Computational Molecular Nanotechnology at NASA Ames Research Center, 1996

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Organization

Introduction

Molecular nanotechnology -- for the purposes of this paper a hypothetical technology of programmable molecular machines -- appears to have great promise for aerospace system design. This technology presupposes manipulation of individual molecules and atoms. There has been substantial skepticism as to the feasibility of molecular nanotechnology, particularly the diamonoid nanotechnology proposed by [Drexler 92a]. However, a number of recent laboratory demonstrations have supported, although not proven, the concept of a technology based on manipulation of individual molecules and atoms. Consider:

- Numerous experiments using AFM and STM to arrange atoms and small clusters on surfaces have been successful. Complex, precise and detailed arrangements of atoms on various surfaces have been achieved. See the IBM STM Image Gallery for some stunning images. Molecules at room temperature have been moved by STM tips at IBM Zurich.
- [Yazdani 96] measured electrical resistance of one and two atom xenon wires.
- [Cluzel 96] and [Smith 96a] have stretched individual DNA molecules and measured the relationship between force (tension) and length.

Also, investigators have reported construction of very small machine components, although on scales somewhat larger than atomic:

- [Sheehan 96] used an AFM to make and manipulate a primitive interlocking machine from MoO_3 nanocrystals on a MoS_2 single-crystal surface.

- Sunny Bains reports in *Science* , volume 273, 5 July 1996, p. 36 on upcoming papers describing how lasers can be used to rotate very small particles.

These laboratory results and others have led us to pursue computational molecular nanotechnology with a particular emphasis on systems that may be synthetically accessible. NASA Ames focuses on **computational** nanotechnology because Ames has been designated as the NASA's lead center for information technology. This paper will discuss the Ames computational molecular nanotechnology program.

Vision

- We envision NASA Ames Research Center leading a nation-wide network of research laboratories
- using computation to understand, design and control programmable molecular machines, their products, and related manufacturing processes.
- Such machines could revolutionize launch vehicles, spacecraft, aircraft, and computer systems.
- This program is high risk, particularly in time-to-completion, but it has a huge potential payoff. Time-to-completion appears to be sensitive to resources allocated.

The early stages of this project are being strongly supported by the NAS supercomputer center in collaboration with computational chemists and computational molecular biologists at Ames and elsewhere. The computational molecular nanotechnology project, if successful, will require massive computational resources [Saini 96]. By supporting an in-house development effort NAS hopes to prepare the supercomputer and support systems necessary to bring aerospace relevant nanotechnology to fruition.

Potential Benefits of Molecular Manufacturing

The hypothetical possibility of building programmable molecular machines has suggested a wide variety of sometimes incredible applications to a variety of authors. Three applications are of particular interest to NASA: launch vehicle structural materials, computer components, and nano-spacecraft.

Launch Vehicle Structural Materials

The dominant problem of space development is the high cost -- about $10,000 per pound -- of transportation from Earth's surface to any orbit within a few hundred miles of Earth. For example, NASA's space shuttle program costs approximately $3 billion per year (see http://venus.hq.nasa.gov/office/budget/fy96/as-1.html) for six to eight launches (see http://www.ksc.nasa.gov/shuttle//missions/); each with 6-8 astronauts and 50-60,000 pounds of payload. Launch costs are a also major component of communication satellite system expenses. Large-scale development of space is unlikely at this price.

One promise of nanotechnology centers on hypothetical diamondoid materials. Since molecular nanotechnology products are (by definition) atomically precise, many interesting products can -- in principle -- be constructed; particularly if macroscopic diamonoid materials can be built. The covalent bonds connecting the atoms in diamonoid structures are very strong. For example, covalently bonded diamond is approximately 69 times stronger than metallically bonded titanium. This may have profound implications for aerospace systems. Consider:

- [McKendree 1995] analyzed existing single stage to orbit designs. He compared vehicle performance of identical vehicle designs differing only in structural materials: titanium vs. diamonoid. McKendree found that using titanium allowed 1-5% of the weight of the vehicle on the launch pad (including fuel) to be devoted to payload. With (hypothetical) diamonoid, 9-12% of launch weight could be payload. Note that this analysis did not modify the designs except to replace structural materials.

