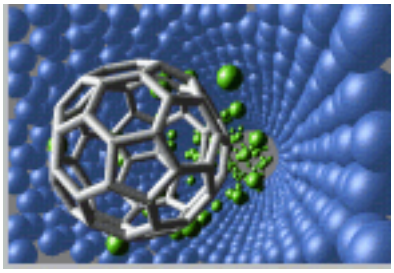
Special Issue:

High Performance Computing Research



In an era of ever restricted budgets, the criterion -- "smaller, better, cheaper" -- is being ruthlessly applied to the design and manufacture of a broad range of products, from complex scientific tools to consumer goods. A government-wide initiative (known as "High Performance Computing Research") has been formed to study these challenges. The NAS Systems Division is investigating solutions in three research areas: petaflops computing, semiconductor device modeling, and molecular nanotechnology.

Need for Computational Simulations Brings Advanced Technologies to Ames

by David H. Bailey

As manufacturing systems increasingly enter the nanometer (10-9 meter) range, the need for computational simulations to understand underlying physical phenomena is acute. The newly created NASA Ames nanotechnology initiative envisions Ames Research Center as the focus of a nationwide network of research laboratories using computation to understand and ultimately control manufacturing processes at smaller and smaller sizes, culminating in atomically precise products.

In the medium term, significant advances can be expected in computing technology as Ames works with Silicon Valley firms, computer vendors, and universities to remove technological barriers that may impede computer hardware progress during the next few years. In the long term, it is expected that petaflops computer systems, atomically precise manufacturing techniques, and other devices developed in this program will revolutionize space launch systems, climate modeling, spacecraft instrumentation, aeronautical design, planetary exploration, and computer manufacturing.

Development of Future Space Vehicles

One example of an important future NASA application of this technology is the development of autonomous intelligent vehicles for the exploration of the solar system and beyond. Since radio signals require up to 40 minutes for a round trip from Mars to Earth, NASA cannot rely solely on ground-based personnel or computers to control Mars-bound spacecraft or Mars-roving robots. An intelligent on-board computer, with sufficient power to ensure reliable real-time operation, is required. For missions to other planets -- or to the stars -- even more powerful computer systems will be required. These systems need to be exceedingly compact in size, highly resistant to radiation damage, and use very little electrical power. Most importantly, they must be affordable in an atmosphere of increasingly tight budgets.

Future spacecraft will also need advanced scientific instruments, such as image sensors, microwave receivers, light spectrometers, mass spectrometers, chemical analyzers, and interferometers -- all of which must be more compact, reliable, and economical than is feasible with current technology. Further, such instruments may require novel designs, such as those inspired by biological systems.

At the same time, the transportation costs of placing humans and equipment into space must be reduced by at least two or three orders of magnitude if large-scale human exploration and development of space is to begin. Much stronger, lighter, and more affordable materials are needed for constructing these

vehicles. One of the more promising approaches is to employ molecular nanotechnology to construct diamondoid materials, which could potentially feature several times the payload-to-launch-weight ratio achievable with titanium. (See related article.) "Smart materials" technology, which can instantly adapt to changing environments, is another intriguing possibility. However, futuristic technologies such as this probably will not be feasible and affordable for at least two to three decades.

Future Missions Need Teraflops, Petaflops

By the year 2010, many important future NASA missions will rely on extra-high performance computer systems, including climate modeling, processing of Earth-observing satellite data, space engineering, aeronautical design optimization, and astrophysics. Each of these areas offers worthwhile applications that today could utilize systems capable of sustained performance rates approaching one teraflops (Tflop/s, or 1012 floating-point operations per second). Future missions are projected to require one petaflops (Pflop/s, or 1015 floating-point operations per second), and beyond.

Unfortunately, it is not certain that the U.S. computer industry by itself will be able to deliver such products in the desired time frames and at acceptable cost. At present, the industry is facing daunting technical challenges just to maintain its current rapid pace of progress. In addition, the scientific computing marketplace is now emphasizing low- and mid-level systems rather than the high-end systems required for key NASA missions. Achieving the ultra-high performance levels (with comparable amounts of memory) needed in the next decade will require major breakthroughs in computer hardware technology, as well as novel architectures, advanced system software, along with programming facilities, innovative algorithms, and clever implementation techniques.

Program Looks at Future Requirements

In light of these challenges, NASA Ames has recently instituted a new program in nanotechnology and advanced computing technologies to ensure that NASA will be able to meet its future requirements in high-performance computing, advanced scientific instruments, and advanced materials and manufacturing technology. The NAS Systems Division, along with other organizations at Ames, has a reservoir of talent and resources that will be leveraged to create a leading center in computer simulations of ultra-small systems.

As part of this program, those involved in the petaflops computing activity will explore designs of computer systems capable of performing at a rate of one Pflop/s by 2010. Issues to be addressed include device components and technology, architectures, system software, algorithms, and applications, and research is being targeted in these areas. The NASA petaflops effort will be conducted as part of the High Performance Computing Research program, an inter-agency initiative now being organized under the auspices of the High Performance Computing and Communications Program to pursue research and development aimed at future high-end systems.

Another component of the Ames plan is an activity to enhance progress in semiconductor technology by

using highly parallel computer systems to simulate semiconductor devices, in partnership with researchers at universities, including Stanford and the University of California, Berkeley, and corporate research labs. In spite of the obvious need for highly parallel computing as a simulation and design tool in this arena, there has been relatively little utilization of parallel systems, up to now. Among the principal impediments are access to parallel testbeds, usable software, and expertise in parallel computing. The Ames program will help remove these impediments.

Later -- Molecular Manufacturing

Looking further into the future (2005 to 2020) Ames is pursuing a program in computational nanotechnology. In this activity Ames scientists are investigating, by means of computational simulations on high-performance computer systems, the future production of components and materials by molecular manufacturing. Two long-term goals have been proposed: the detailed design and simulation of "nanotechnology replicators" (for example, self-assembly systems), and the development of a molecular manufacturing computer-aided design system.

Related to the computational nanotechnology activity, which focuses on molecular (or "dry") nanotechnology, is an activity in biological nanotechnology (also called "neuro-nanotechnology" or "wet nanotechnology"). This activity involves the computer-aided development of sensors and computer devices based on biological models. Recent successes in the latter field, such as the development of an artificial retina, suggest potential for valuable NASA applications. The long-term objective is to abstract principles from biological systems to produce computer devices, sensors, and intelligent computer systems that replicate human analytical power and versatility.

Emphasis on `Potential'

It should be emphasized that at present it is by no means certain when atomically precise molecular manufacturing will be possible, so potential applications are still somewhat speculative. Still, enough progress has been made, particularly in recent laboratory demonstrations of atomic manipulation, that molecular nanotechnology appears to be worth serious investigation by NASA.

Computational Support at NAS

Overall, it is expected that the majority of the program's research work will be performed outside NASA, either by grants and cooperative agreements monitored by NASA scientists, or by scientists sponsored through their own organizations or other government grants, with computational support provided by the NAS Program. There are no plans to do experimental work or produce any materials, computer devices, or commercial-grade software. Instead, the focus will be on basic research, the results of which will be transferred through publications and prototype computer programs to computer and software vendors, aerospace firms, and other NASA centers for subsequent use in its missions.

The program will be re-evaluated in the year 2000 to see if further staffing, grant, or contract funding should be pursued.

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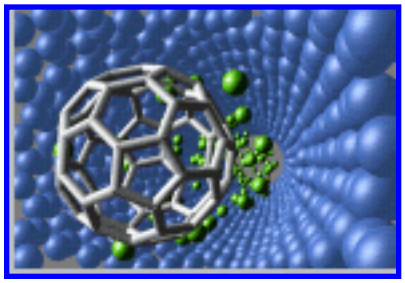
Device Modeling Holds Key to Future NASA Missions



by Elisabeth Wechsler

"Unless there are major breakthroughs in semiconductor technology, NASA's future space missions will be imperiled," observed scientist David Bailey in his introductory remarks at the NAS-sponsored Semiconductor Device Modeling Workshop, March 28-29. What is needed are "very high density (ultracompact) systems with very high reliability and performance that can be built at very low cost -- no one will buy a petaflops computer for $500 million."

Among the important technical challenges facing semiconductor manufacturers, according to Bailey, are two that the NAS Systems Division is particularly well-positioned to help tackle:

- performing accurate 3D simulations of physical effects
- porting advanced TCAD [technology CAD] software to highly parallel systems

`Complementary Role' to Other Programs

"We see our role as complementary with industry and other government research programs," Bailey explained. To that end, he views Ames as Silicon Valley's government laboratory, and proposes research cooperation with local semiconductor manufacturers, universities, and other government labs.

The NAS initiative in semiconductor device modeling (see *Need for Computational Simulations Brings Advanced Technologies to Ames*) includes access and computer time on parallel supercomputers for selected researchers.

In terms of setting NAS's priorities in this area, Bailey mentioned: studying classes of devices critical to future NASA missions; conducting basic research to understand physical effects that may limit future devices; performing landmark computations not previously possible; testing device modeling codes on parallel systems configurations not otherwise available to researchers; comparing performance of various vendor systems on device codes; and porting key multi-vendor design codes to highly parallel systems.

Bailey commented that the following use of NAS capabilities would "probably not be appropriate": production runs using conventional single-processor codes; production runs using proprietary codes for

commercial vendors; and production runs for projects sponsored by other government agencies "when adequate computational resources are already provided."

Diverse Representation at NAS Workshop

About 110 participants from Silicon Valley computer manufacturers, as well as academia and Ames Research Center, attended the two-day program, which focused on a broad range of topics. Presentations were given by 23 invited speakers from -- among others -- IBM, Intel Corp., Sun Microsystems Inc., Lawrence Livermore and Lawrence Berkeley national laboratories, Stanford University, and University of California, Berkeley.

