircraft or space vehicle concepts early in the design process. The end result is that better design decisions can be made, ultimately leading to much better vehicles at a lower cost," says Henry McDonald, Ames center director. Designated *Lomax*, after NASA Ames computational fluid dynamics (CFD) pioneer Harvard Lomax (1922-1999), this 512-processor SGI 2800 shared memory system is a dynamic new tool for NAS Facility researchers. Overflow-MLP (Multi-Level Parallelism), a production CFD code, was modified to run on *Lomax* by NAS scientist Jim Taft. The 512-processor has enabled the code to model a 35-million-point CFD problem in less than two hours. This performance is roughly 32 times faster than the CRAY C90, and it is done at 75 percent of the C90's cost.

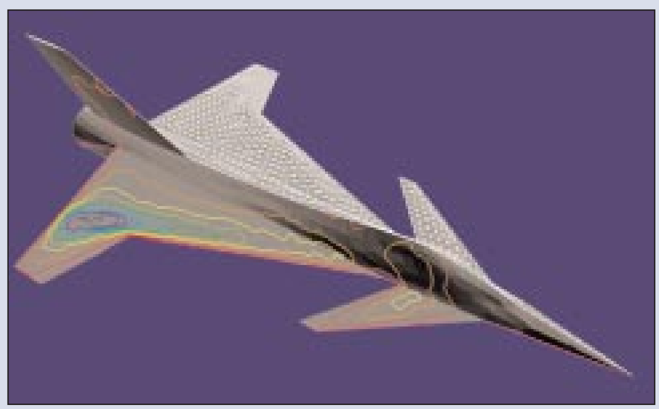
Nanotube Biosensors Developed for Cancer Research

Another division research project is the development of novel carbon nanotube-based molecular electronic biosensor technology. This science will detect specific DNA sequences of cancer cells, and aims at early clinical detection and diagnosis of cancer. Results of these experiments will also be used by NASA's astrobiology program.

Biosensor research is also the first step in building future molecular electronics computers in which nanotubes and DNA will be essential computing elements in the form of an electronically modulated DNA/nanotube chip. Nanotubes will effectively connect electronics and biomolecules for biological sensing and information processing.

Software Releases: FEL and GLIC

The Field Encapsulation Library (FEL) is a C++ library for representing fields and meshes. FEL supports existing



Langley Research Center/T. Sandstrom, P. Moran

applications, such as the Virtual Wind Tunnel, as well as the rapid development of new applications including visualization tools for problem solving environments.

The January release of FEL version 2.1 features: compatibility with NAS's VisTech library, a set of visualization techniques supporting rapid applications development; upgraded support for large data handling via paged mesh and field classes; and modifications and extensions for compatibility with Windows NT. Patrick Moran of the NAS data analysis group headed the design team. (Version 2.2 was released in January 2000.) The beta version of GLIC (Graphical Line Integral Convolution), an interactive flow visualization software, was also released. This software features LIC (Line Integral Convolution), a visualization technique that can effectively convert numerical flow simulation results into animated surface textures to depict steady and unsteady flow directions. This helps scientists discover important flow features. Users from NASA and industry are now employing the software.

NAS Researcher Wins Best Paper at SC99

Rupak Biswas of the NAS Systems Division's algorithms, architectures, and applications group, and co-author Leonid Oliker of the National Energy Research Scientific Computing Center, were awarded SC99's prestigious Best Paper Award. Their study, titled "Parallelization of a Dynamic Unstructured Application Using Three Leading

Lenny Oliker, center, and Rupak Biswas, right, received SC99s' "Best Paper" award. Bob Borchers, left, from the National Science Foundation was the presenter.
(Steve Reed, Oscar and Associates)

Paradigms," reported their comparison of a mesh adaptation code run on the CRAY T3E, SGI Origin 2000, and the Tera MTA computers (see *Gridpoints*, Winter 1999, page 12). Steven F. Zornetzer, director of Information Systems at Ames, said: "Biswas' work is a strong indication that NAS has been revitalized and is leading the efforts in high performance computing for the 21st century."

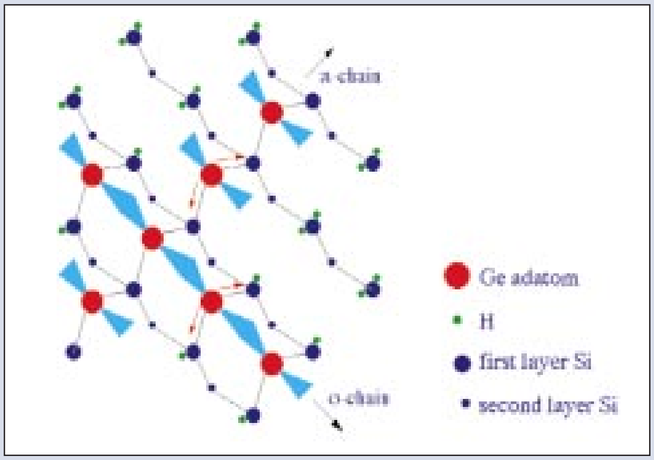
Global File System Workshop

The NAS Systems Division, in cooperation with the Parallel Computer Systems Laboratory at the University of Minnesota, coordinated and hosted the Global File System Workshop on March 5-6, 1999, as a follow-on to the Linux World event held in Silicon Valley.