- [Drexler 1992b] analyzed single stage to orbit vehicles specifically designed around diamonoid materials. His speculative, but physically based, analysis suggests that a three ton (including fuel) single stage to orbit spacecraft for 4 passengers can be built.
- The application which first interested this author in nanotechnology is the orbital tower [Pearson 1975]. An orbital tower is a cable stretching from the Earth's surface to twice geosynchronous orbital altitude (this length is necessary to stay over one point on the Earth's surface). Orbital towers don't collapse since they're held in tension by orbital dynamics. Unfortunately, orbital towers require materials of tremendous strength. The point of maximum stress is at geosynchronous orbit. Thus, for a given material, the tower must be thickest at geosynchronous orbit and then exponentially taper to a smaller radius at the Earth's surface and at the high point. Diamondoid could be used to build an orbital tower with a taper factor of about 22 [McKendree 1995] vs. >10,000 for steel. Once built, an elevator is attached to the cable to get to orbit. An orbital tower is the only launch/return system known that does not require the vehicle to enter the atmosphere at high speed. Lower speeds generate less heat reducing the probability of unacceptable atmospheric environmental changes when millions of people travel between Earth and space as they do between continents today.

It should be noted that aircraft are also limited by the strength-to-weight ratio of materials, so vastly superior aircraft should result from diamonoid materials.

Computer Components

Aerospace systems depend heavily on computer technology. Improvements in computer technology depend heavily on smaller and smaller feature size. To continue current trends will require atomic precision early in the next century [Saini 96]. Computational molecular nanotechnology hopes to develop atomically precise computer components and there has been some theoretical work:

- A write-once-read-many memory concept was developed at NASA Ames in collaboration with Xerox PARC. In a perfect diamond crystal, the outer-most layer of atoms are hydrogen. Some of these may be replaced by fluorine. Fluorine is chosen since it binds to carbon in the same way as hydrogen, but fluorine is larger. Using hydrogen to represent 0 and fluorine to represent 1, this modified diamond becomes very high density memory (approximately 10^{15} bytes/cm^2). However, a probe must be designed that can sense the difference between a hydrogen and a fluorine on the surface. Bauschlicher and Merkle have designed such probes and computationally validated them using using quantum chemistry codes. For details see [Bauschlicher 96].
- To establish a lower bound on the computational capabilities of an atomically precise CPU, [Drexler 1992a] designed mechanical computer components made of small diamond rods. Such a three dimensional CPU should be able to achieve 10^{18} MIPS in a highly parallel desktop computer. This is only a lower bound on performance, atomically precise electronic computers can be reasonably expected to outperform diamond rods since electrons are smaller and move faster.

Nano-Spacecraft

Current trends in spacecraft design, particularly scientific spacecraft, are to shrink components allowing more capable spacecraft to be launched on small and medium capacity launch vehicles. Atomically precise components, if they can be constructed, can reasonably be assumed to radically decrease spacecraft size and enable radically new missions using very large numbers of very small spacecraft.

Computational Nanotechnology

As NASA's Information Science lead center, Ames' role is computational rather than experimental. Computational nanotechnology is **necessary but not sufficient** to achieve NASA goals. Specifically, computation will allow Ames and partners to:

- Compute what the laws of physics and chemistry allow but is beyond the state-of-the-art in fabrication.
- Work with experimentalists to gain deeper understanding of results leading to faster progress.
- Design molecular systems with billions of interconnect parts executing complex software instructions. Note: a flawed molecular manufacturing system may convert to carbon dust on failure making debug difficult. Test and validation via simulation are essential.
- Control complex molecular manufacturing systems and products.

As important as it is, computation alone cannot reap the anticipated benefits of nanotechnology. A major future requirement is for a partner center to take responsibility for experimental and manufacturing progress.

NASA Ames' Strengths

A robust program in computational molecular nanotechnology requires massive computational capabilities, excellent computational chemistry expertise, and expertise in the most capable existing "nanotechnology" -- molecular biology. Ames has all three.

- **Supercomputers**. The NAS supercomputer center at Ames, originally developed for computational fluid dynamics, is an excellent computational resource. In addition to large scale operational vector supercomputers, NAS has experimented for many years with massively parallel supercomputing. The Ames nanotechnology initiative has focused on these resources.