Workshop presentation topics included:

- "Challenges in Computational Prototyping of Deep Sub-micron Integrated Circuit Technology" (Robert Dutton, Stanford University)
- "Modeling in the Sub-0.07 Micron Gate Length Regime" (David Ferry, Arizona State University)
- "TCAD at National -- A Study in Diversity" (Ronald Goossens, National Semiconductor Corp.)
- "Predictive Simulation Tools and Techniques for Silicon Technology Research, Development, and Manufacture" (Mark Pinto, Bell Laboratories and Lucent Technologies)
- "Level Set Methods for Etching, Deposition, and Photolithography Development
- (James Sethian, Lawrence Berkeley National Laboratory)
- "Issues in the Parallelization of Large-scale Semiconductor Device Simulators" (Bruce Herndon, Stanford University)
- "Parallel and Distributed Computing for Monte Carlo Device Simulation" (Henry Sheng, University of California, Berkeley)
- "Modeling and Simulation Issues in Next Generation Integrated Circuit Development" (Francisco Leon, Intel Corp.)
- "Computational Modeling of Ultrafast Optical Pulse Propagation in Nonlinear Optical Material" (Peter Goorjian, NASA Ames Research Center)
- "Large-scale Application Issues for Full Band Monte Carlo Simulation of Semiconductor Devices" (Umberto Ravaioli, University of Illinois, Champaign-Urbana [paper only])

Hard-copy proceedings and/or videotapes for workshop presentations are available at no charge. Send an email request with your postal address to **doc-center@nas.nasa.gov**.

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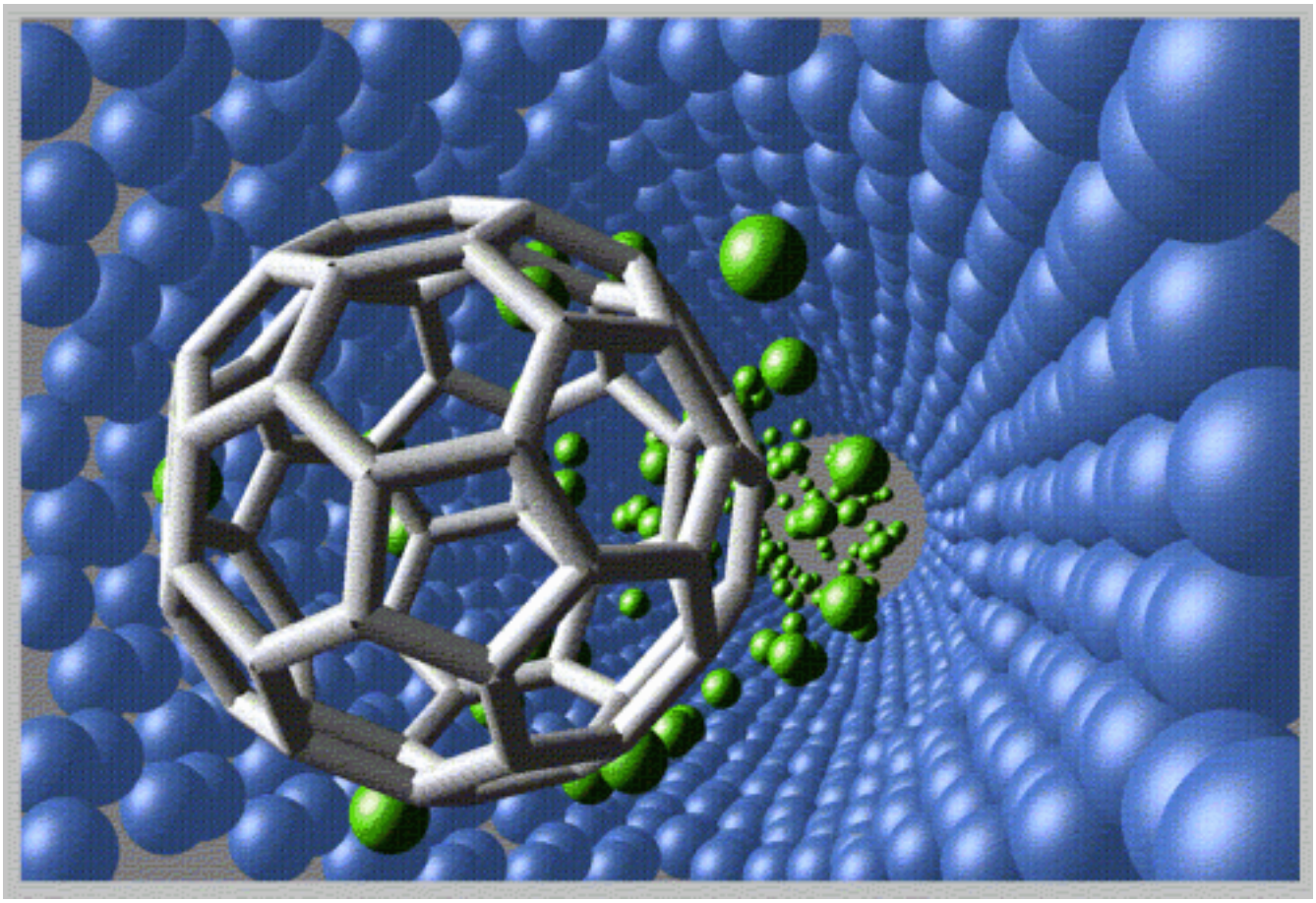

Close-up of a simulation of a buckyball and helium atoms passing through a graphite nanotube. The blue spheres are carbon, the green spheres are helium, and the gray structure (buckyball) is composed of the bonds between carbon atoms in a C60 molecule. This simulation showed substantial interaction between molecules flowing through the nanotube and the surrounding walls, especially when tube walls were allowed to respond to interatomic forces.

Graphic courtesy of Robert Tuzun, Oak Ridge National Laboratory, a speaker at the NAS Computational Nanotechnology Workshop, March 4-5.

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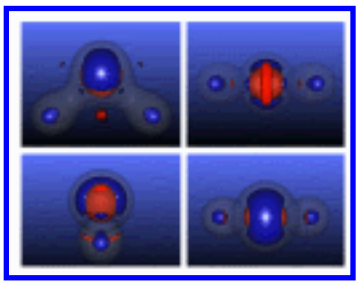
NASA, NAS `Well Placed' to Lead Computational Molecular Nanotechnology Effort

by Al Globus



The NAS Systems Division's strength in supercomputing and computer science, the world class expertise of NASA Ames Computational Chemistry Branch, and computational biology expertise -- along with a Silicon Valley location -- places Ames in an excellent position to lead computational nanotechnology research and make major contributions to NASA's missions. The new program (see *Need for Computational Simulations Brings Advanced Technologies to Ames*), involves related efforts in semiconductor device modeling, petaflops computing, aerospace materials simulation, and computational support for microelectrical mechanical systems (MEMS) technology.

In this context, nanotechnology refers to molecular fabrication -- that is, creating programmable molecular machines. These tiny hypothetical machines would create products by precisely placing each atom in a specified position. Polypeptide synthesizers already exist that can create molecules, given a specification; however, this capability must be expanded to aerospace products. Although programmable machines can already make microscopic, atomically precise products (such as proteins), producing macroscopic engine components, for example, would require replication or self-assembly because of the huge number of atoms in any large object.

Self-replicating Machines -- Hypothetically

One hypothetical approach is to construct a programmable molecular machine, which is instructed to reproduce until a large number of copies are created. Then, the instructions are changed and the desired macroscopic product is built. (See an article by K. E. Drexler, of the Foresight Institute, Palo Alto, CA, entitled, "Nanosystems: Molecular Machinery, Manufacturing, and Computation.") Although this concept may seem fantastic, it should be observed that living organisms routinely replicate themselves.

Another approach is self-assembly, where the components of the end product are designed to attract each other in the preferred configuration via intermolecular forces. The product is created from a large number

of these randomly interacting components. Again, there is a biological model in viruses; similarly, cell-sized membranes have been self-assembled in the laboratory by Fred Manger at Emery University.

Potential Benefits for NASA

The dominant problem of space development is the high cost -- at least $10,000 per pound -- of transportation from Earth's surface to any orbit within a few hundred miles of Earth. NASA's space shuttle costs over $3 billion per year for six to eight launches. Large-scale development of space is unlikely at this price.

The promise of nanotechnology centers on hypothetical materials, particularly diamondoid. Since nanotechnology products are atomically precise, such products can -- in principle -- be constructed. The covalent bonds connecting the atoms in such structures are very strong. For example, covalently bonded diamond is 69 times stronger than metallically bonded titanium.

The potential strength of diamondoid materials has profound implications for aerospace systems. For example, the payload-to-launch-weight ratio of single-stage-to-orbit vehicle designs could be increased from 1-5 percent to 9-12 percent by replacing titanium with diamondoid. (See *Future Space Applications to Benefit From Molecular Nanotechnology Advances*.) A more speculative analysis by Drexler suggests that a 3-ton, four-passenger, single-stage-to-orbit vehicle could be built.

Work Underway at NAS, Ames

One area of interest to the NAS Systems Division is potential applications in computer technology. The graphic on the opposite page illustrates a write-once-read-many memory concept being developed by Charles Bauschlicher, a NAS user in the Ames Computational Chemistry Branch, in collaboration with Ralph Merkle, Xerox PARC (see *Modeling a Simple Assembler for Molecular Manufacturing `Possible Today'*). In a perfect diamond crystal, the outermost layer of atoms are hydrogen. Imagine that some of these hydrogen atoms could be replaced by fluorine (chosen because it binds to carbon in the same way as hydrogen). Using hydrogen to represent 0 and fluorine to represent 1, this modified diamond structure then becomes an extremely high-density memory (approximately 1015 bytes/cm2).