Approximately 70 participants attended, including vendors, users, and researchers interested in building high performance input/output and storage systems using open source operating systems such as Linux. Presentation slides can be viewed online at:
http://www.globalfilesystem.org/Pages/workshop_slides.html

Atom Manipulation Technology Patent

On June 4, Toshishige Yamada, a member of NAS's semiconductor device modeling team, filed a patent application for his research in atom manipulation technology titled "Atomic-Scale Electronic Devices and Methods Of Fabrication." Yamada's research into atomically precise



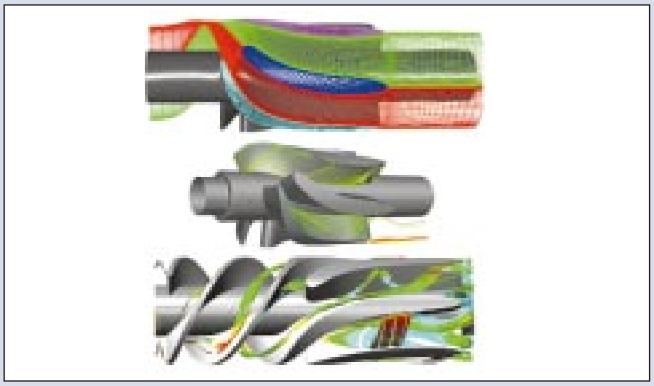
structures for electronics applications shows how an atomic structure can be chemically bonded to a substrate without the occurrence of an electrical short circuit. The patent, which is currently pending, also provides a list of preferred combinations of atoms and substrates that provide excellent isolation properties. In addition, Yamada published two papers on the technology; T. Yamada, C. W. Bauschlicher, Jr., and H. Partridge, "Substrate for Atomic Chain Electronics," *Physics Review*, June 1999; and T. Yamada, "Substrate Effects on Electronic Properties of Atomic Chains," *Journal of Vacuum Science Technology*, July/August 1999.

Photonic Switching Device Patent Granted

On October 5, NASA was granted a patent titled "Photonic Switching Devices Using Light Bullets," an invention by Peter Goorjian of the NAS science and technology group. The patent proposes an ultra-fast, all-optical switch made with nonlinear optical materials, in which colliding light bullets form the basis of the optical switch. These switches may be used to make logic devices and optical interconnections for data processing. Light bullets are expected to improve data transmission from the current electronic means of approximately 50 gigabits per second to an expected rate for optical means of over one terabit per second. The patent was based partially on Goorjian's earlier computer simulations of light bullets. Recent laboratory experiments suggest that "there is a stable regime where light bullets may exist," says Goorjian.

Patent Awarded For Heart Assist Device

On September 7, Houston's Baylor College of Medicine, Johnson Space Center, MicroMed Technology Inc., and



NAS researchers Cetin Kiris and Dochan Kwak were granted a patent for improvements made to the DeBakey Ventricular Assist Device. Using CFD technology, Kiris and Kwak substantially improved the performance of the device. The project's ultimate goal is an implantable unit that will become an alternative to heart transplant surgery. For more on Kiris and Kwak's work, see page 4.

The achievements in science and technology within the division are numerous and cover a broad spectrum. Research work completed in 1999 forms the building blocks for tomorrow's technological advances.

To view additional NAS Facility achievements, research papers, and highlights visit our new website: http://www.nas.nasa.gov

—Nicholas A. Veronico

NAS 1999 Technical Reports

Technical reports are one of the ways NAS Facility researchers share their work with others in the scientific community. A large number of reports are available electronically in PDF format at the division's web site, including an archive dating back to 1998. To learn more about NAS research, visit: http://www.nas.nasa.gov/Research/Reports/reports.html

Energetics and Dynamics of GaAs Epitaxial Growth Via Quantum Wave Packet Studies
Author: Fedor Dzegilenko
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-001-abstract.html

Visualization, Extraction and Quantification of Discontinuities in Compressible Flows
Author: Ravi Samtaney
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-002-abstract.html

A Method to Solve Interior and Exterior Camera Calibration Parameters for Image Resection
Author: Ravi Samtaney
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-003-abstract.html

Efficient Parallelization of a Dynamic Unstructured Application on the Tera MTA
Author: Rupak Biswas
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-004-abstract.html

Automatic Molecular Design Using Evolutionary Techniques
Authors: Al Globus, John Lawton, Todd Wipke
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-005-abstract.html

AsterAnts: A Concept for Large-Scale Meteoroid Return and Processing using the International Space Station
Authors: Al Globus, Bryan A. Biegel, and Steve Traugott
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-006-abstract.html

Measurement of a Scientific Workload using the IBM Hardware Performance Monitor
Author: Robert J. Bergeron
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-007-abstract.html

BSD Portals for LINUX 2.0
Author: David McNab
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-008-abstract.html