  In addition to acquiring, configuring and maintaining the supercomputers, a nationwide network, and a large local network of workstations, NAS has developed tremendous expertise and capabilities in supercomputing related software such as:

  - Parallel algorithms and tools
  - Visualization
  - Virtual reality
  - Supercomputer benchmarks
  - Mass storage
- **Computational chemistry**. The NASA Ames computational chemistry branch has long exercised their world class expertise to understand atmospheric and space chemistry (such as the effects of low Earth orbit atomic oxygen bombardment) affecting aircraft and spacecraft. Turning to nanotechnology, they have used their molecular structure and classical dynamics expertise to design nanosize tools and components, determined reaction mechanisms and rates to address questions of mechanosyntheses, and

are addressing questions of entropy and finite temperature on the stability of nanodevices.

- **Computational molecular biology**. Collaboration between the nanotechnology group and computational molecular biologists at Ames has just begun. The biologists have been studying hypothetical molecular mechanisms that may have existed in early proto-cells. This is part of investigations into the origin of life. Similar mechanisms are of considerable interest in nanotechnology. This group has recently made a very interesting biological computational nanotechnology proposal.

In addition to world class expertise in the science and technology critical to computational molecular nanotechnology development, Ames is located in California's Silicon Valley. This provides close proximity to first rate universities such as Stanford and U. C. Berkeley as well as many of the finest high technology commercial laboratories and manufacturing facilities in the world.

Current Activities

As of the summer of 1996, the Ames computational molecular nanotechnology initiative is involved in the following activities:

- Fullerene nanotechnology. The NanoDesign project is developing a hypothetical functionalized fullerene based nanotechnology. This project is presently focused on development of gears made of carbon nanotubes with o-benzyne teeth [Han 96], design software [Globus 96], parallelized molecular dynamics based on Brenner's potential [Brenner 90], and quantum calculations characterizing the teeth [Jaffe 96a]. This work points to a nanotechnology that is relatively synthetically accessible.
- Diamonoid mechanosynthesis. This work investigates reaction pathways for diamond creation.
- Properties of clusters. This work investigates the properties of matter for clusters up to sizes exhibiting bulk properties.
- Nanotube strength. The tensile strength of various carbon nanotubes is determined using Brenner's potential [Brenner 90].
- Entropy and temperature effects. Methods are under development to address questions of entropy and finite temperature on stability of nanodevices.
- High density atomically precise memory. See above [Bauschlicher 96].
- Laplacian of the Electronic Charge Density. This project uses FAST to visualize and understand molecular electronic structure and reactivity.
- A grant program in computational nanotechnology (see the synopsis). Proposals were due on 15 October 1996. We expect another call for proposals next year.
- The NAS parallel supercomputers are supporting six 1997 operational year proposals in computational molecular nanotechnology; up from one in 1996. Computational scientists from CalTech, Harvard University, North Carolina State University and the University of Kentucky, among others, will use the NAS computers to study nanotechnology. Parties interested in access to the NAS parallel supercomputers for preliminary investigations to prepare for 1998 operational year proposals should contact the author.
- A workshop on computational molecular nanotechnology sponsored by NAS was held on March 4-5, 1996 at NASA Ames Research Center.

A number of collaborations with major universities and industrial laboratories are underway:

- Dr. William Goddard at CalTech and Ralph Merkle at Xerox PARC to use NASA computers to

simulate the dynamics of large nanotechnology systems. The first results of CalTech's work is a molecular dynamics simulation of a Drexler and Merkle's Molecular Planetary Gear [Gao 96].
- Dr. Don Brenner of North Carolina State University to parallelize his reactive hydrocarbon potential.
- Dr. Todd Wipke at UCSC to develop software to automatically design molecular parts for nanotechnology, with particular emphasis on self-assembly.
- Tom McKendree at Hughes to explore software issues common to automated automobiles and a replicating swarm concept under development at NASA Ames.