Bauschlicher and Merkle have designed probes that can sense the difference between a hydrogen and a fluorine, and have computationally validated them using quantum chemistry codes.

To establish a lower bound on the computational capabilities of an atomically precise CPU, Drexler designed a mechanical computer consisting of small diamond rods. Such a three-dimensional CPU should be able to achieve 1018 MIPS in a highly parallel desktop computer. Even faster rates should be possible with nanocomputers based on electronic principles.

Computational vs `Experimental' Role

As NASA's lead center for information technology, the Ames role is computational rather than experimental. Although computational nanotechnology is necessary to achieve long-term goals in nanotechnology, experimental work will also be required. Still, computational simulation will allow NASA to:

- Compute what physics laws and chemistry allow, but which is beyond the current state-of-the-art fabrication.
- Work with scientists to gain deeper understanding of experimental results, leading to faster progress.
- Design molecular systems with billions of interconnecting parts executing complex software instructions. Testing and validation through simulation are essential.
- Control complex molecular manufacturing systems and products.

Collaborations in Progress

Several scientists have begun informal collaborations with Ames or have become users of computer systems at the NAS Facility, including:

- Don Brenner, North Carolina State University, is collaborating with Jie Han, IBM contractor in the Ames Computational Chemistry Branch. They are parallelizing Brenner's potential/molecular dynamics code, which can model chemical reactions in hydrocarbons.
- Using the NAS-developed NanoDesign software to create gears from benzyne fused onto carbon nanotubes, Han has used the parallelized Brenner's potential to demonstrate preliminary feasibility of these atomically precise gears.
- Tom McKendree, Hughes Aircraft Co., is working with NAS staff to simulate the behavior of large numbers of independent, cooperating machines. This work is aimed at understanding software issues. (See *Future Space Applications To Benefit From Molecular Nanotechnology Advances*.)
- Todd Wipke, University of California, Santa Cruz, is collaborating with NAS scientists to develop software that "invents" molecules. (See *UCSC's INVENTON Software Creates Molecules in 3D*. Wipke's primary interest is pharmaceutical design, and he is investigating the application of similar techniques for nanotechnology.

NAS and Ames computational chemistry staff involved in nanotechnology research include:

- Timur Halicioglu, Eloret Institute, who has used Brenner's potential to study the properties of carbon clusters from one atom to sizes exhibiting bulk properties.

- Richard Jaffe, Computational Chemistry Branch, who has studied self-assembly.

- Creon Levit, NAS applications and tools group, who has developed simulations and visualization of the molecular charge density field, its gradient, and its Laplacian.

- Steve Walch, Eloret Institute, who has used quantum calculations to elucidate the energetics of adding carbon atoms to diamond surfaces.

Al Globus, a member of the NAS applications and tools group, is developing the NanoDesign molecular design software. He was instrumental in planning the Computational Molecular Nanotechnology Workshop, held March 4-5 at the NAS Facility.

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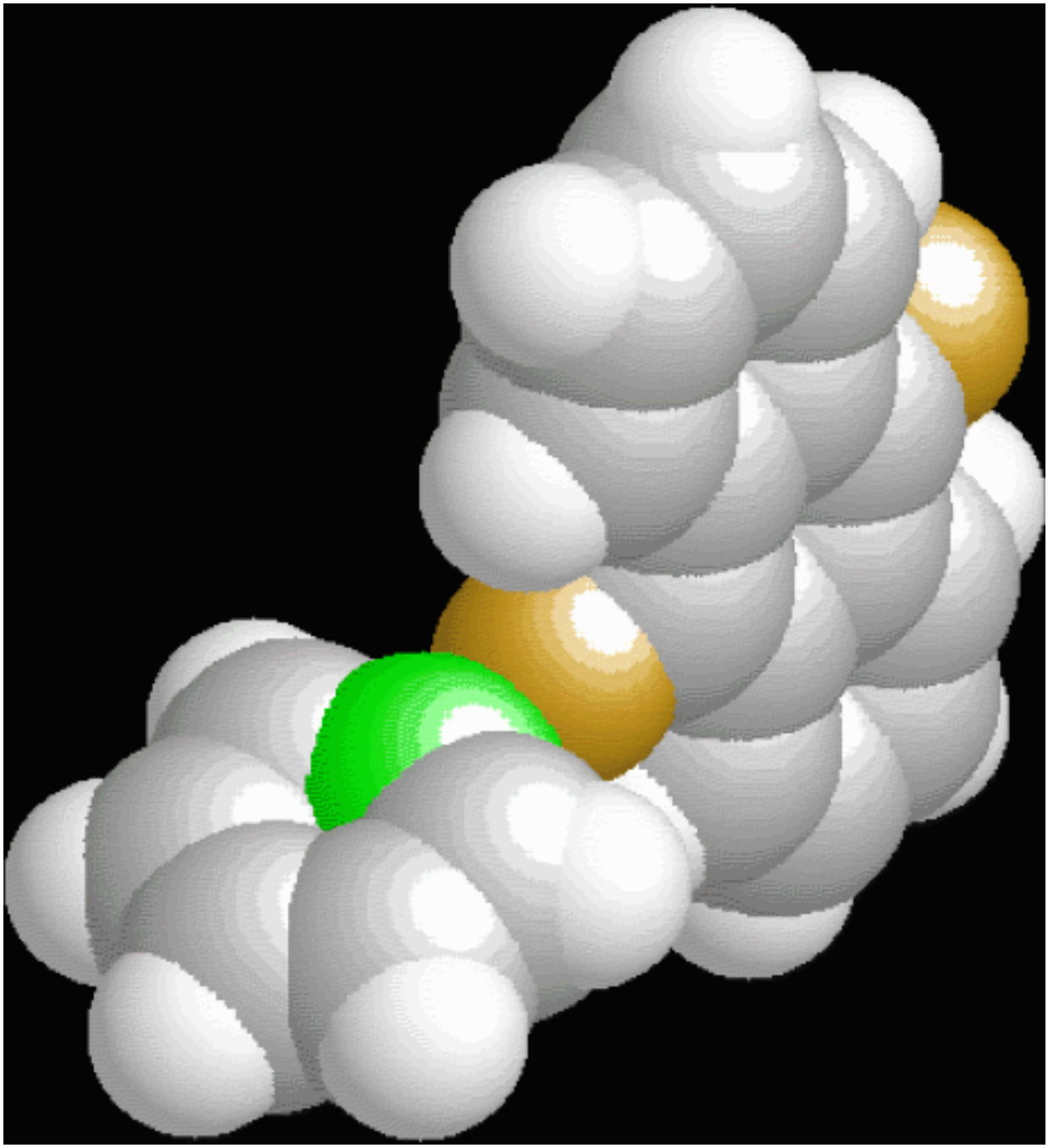

A model of the high-density memory concept under investigation by Charles Bauschlicher (Ames Research Center) and Ralph Merkle (Xerox PARC). The smaller molecule is the data sensor in this model. The larger memory molecule is like tape wrapped around a spindle; it exhibits the most important characteristics of a diamond surface-based memory. Because a representative piece of diamond contains too many atoms to model in reasonable time with highly accurate quantum computational chemistry techniques, a lower-dimensional memory model, such as this one, is used instead.

Graphic courtesy of Al Globus.

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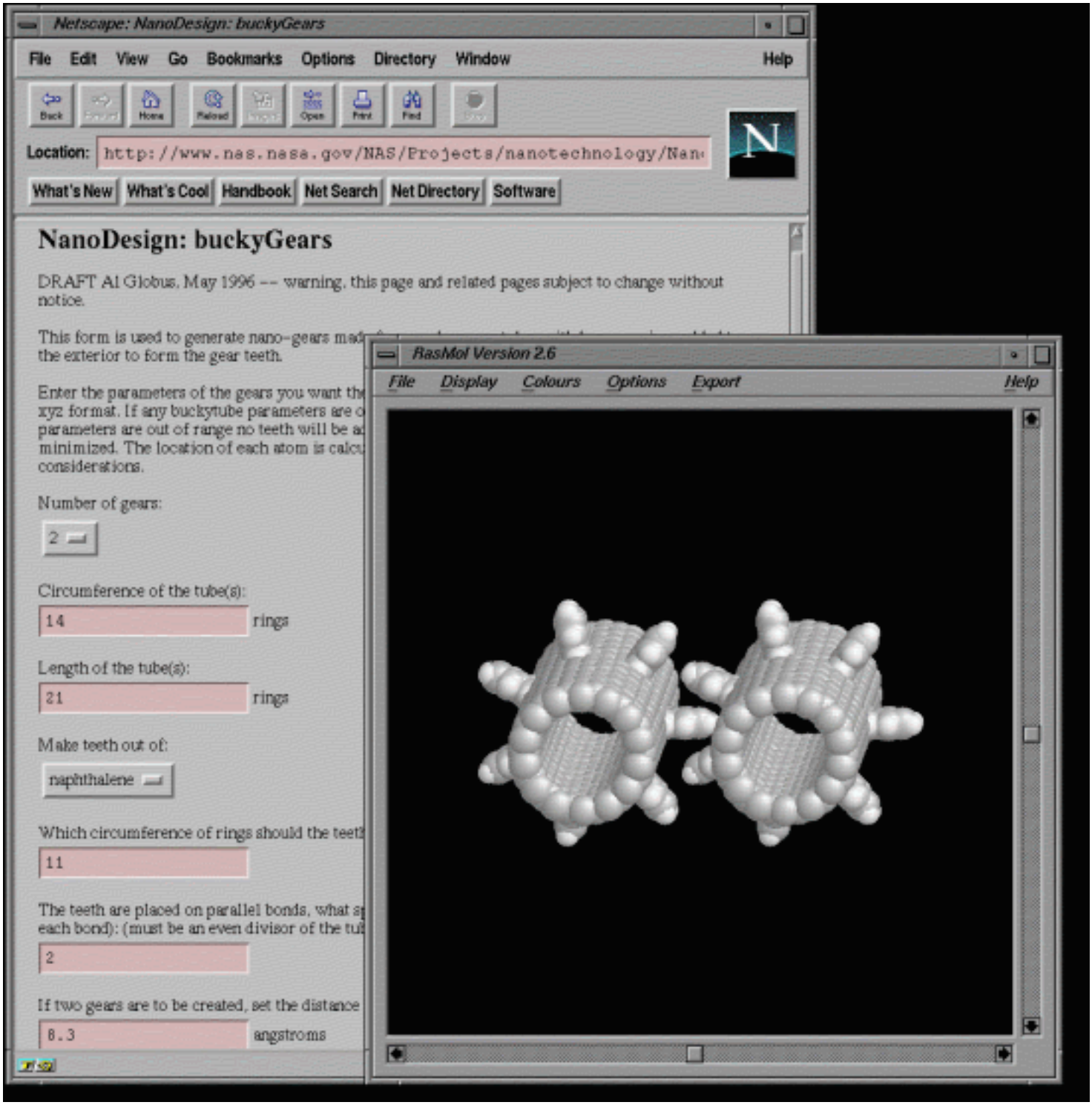