Simplified Discontinuous Galerkin Methods for Systems of Conservation Laws with Convex Extensions
Author: Timothy J. Barth
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-009-abstract.html

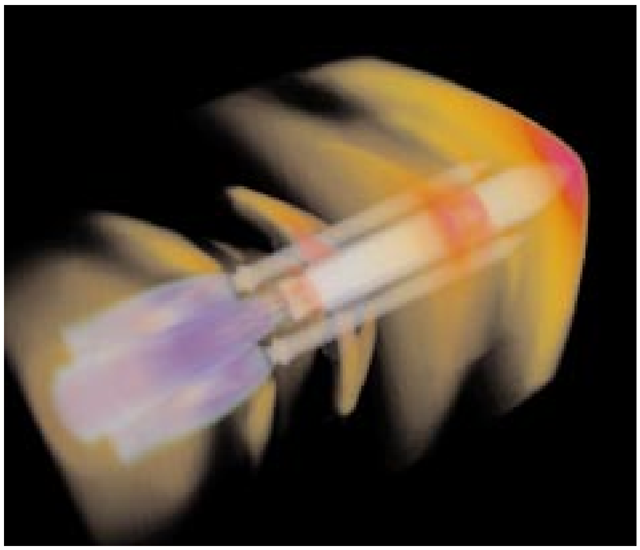
A Posteriori Error Estimation for Discontinuous Galerkin Approximations of Hyperbolic Systems
Authors: Timothy J. Barth, Mats G. Larson
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-010-abstract.html

The OpenMP Implementation of NAS Parallel Benchmarks and Its Performance
Authors: Haoqiang Jin, Michael Frumkin, Jerry Yan
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-011-abstract.html

Automatic Data Distribution for CFD Applications on Structured Grids
Authors: Michael Frumkin, Jerry Yan
www.nas.nasa.gov/Research/Reports/Techreports/1998/nas-98-012-abstract.html

Calendar of Events

April 3-5 — Moffett Field, California
Astrobiology Science Conference: NASA Ames will host an international conference on astrobiology science to be held this spring at NASA Ames Research Center in the Moffett Conference and Training Center. The focus of the meeting is on scientific results that illustrate the broad multidisciplinary nature of astrobiology. This conference will complement other, more narrowly focused meetings that deal primarily with one or two subdisciplines of astrobiology. Further details are available on the conference website at: http://astrobiology.arc.nasa.gov/


Reynaldo J. Gomez – NASA Johnson Space Center

May 1 — Cancun, Mexico
Heterogeneous Computing Workshop: This seminar is run in conjunction with the International Parallel and Distributed Processing Symposium, and is co-sponsored by the IEEE Computer Society and the U.S. Office of Naval Research. For more information, visit: http://myrtle.cs.umanitoba.ca/hcw/

May 1-5 — Cancun, Mexico
International Parallel and Distributed Processing Symposium (IPDPS 2000): Co-sponsored by IEEE Computer Society and the Association for Computing Machinery. Information is available at: http://www.ipdps.org/

May 8-11 — Sante Fe, New Mexico
International Conference on Supercomputing: Sponsored by the Association for Computing Machinery Special Interest Group on Computer Architecture. Additional details are available at: http://www.ics.uci.edu/~ics00/

June 3-4 — San Francisco, California
The Java Grande Conference focuses on the use of Java in the broad area of high-performance computing; including engineering and scientific applications, simulations, data-intensive applications, and other emerging application areas that exploit parallel and distributed computing or combine communications and computing. The conference is sponsored by the Association for Computing Machinery. For information, visit:
http://www.extreme.indiana.edu/java00

June 26-29 — Las Vegas, Nevada
The International Conference on Parallel and Distributed Processing Techniques and Applications will be held concurrently with the first International Conference on Internet Computing and The International Conference on Imaging Science, Systems, and Technology. In addition, during the same time frame, The International Conference on Artificial Intelligence and the International Conference on Communication in Computing will be held at the same convention site. Full details are available at: http://www.cs.umanitoba.ca/~iwic/

July 13-15 — Palo Alto, California
The Second NASA/DoD Workshop on Evolvable Hardware, sponsored by NASA and the Defense Advanced Research Projects Agency, will be held at The Crowne Plaza Cabana, Palo Alto, California. The event is co-hosted by Ames Research Center's Information Sciences and Technology Directorate and Jet Propulsion Lab's Center for Integrated Space Microsystems.

Evolvable hardware is an emerging field that applies simulated evolution to the design and adaptation of physical structures, particularly electronic systems. Application techniques enable self-reconfigurability and adaptability of programmable devices and have the potential to significantly increase the functionality of deployed hardware systems. Moreover, these techniques have the potential to reduce costs by automating numerous design and optimization tasks encountered in engineering design.

A focus of this year's workshop is real-world applications of evolvable hardware. Current application areas include adaptive and reconfigurable computing, circuit and antenna design, and evolutionary robotics. Evolvable hardware methods could also be effective in dealing with increased complexity and reliability requirements in areas such as sensors, MEMS, biomolecular design, quantum computing, and nanoelectronics.

More information about the workshop can be found at: http://ic.arc.nasa.gov/ic/eh2000