Current Resources

The NAS computational nanotechnology group consists of one civil servant and three contractors, all working full time. The group has six SGI and two IBM workstations. The workstations run Cerius2, Insight/Discover, Gaussian, rasmol, and xmol computational chemistry software in addition to codes developed in-house and with our collaborators. Most large scale computation is performed on the NAS parallel supercomputers. In addition, the NAS budget includes $600,000 in research grants for fiscal 1997. Finally, the entropy work discussed above is supported by the Ames' Director's Discretionary Fund.

Milestones

Our ultimate goal is to use programmable molecular machines to build aerospace systems; and our piece of the problem is the computational aspect. This is a long range research problem which is not yet well understood. Therefore, detailed monthly milestones are not only meaningless, but potentially counterproductive since promising avenues may be abandoned to meet possibly irrelevant short term goals. With this in mind, we have established ambitious long term goals for the project:

- Develop a software environment conducive to research within one year. The project is approximately one year old and two software environments are in place: 1. the NanoDesign [Globus 96] software for development and 2. the Cerius2 and Insight/Discover commercial computational chemistry software for standard operations and small, special purpose development efforts.
- Develop a numerically validated atomically precise replicator point design within five to seven years. The system should be able to reproduce and build something of aerospace interest. The chosen product is any long thin structure with tensile strength comparable to diamond. Such structures are necessary for orbital towers in the very long term. However, any increase in fiber length should be of great near term value in aerospace composites production. The replicator design may use either terrestrial or orbital conditions and does not necessarily need to be efficient or synthetically accessible although these properties are desirable.
- Develop a molecular manufacturing CAD system in ten to fifteen years. Searching the space of all possible molecular manufacturing systems for efficient and synthetically accessible systems is extremely difficult. The CAD system is to support such an engineering development. The system must support environmental conditions consistent with terrestrial laboratories and orbital conditions where micro-gravity and hard vacuum are readily accessible.
- Develop a numerically validated, synthetically accessible, efficient molecular manufacturing system design within fifteen to twenty-five years.

Along the way most results will be published in the literature and made available on the NAS WWW server. Also, wherever possible collaborations with experimentalists will be established to validate numerical results.

The second milestone is expected to be a research project using in-house staff and research grants to universities and industrial research laboratories. The last two milestones are expected to be, in part, achieved through contracts to develop specific, specified software and produce molecular designs. In all cases, heavy use of the NAS supercomputer center is expected to be crucial.

We recognize that these are ambitious goals that probably cannot be reached without additional resources, but there is some reason to believe that the nanotechnology effort may be expanded in the future.

Research Areas

The following research areas have been identified as important to computational molecular nanotechnology. Those under active investigation by Ames or our partners are **strong**.

fullerene nanotechnology	**diamonoid mechanosynthesis**	synthetic self assembly	protein design
ab initio simulation	**molecular dynamics simulation**	meso-scale simulation	long time scale molecular simulation
finite element simulation	simulation integration	**visualization** and virtual reality	artificial intelligence application
meso-scale concepts	**materials simulation**	test and validation	**software concepts**
terrestrial replicator-assemblers	orbital replicator-assemblers	**molecular manufacturing CAD**	**component design**

Closely Related Projects

There are a couple of closely related projects. Plans for nanotechnology and these projects have been developed together. The other two projects are:

- Petaflops computing: development of these supercomputers benefits from near-molecular manufacturing and provides necessary computer power for advanced computational molecular nanotechnology.
- Semiconductor device modeling using NAS parallel computers: aids in development of faster supercomputers for computational molecular nanotechnology and provides near/mid term practical results such as the optimization of CVD process by designing virtual reactors.

See the NAS business plan for details of these projects and computational nanotechnology.

Conclusions

- Nanotechnology, while high risk, promises enormous payoffs for NASA missions.
- Computational nanotechnology is necessary, but not sufficient, for success. A corresponding experiment effort is required to realize full potential of this research effort.
- Massive computational resources will be required, and computational nanotechnology requirements must influence supercomputer center development.

- NASA Ames has the necessary expertise, facilities and charter to lead computational molecular nanotechnology research.
- Substantial spin-offs can be expected.
- NASA Ames has a small but growing program in computational molecular nanotechnology and is well placed to lead computational nanotechnology into the next century.

References

To companion papers.

Web Work: Al Globus