A World Wide Web user interface is used by NanoDesign software to generate molecular models of nanogears. Molecular fragments are fused to the outer surface of the carbon nanotubes to form the gear's teeth. Gray spheres represent carbon atoms, white spheres represent hydrogen atoms. The researcher fills in the form with parameters such as tube circumference and length, tooth spacing, and tooth type. By clicking the Create button (not shown), a C++ language program is invoked to generate the gears in XYZ format. The resulting data may be displayed with programs such as XMOL, used in this image.

Graphic by Al Globus.


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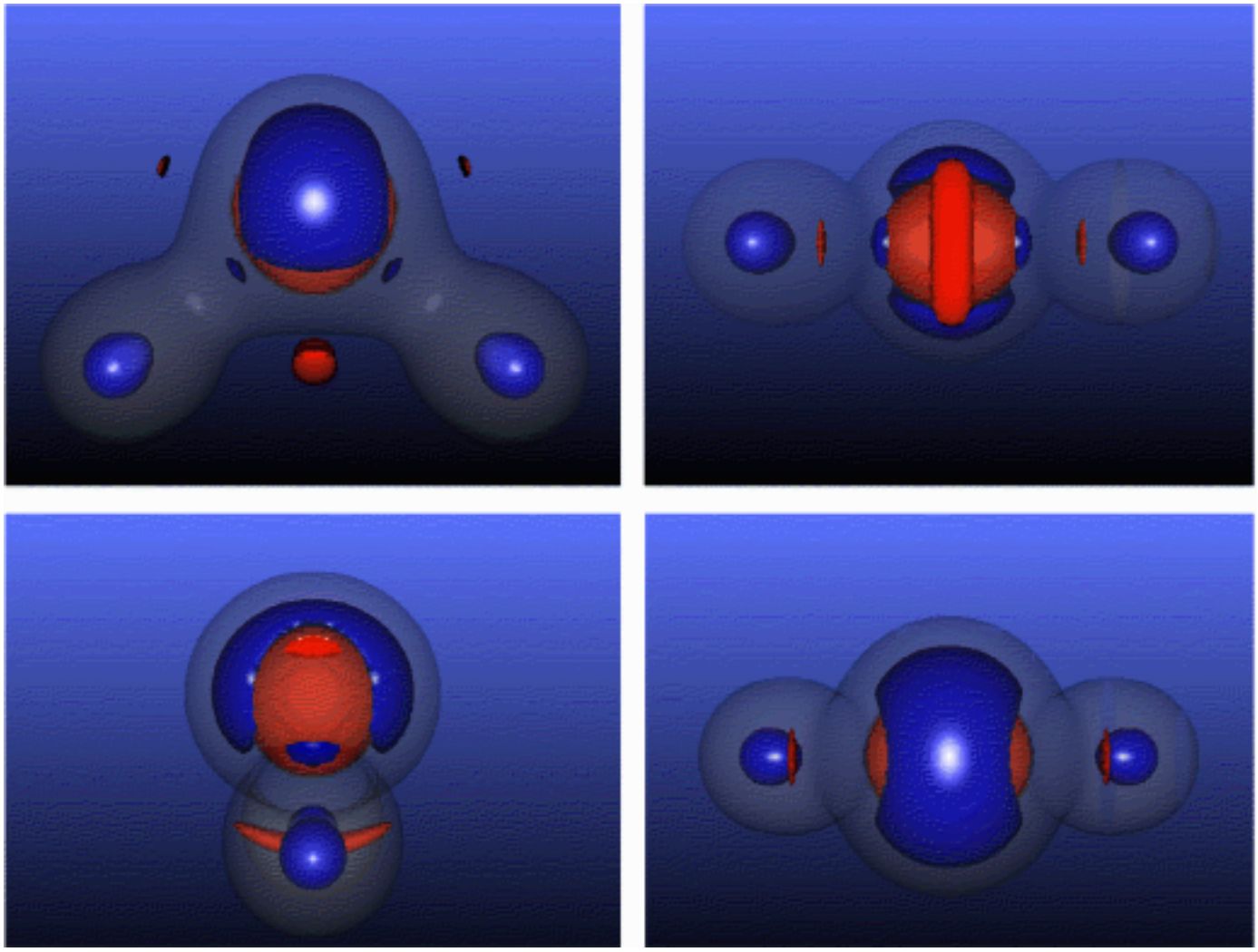

Four views of a water molecule in the ground state. The blue surfaces isolate regions of electronic charge accumulation (lap(rho) < 0), the red surfaces surround regions of charge depletion (lap(rho) > 0), and the transparent surface is at lap(rho)=0. The blue surfaces surround the bonds, the lone pairs, and the nuclei (there is a hidden blue surface around the oxygen).

The molecule was optimized using Gaussian 94 at the b3lyp/6-311++G(2d,2p) level of theory -- that is, using density functional theory and a large basis set.

(Graphic by Creon Levit, using FAST, the Flow Analysis Software Toolkit.)

to the article

One Researcher's Perspective on Semiconductor Technology Modeling for the Next Millenium

by Subhash Saini

Many experts agree that semiconductor technology is the foundation for progress in information technology. It plays a pivotal role in shaping U.S. economy, and this role is expected to continue in the next millennium. Information technology needs devices that are ultra-fast, and cheaper, more robust, and more reliable -- with higher gigaflops per watt and higher Gflop/s per square foot -- than current technology can offer. This requires a need to discover new materials, new processes, new devices -- and to manufacture them cheaply.

Computer Modeling is `Critical'

The attraction of computer simulation and modeling is that it can accelerate the development of semiconductor technology. The current method for developing a new technology is to perform a series of experiments to determine a sequence of processing steps and conditions that lead to satisfactory results. The drawbacks to this approach are time -- since each experimental cycle takes several weeks -- and expense -- because major capital resources are required. According to Forbes magazine (February 26, 1996), these fabrication facilities currently cost between $500 million and $1.5 billion.

The promise of computer simulation and modeling is a reduction in the number of experiments required to develop new materials and devices, thereby saving time and money as well as providing additional insight into the physics involved. Predictive modeling and simulation of materials, processes, and devices are critical to the timely development of semiconductor technology.

The successful development of integrated circuits (ICs) requires a complex interplay of advances in circuit, transistor, and process technology. In the 1980s, computer simulations occupied a predominant role in the area of circuit design. Today, first-pass success has become a standard and traditional methods have been totally eliminated, leading to an order-of-magnitude reduction in circuit design costs. The ever-increasing costs of process and device design warrant a similar role for computer simulations in the 1990s.

`Revolutionary New Design Capabilities'

It has been demonstrated that detailed one-dimensional and two-dimensional computer simulations of the IC fabrication process can save as much as 50 percent of the cost involved in developing a new process technology. The national Grand Challenge of making 3D CAD technology a viable alternative to "cut-and-try" technology requires high-performance parallel computers. The ability to directly link IC mask information (the design media of circuit architects) with the underlying IC technology base (the "engine" that drives the IC revolution base) will provide revolutionary new design capabilities.

Through the drastic reduction of feature size (currently, 0.35 microns in the Digital Equipment Corp. Alpha Chip 21164), IC technology has reached a point where the complexity of the devices requires a fine-grain 3D analysis to obtain adequate accuracy in computer simulations. The potential gains from such 3D simulations are very high -- both in terms of enhanced performance and manufacturing capabilities of existing device structures -- as well as in future breakthroughs in new technology such as merged-bipolar and CMOS (Complementary Metal Oxide Semiconductor) devices.

One example is the study of the scaling trade-offs in designing a submicron bipolar transistor. In the submicron regime, the interplay of 3D geometry, distribution of dopants (an element that is diffused into pure silicon in order to alter its electrical characteristics), and the carrier transport under bias, combine to create a multidimensional design space that cannot be explored by cut-and-try prototypes. In addition, internal IC device information (the trade-off between current flow and parasitic resistive drops) is not directly measurable.

Semiconductor Technology Simulation

Key activities in semiconductor technology simulation (often referred to as TCAD) are process and device simulation. Process simulation refers to predicting the physical structure that results from a given sequence of processing steps. Device simulation refers to predicting the electrical characteristics of a given physical structure.

Accurate simulation of a silicon device structure begins with an accurate description of the geometry and material properties of that structure. This is done by simulating the individual process steps involved in fabricating the device. Once a profile of acceptors and donors within the device is simulated, this profile can be used as input for a device simulator to predict device characteristics prior to fabrication.

Device modeling is performed by solving the basic equations governing the behavior of semiconductor devices. In semiconductor simulation, equations to be solved are Maxwell equations and the Boltzmann Transport Equation (BTE). One approach to solving the BTE is the Monte Carlo method. This method simulates, at a microscopic level, the transport process of mobile carriers. However, this method is very CPU intensive, particularly when coupled with Poisson's equation. The hydrodynamic model is an alternative to solving the BTE. A drift and diffusion model can be derived from the hydrodynamic model

and comprises electron and hole current continuity equations coupled with Poisson's equation.

Semiconductor simulations are also highly CPU intensive. To become mainstream in the industrial world, they need to be done quickly, which requires very powerful parallel computers.

`Virtual Design' and `Virtual Factory'

The ever-increasing complexity of designing high-performance devices requires new concepts and paradigm shifts, such as "Virtual Design" and "Virtual Factory." Virtual Design is a new approach to designing new devices, whereby the entire process is completed on a computer without the actual implementation in silicon. Design trade-off and implementation decisions are made solely with the help of software tools. Only when specifications are met and the designer is satisfied with the results does the actual implementation take place. The Virtual Factory concept involves a rapid prototyping software environment for factory design and manufacturing, based on computer simulations at various levels (such as material, process, device, logic, and circuit).

As in computational fluid dynamics, 3D simulation of the electrical behavior of semiconductor devices is given by a set of highly non-linear coupled partial differential equations, combined with parametrized and highly solution-dependent models for the coefficients. In some situations, this amounts to solving Poisson's equation governing the electrical potential distribution in the device, and two continuity equations for the electrons and holes governing their density distribution and transport through the device.

Using Non-uniform Mesh

Again, as in CFD, a structured, non-uniform mesh is used to discretize the computational domain leading to a large system of non-linear coupled algebraic equations. An iterative method is used to solve this system of equations. In each non-linear iteration, a linearized version of the system of equations needs to be solved. This large sparse matrix can be solved by direct or indirect methods. If one takes ten million grid points with three unknowns per point, one has to solve a matrix of rank 30 million. Parallel direct or indirect methods for solving large sparse systems developed for CFD can be used for device simulations.

Mesh generation technology (structured and unstructured) and algorithms developed in CFD at Ames are expected to play a crucial role in semiconductor simulation and modeling. Fast, high-quality algorithms developed at NAS for graph partitioning would also be very useful for device simulations. For 3D device simulations, adaptive mesh refinement methods, in conjunction with fast graph partitioning methods, would be of immense value.

Besides the similarities between CFD and semiconductor simulations, there are some subtle differences. In CFD, it can be assumed that velocity and momentum are proportional to mass. In semiconductor simulations, going beyond parabolic form complicates the problem, and one must solve velocity and momentum conservation equations and then model the effective mass as a function of energy. In CFD,

this can be assumed as a small source term. In semiconductor simulations, non-linear behavior of this source term complicates the problem. Eigenvalue analysis shows that initially the problem is a mixture of parabolic and hyperbolic type, and over time, it changes to hyperbolic type -- and thus needs different numerical schemes.

Technology developed for CFD at Ames can dramatically accelerate the understanding and designing of TCAD.

Subhash Saini leads the NAS algorithms, architectures, and applications group. He has a Ph.D. in computational physics from the University of Southern California, and has been doing research at NAS since 1989.

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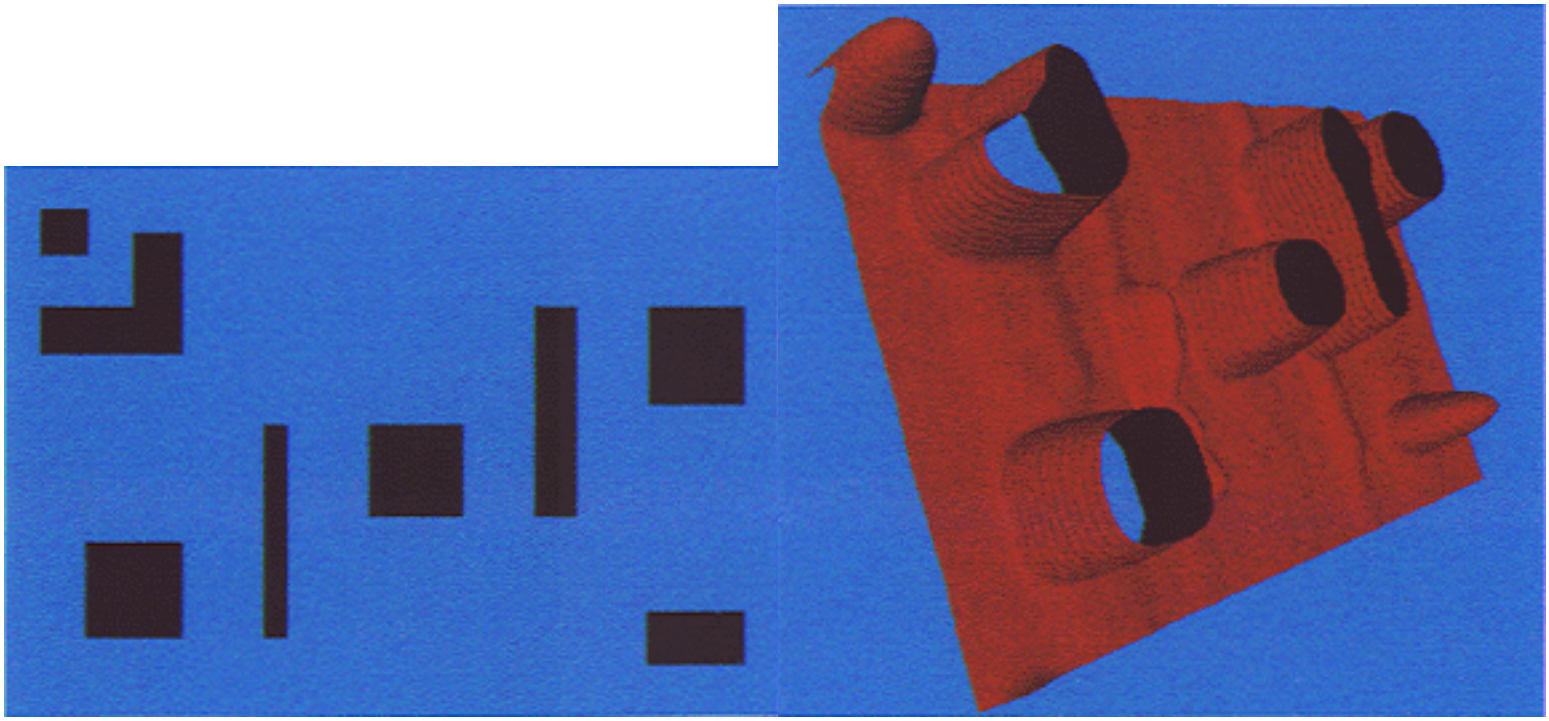

Level-set methods can be used to model the manufacturing of semiconductors. The fisrt image shows a pattern mask in the photolithography process. When the entire area is exposed to light, the chemical properties of the material are changed depending on whether the light is blocked. The second image shows the development of a 3D profile as the material is etched away. This graphic was part of a presentation by James A. Sethian at the NAS Semiconductor Device Modeling Workshop, March 28-29.

Graphic courtesy of D. Adalsteinsson and J. A. Sethian, Department of Mathematics and Lawrence Berkeley Laboratory, University of California, Berkeley.

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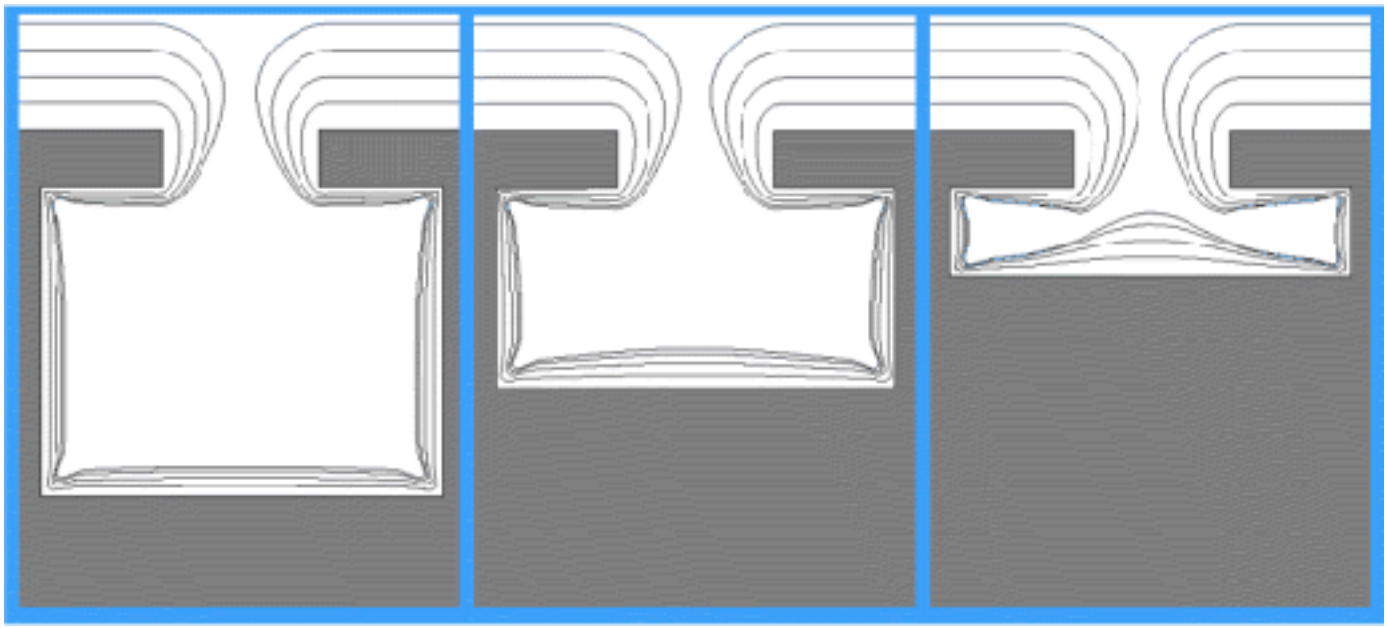

During a deposition process, material is laid down on an etched-out shape. To analyze the width and distribution of the layer deposited on various shapes, the above figure shows the effect of the sticking coefficient, which measures the fraction of material re-emitted when particles are deposited at the surface. As the depth of the cavity decreases (from left to right), the width of the surface layer changes.

Graphic courtesy of D. Adalsteinsson and J. A. Sethian, Department of Mathematics and Lawrence Berkeley Laboratory, University of California, Berkeley.

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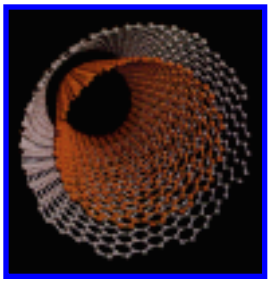
UCSC's INVENTON Software Creates Molecules in 3D



by Elisabeth Wechsler

A software package under development at the University of California, Santa Cruz (UCSC) uses artificial intelligence techniques and a knowledge of chemistry to "invent" molecules in 3D space -- something that has been lacking to date, according to Professor Todd Wipke, of UCSC's Molecular Engineering Laboratory.

"Chemists have no good algorithms for manually enumerating the molecules that can satisfy a set of constraints in 3D," he said, in his March 5th presentation at the NAS Computational Molecular Nanotechnology Workshop. Wipke believes that "computers, when properly programmed, [can] be more creative than chemists in the task of inventing new chemical structures."

Called INVENTON, the program automatically constructs chemical frameworks that position atoms in a desired 3D arrangement, giving researchers new ideas for building blocks. Wipke summarized the paradigm as: "Chemist describes objectives and constraints. Computer formulates strategy and tactics, then invents structures and ranks them. Chemist reviews resulting candidates." More specifically, INVENTON creates molecules by adding molecular fragments to span the space from one point to another. The points are given in the problem description provided by the chemist or are generated as subgoals. The molecular fragments come from a basis set established by the investigator. INVENTON also can build structures from individual atoms. Finally, the program ranks the candidate structures by scoring functions selected by the chemist, Wipke explained.

Productive Approach To Design

"A computer program can invent molecules that have never been conceived of and do not exist in any database anywhere," he commented. In its six years of existence, INVENTON has designed structures in the domains of nanotechnology (self-assembling molecules in nanoscale systems) and pharmaceutical drugs (such as mimics of known drugs for cancer and enzyme inhibitors for AIDS).

"Designing a system like this is a complex task -- one that requires really logical thinking. AI methods are already being used by INVENTON to prioritize tasks, and heuristic search is used to reduce the number of `relevant' constraints." In addition, bringing "engineering principles across boundaries to assist chemical design" has been useful, Wipke noted.

Automated molecular design will benefit from greater CPU speed, more knowledge and understanding, and larger organized collections of chemical information readable by computer, he said, adding that "having more complex problems will accelerate our abilities to problem solve."

Collaboration with NAS

Collaborative work between Wipke's group at UCSC and Al Globus (NAS applications and tools group) has included modifications to the search strategy and solving simple initial problems. Current work is focused on developing fragment libraries designed for nanotechnology and then applying them to problems requiring very stiff molecules. A more difficult future problem is taking advantage of the high degree of symmetry common in nanotechnology problems and spanning space with molecular fragments that can be repeated an indefinite number of times.

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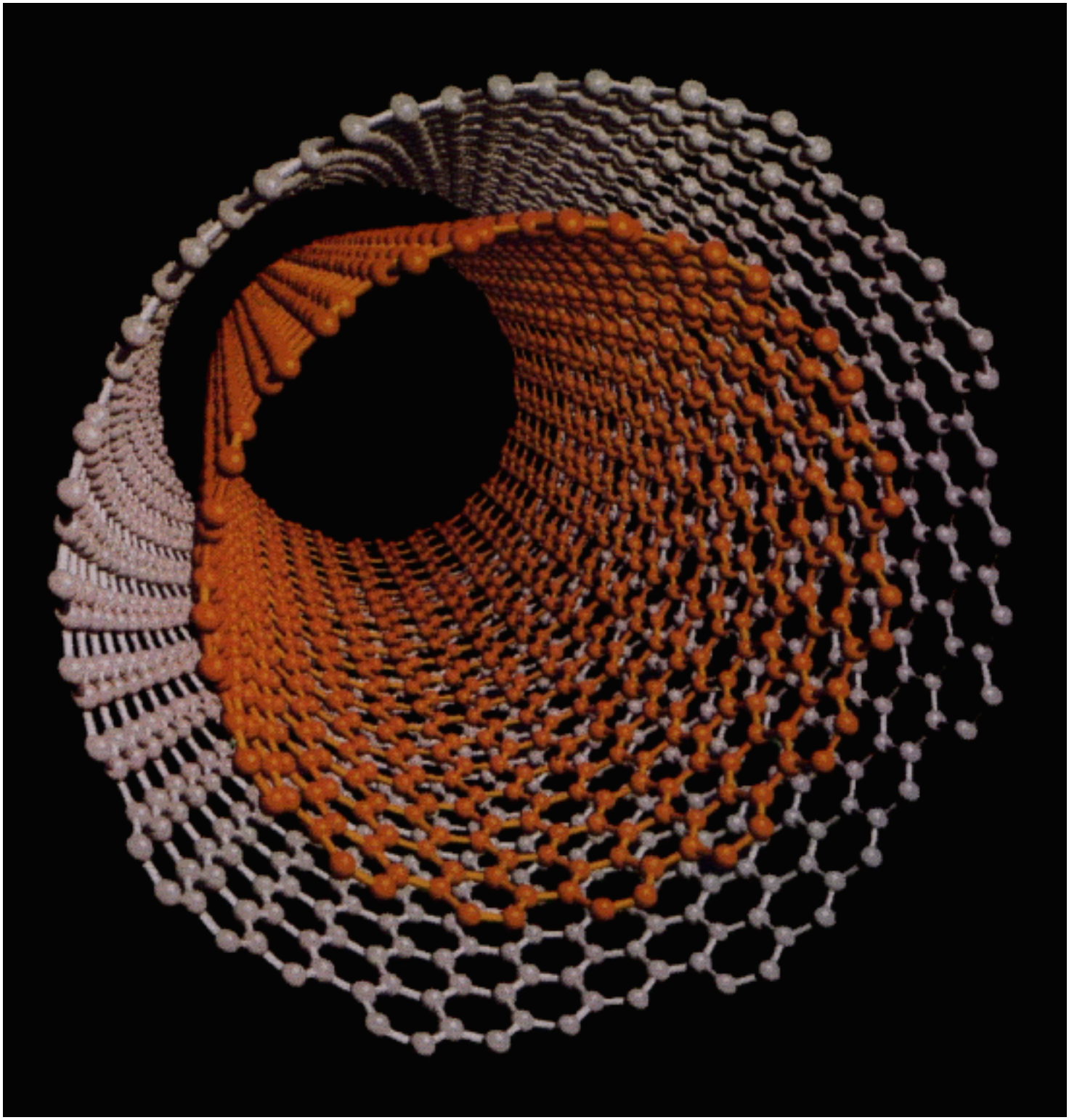

Two nested carbon nanotubes, separated by about 3 angstroms. Close examination reveals that the bonds in the outer tube are not parallel to the bonds in the inner tube. This phenomenon, called helical winding, is associated with different electrical properties and may be helpful in building nanocomputers.

Graphic courtesy of Naval Research Laboratory.

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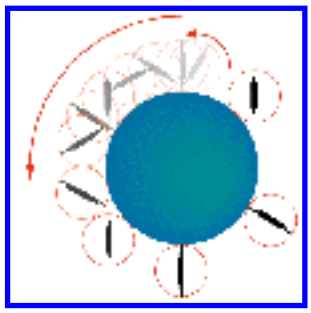
Future Space Applications To Benefit From Molecular Nanotechnology Advances



by Elisabeth Wechsler

Molecular nanotechnology -- defined as the future general ability to design and build to atomic precision -- can contribute "significant increases in technical performance parameters for future space applications, especially in areas of materials strength and density," said Tom McKendree, systems engineer at Hughes Aircraft Co, Fullerton, CA.

However, he emphasized in a March 15th presentation at the NAS Facility that improvements in computer hardware and systems software are needed to take full advantage of the new technical possibilities.

McKendree believes that molecular nanotechnology will support "powerful and cost-effective space systems once we develop and deploy mature nanotechnology." To prepare, further study will be necessary in the areas of system architectures, operational concepts, grand strategies, and enabling technologies.

Building Lighter Vehicles

Traditional aerospace materials leave little room for the payload portion -- such as scientific equipment and personnel -- of total vehicle weight, McKendree explained. One of the first space applications of molecular nanotechnology may be creating spacecraft from diamondoid materials to achieve "significantly less mass for the same structural capability."

"If diamondoid can be protected from the heat of engine combustion and atmospheric temperatures, an immediate improvement in overall payload size could be realized," he said.

The building materials so affect the vehicle's overall weight that "differences between nanotechnology-based and traditional architectures become more important than the issue of one- or two-stage-to-orbit designs," McKendree said. "The worst launch concept examined using nanotechnology material is still better than the best concept using conventional materials," he said.

Skyhook a Potential Application

Other potential space applications based on developing a molecular manufacturing capability include tools, such as the geosynchronous skyhook. This long cable is designed to reach down to a planet for transferring supplies, personnel, and equipment and would work "by stealing momentum from the rotating planet," McKendree said.

One problem of the skyhook is "severe stress." A structure designed with constant thickness would break, he explained, so the skyhook needs to be tapered at both ends and thicker in the middle. "Molecular nanotechnology materials will allow the development of narrower geosynchronous and rotating skyhooks," he said. (See figure)

Additional space applications for molecular nanotechnology include: light sails, which create thrust by reflecting sunlight and do not consume propellant; solar electric engines; and even human-inhabited space colonies and "personal asteroid settlement systems," McKendree said.

Risk Factors Noted

During a question-and-answer session, McKendree noted several risk factors that could impact the development of molecular nanotechnology and, ultimately, the likelihood that such space applications could be built. One of McKendree's primary concerns is "better software, better computers -- or both."

Some audience members were more hopeful about solving molecular nanotechnology problems with current system capabilities. "There's tremendous opportunity for improved algorithms based on the progress we've made in solving fluid dynamics problems," observed NAS scientist David Bailey. "I don't think the future scaling of nanotechnology computations is going to be as bad as people expect, because we'll find algorithmic ways to reduce the cost."

Potential for Fundamental Flaws

Another big risk, according to McKendree, is the discovery of "some fundamental flaw" that would shoot down the whole concept. "We've got real issues to address and we're going to have to engineer around these constraints. However, so far, we [nanotechnology researchers] haven't found anything that kills the concept."

McKendree noted comparisons between molecular nanotechnology and biological systems. "We know [the latter] work, so that gives a lot of people the confidence that molecular nanotechnology should work as well, even though it's much more mechanistic at a lower level."

"At the smallest scale things look like mechanical engineering more than living cells," he explained. "The advantage of [a certain inherent brittleness] means easier control if you take advantage of it."

Another question from the audience concerned the progress of other countries, including Japan, in this field: "If other nations get there first, what can they do with the technology before we catch up?"

McKendree commented that Japan seems "to have a leg up on several components that we're trying to do here, but I don't see enough of a system focus yet. They're doing well on the technical base issues and could ramp up if they wanted to. They're working on a long-range grand strategy, which appears to be viewed seriously by the general public."

Beyond Microelectronics

Bailey commented that references to nanotechnology "often mean what we consider to be microelectronics." He added that he doesn't believe Japan has the same focus on long-term molecular nanotechnology as the U.S.

McKendree concurred, in part. "They do have micro-electromechanical systems (MEMS) in Japan, and there are people thinking specifically about nanotechnology as we know it."

In responding to a question about specific software building blocks needed for molecular nanotechnology, McKendree emphasized the component level. In the far term he called for an "assembly compiler," which he defined as a large software program that will take the 1017 number of mechanisms needed for large molecular manufacturing systems and control them to build specific objects.

Computational Chemistry Role

McKendree hopes that computational chemists will attempt solutions for certain computational nanotechnology problems -- "to see where the differences are between that field and nanotechnology. Then, we'll really have a handle on molecular nanotechnology concepts."

Another issue involves designing an appropriate ladder of simulations at a number of different scales and being able to hand off the results of one set to feed into the larger scale. "Designing molecular nanotechnology pieces properly is an important issue -- we're part way but we have a way to go," he said.

To obtain a copy of the March 15th presentation handout or a videotape, send email to **doc-center@nas.nasa.gov**. For more information about McKendree's research, send email to **tmckendree@msmail3.hac.com**.

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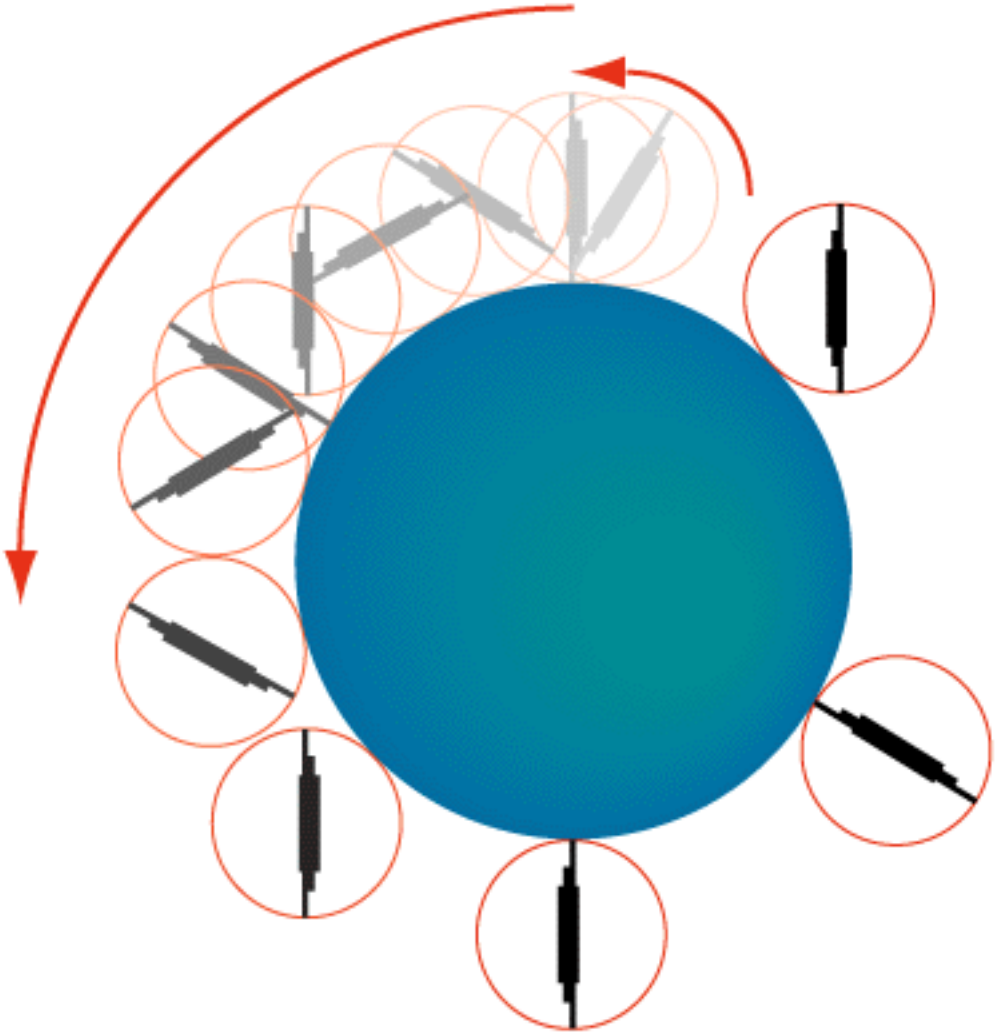

The rotating skyhook spins and orbits counterclockwise, as if it were the spoke of a wheel rolling on the planet's surface. The tip of the skyhook is temporarily stationary at its closest approach, so that a vehicle could grab hold of it and be flung into space. To avoid drag, a skyhook used for this purpose would need to be positioned just above the atmosphere. Design requirements for such a skyhook include both very strong and light cabling -- such as that produced by molecular nanotechnology.

Graphic courtesy of Tom McKendree.

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Modeling a Simple Assembler for Molecular Manufacturing `Possible Today'

by Elisabeth Wechsler

"We could design and model computationally a simple assembler using today's software tools, computational capabilities, and understanding to perform that task," said Ralph Merkle, of Xerox Palo Alto Research Center. However, he acknowledged "some uncertainties about the number of people needed and the time it would take" in his March 4th presentation at the two-day NAS Computational Molecular Nanotechnology Workshop. Of course, it's another issue to actually build a simple assembler, Merkle acknowledged, explaining that that phase will require an "entire new technology of molecular tools and positional devices."

The reasons to design and model a simple assembler include clarifying the longer-range capability and approach to molecular nanotechnology research, as well as exploring and discarding poor designs early and cheaply before manufacturing.

"As we move toward more and more complex structures, we'll find it increasingly important to model them computationally before building them," Merkle said, adding that "we'll need large piles of computer time to chew on the large problems."

Design Based on Simple Subsystems

"Besides needing people with computational chemistry backgrounds and the right skill sets, we'd also need architectural proposals -- broad descriptions of what a simple assembler looks like on a large scale -- and that define the basic strategy to achieve the goal," he continued. "It's useful to break down the design of a large and complex system into simpler subsystems, and then to propose and analyze different ways of making those subsystems."

For example, he believes that "positional control" is quite important: "There are several possible positional devices to choose from, including rather conventional robotic arms and the somewhat more rigid Stewart platforms (robot-like devices that can move a platform to any place and orientation within some region of space used in six-degree-of-freedom flight simulators). The positional device would pick up molecular tools -- so we'd need multiple proposals for what a `molecular tool' would look like, and

what reactions it would participate in. The basic idea is to make sure there are always several different ways of implementing each critical subsystem -- that way, a single bad proposal for a subsystem won't cause the whole system to fail."

A Series of Designs

There should also be a series of designs, ranging from full-blown diamondoid systems, to intermediate systems that could synthesize useful (reasonably stiff) structures in solution, to systems that are more experimentally accessible today.

At the molecular scale, the most common method of assembling parts is some form of self-assembly, Merkle explained. "By exercising great ingenuity, chemists routinely synthesize a remarkably wide range of small molecular structures without the molecular equivalent of human hands -- the parts spontaneously arrange themselves in the desired pattern."

Self-replication `Difficult to Understand'

Self-replication has been proposed as a way to reduce manufacturing costs. Merkle noted that many people find the concept of self-replication difficult to understand, which he thinks is often due to "an erroneous intuition that the thing manufactured must be less complex than the thing doing the manufacturing itself -- for example, the notion that a box can't make another box." He emphasized that devices need not be inherently complex to make copies of themselves.

Horizons Beyond a Decade

To pursue these nanotechnology projects "requires horizons on the order of a decade or two," Merkle said, adding that organizations with computing, chemistry, and manufacturing expertise -- as well as long-term planning horizons -- are needed to bring this type of project to fruition. NASA and the Department of Defense (including the Naval Research Laboratory) are well-positioned for this time frame, with the added advantage that project findings would remain in the public sector. "This is very helpful for developing the new technology and examining its ramifications."

Private companies, on the other hand, "tend to go for certain capabilities that can lead to profitable intermediate goals -- like products. This approach will advance [molecular manufacturing] in the long run, though not as directly as a project mounted by NASA or some other organization with a long planning horizon," Merkle said.

Nature's Limitations

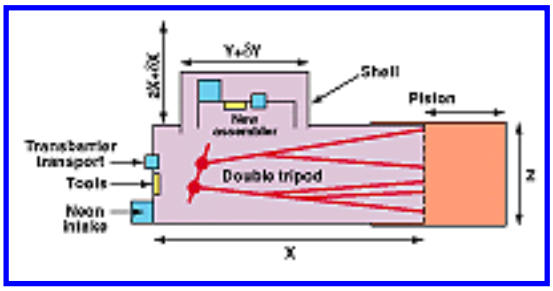
One workshop participant asked about getting around "the intrinsic limitations that exist in nature," stating that "there's an element of simplicity in assuming that just because you can position atoms and

molecules together you'll be able to assemble [anything you want]. No matter how you position certain molecules," this participant said, "you can't necessarily make them stick together" when you remove them from the assembler.

Merkle responded that "synthetic chemistry is a big complex field with no guarantees that we can build things." However, he believes that "if we restrict ourselves to hydrocarbons, and look at the kinds of tools that are `plausible' [because they can be modeled computationally], you don't need a large tool set to perform basic operations."

Structures Need Inert Environment

"It should be possible to build a remarkably broad range of structures with positional control if you combine it with an inert environment -- such as neon gas or a vacuum," Merkle said.



"Initial architectures could be powered by acoustical transmission (see figure), then as systems became more complex, you could use electrical, chemical, optical, or solar power," Merkle said. "There are many ways to provide energy. After computational modeling is done, the odds that we'll come up with something better than the present proposals are very good."

"At present, we don't have a fleshed out version of a diamondoid assembler model, so more work needs to be done," he said. Merkle is also collaborating with Ames researchers on computational modeling issues.

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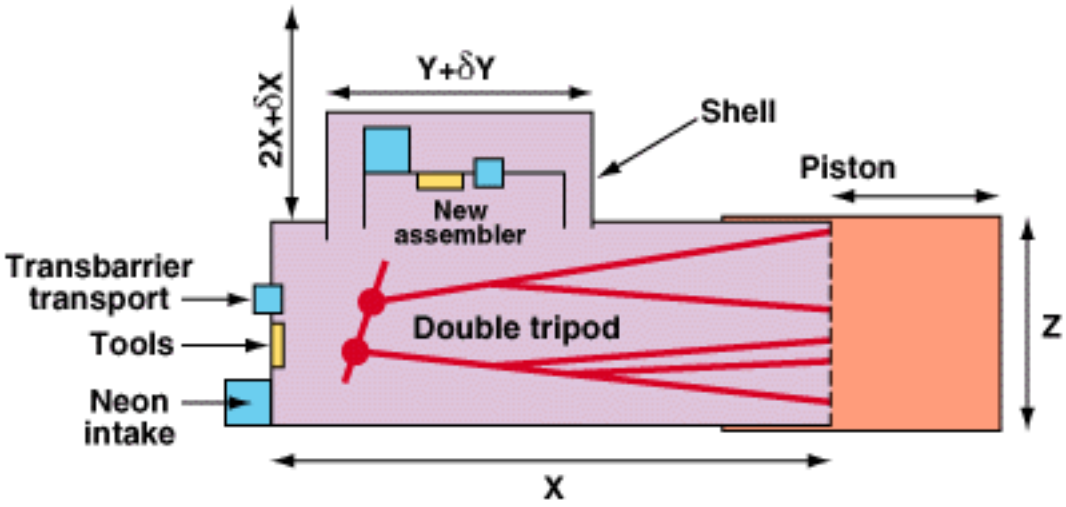

This theoretical simple diamondoid assembler gets its power from broadcast acoustic waves, which are carried in the interior of the assembler by compressed neon. Pressure actuated ratchets, located at the joints of the positional device (a double tripod) drive it directly. The pressure waves send both power and information to the assembler, and are generated by a macroscopic system (loudspeaker) controlled by a conventional computer. The positiional device can "pick up" and "put down" molecular tools, and can place them over a molecular workpiece: here, the positional device is building a copy of the simple diammondoid assembler. Raw materials enter in the form of feedstock molecules (used to build molecular structures), bound from the external solution by binding sites, which can be moved into the interior of the assembler. The feedstock molecules are then manipulated directly by the positional device.

Graphic courtesy of Ralph Merkle

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Special Issue

High Performance Computing Research Vol. 2, No. 19

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NAS

Special Issue

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High Performance Computing Research

In an era of ever restricted budgets, the criterion—"smaller, better, cheaper"—is being ruthlessly applied to the design and manufacture of a broad range of products, from complex scientific tools to consumer goods. A government-wide initiative (known as "High Performance Computing Research") has been formed to study these challenges. The NAS Systems Division is investigating solutions in three research areas: petaflops computing, semiconductor device modeling, and molecular nanotechnology.

Device Modeling Holds Key to Future NASA Missions

by Elisabeth Wechsler

"Unless there are major breakthroughs in semiconductor technology, NASA future space missions will be impaired," observed scientist David Bailey in his introductory remarks at the NAS-sponsored Semiconductor Device Modeling Workshop, March 28–29. "What is needed are very high density, ultraminiaturized systems with very high reliability and performance that can be built at very low cost.... At any cost we'll buy a petaflops computer for $800 million."

Among the important technical challenges facing semiconductor manufacturers, according to Bailey, are two that the NAS Systems Division is particularly well-positioned to help tackle:

- performing accurate 3D simulations of physical effects
- porting advanced TCAD [technology CAD] software to highly parallel systems

'Complementary Role' to Other Programs

"We see our role as complementary with industry and other government research programs," Bailey

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Need for Computational Simulations Brings Advanced Technologies to Ames

by David H. Bailey

As manufacturing systems increasingly enter the nanometer (10^{-9} meter) range, the need for computational simulations to understand underlying physical phenomena is acute. The newly created NASA Ames nanotechnology initiative envisions Ames Research Center as the focus of a nationwide network of research laboratories using computation to understand and ultimately control manufacturing processes at smaller and smaller sizes, culminating in atomically precise products.

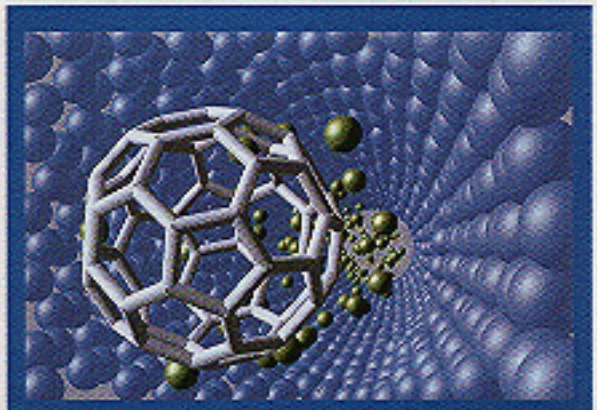
In the medium term, significant advances can be expected in computing technology as Ames works with Silicon Valley firms, computer vendors, and universities to remove technological barriers that may impede computer hardware progress during the next few years. In the long term, it is expected that petaflops computer systems, atomically precise manufacturing techniques, and other devices developed in this program will revolutionize space launch systems, climate modeling, spacecraft instrumentation, aeromedical design, planetary exploration, and computer manufacturing.

Development of Future Space Vehicles

One example of an important future NASA application of this technology is the development of autonomous intelligent vehicles for the exploration of the solar system and beyond. Since radio signals require up to 40 minutes for a round trip from Mars to Earth, NASA cannot rely solely on ground-based personnel or computers to control Mars-bound spacecraft or Mars-roving robots. An intelligent on-board computer, with sufficient power to ensure reliable real-time operation, is required. For missions to other planets—or to the stars—even more powerful computer systems will be required. These systems need to be exceedingly compact in size, highly resistant to radiation damage, and use very little electrical power. Most importantly, they must be affordable in an atmosphere of increasingly tight budgets.

Future spacecraft will also need advanced scientific instruments, such as image sensors, microwave receivers, light spectrometers, mass spectrometers, chemical analyzers, and interferometers—all of which must be more compact, reliable, and economical than is feasible with current technology. Further, such instruments may require novel designs, such as those inspired by biological systems.

At the same time, the transportation costs of placing humans and equipment into space must be reduced by at least two or three orders of magnitude if large-scale human exploration and development of space is to begin. Much stronger, lighter, and more affordable materials are needed for constructing these vehicles. One of the most promising approaches is to employ molecular nanotechnology to construct diamondoid



Close-up of a simulation of a buckyball (a C60 fullerene molecule) passing through a graphite nanotube. The blue spheres are carbon, the green spheres are helium, and the gray structure (buckyball) is composed of the bonds between carbon atoms in a cell's nanotube. This simulation showed substantial interaction between molecules flowing through the nanotube and the surrounding walls, especially when tube walls were allowed to respond to atomistic forces. (Graphic courtesy of Robert Tuzun, Oak Ridge National Laboratory, a speaker at the NAS Computational Nanotechnology Workshop, March 4-5.)

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