Brian Helfrich has more than 10 years of experience in computer technology research and development. Brian designed and implemented NanoHive-1, a modular, cross-platform simulation framework for molecular modeling. He's also the creator of NanoHive@Home, a distributed computing system used to simulate large-scale nanotech systems that draws its computing power from otherwise idle computers sitting in people's homes. Brian came to Nanorex with the acquisition of Nano-Hive. Prior to Nano-Hive, he was a senior member at Telelogue, a company he helped spin out of Telcordia Technologies (formerly Bellcore Labs) where he designed, managed, and patented the development of high-throughput, high-availability, distributed computing systems. Before Telelogue, he was the Director of Technology at Aspen Marketing where he directed their marketing technologies initiative in the web and wireless applications space. And prior to Aspen, he worked at Telcordia Technologies where he was a research scientist working on automated speech recognition applications, visualization of complex systems, and new business development. Brian holds a B.A. degree in Computer Science from Berkeley. While earning his degree, he worked as a programmer and general technologist for a handful of Internet and technology start-ups such as Rubric (acquired by Kana), Internet Profiles (acquired by Topicalnet), and NonStop Logistics. Brian is an accomplished technologist and is expert in translating a business's technology needs into innovative technology solutions.

NanoHive@Home – Nanosystems Simulation

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Abstract

NanoHive@Home is a distributed computing system used to accurately simulate nanosystems too large to be calculated via conventional means, thereby enabling further scientific study in the field of nanotechnology.

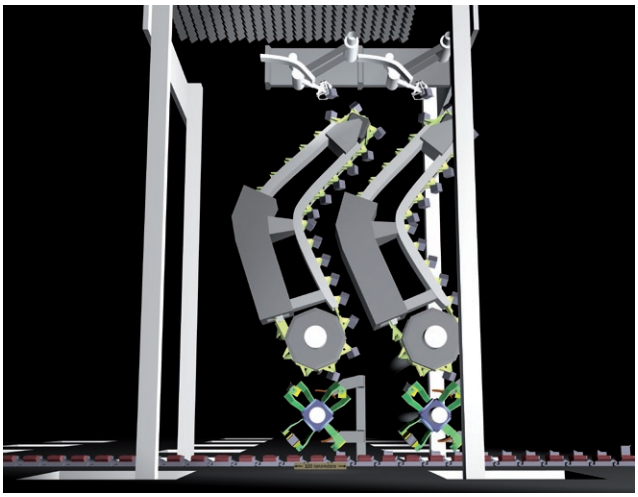
Introduction

Nanotechnology is the science and engineering of matter at the atomic and molecular scale. At this scale, the physical and chemical properties of materials are fundamentally different from materials at micrometer or larger scales. These fundamental differences are both the cause of amazing challenges today and potentially amazing benefits in our future.

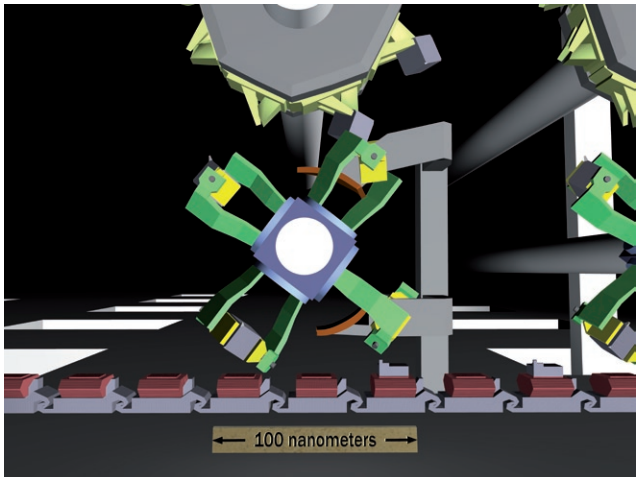
As we increase our understanding of nanotechnology and our ability to manipulate matter at this scale, a broad range of vital applications begin to emerge. For example, pathologists currently diagnose most cancers based on the shape or other visual characteristics of a tumor and its cells. This technique does not allow for early detection since a tumor must already exist. Recently, scientists have developed a strategy to recognize cancer cells amidst normal cells using the differences, at the molecular level, between any two types of cells[1]. This cell selection technique holds great promise in developing specific molecular probes for early cancer diagnosis, and is an example of how expanding our working knowledge into the nanoscale can benefit humanity.

Another goal of nanotechnology that will ultimately have the most profound influence in our world is molecular manufacturing. Molecular manufacturing would enable the construction of nanometer scale components, and then the assembly of those components into micrometer-scale mechanisms, or *nanosystems*. Nanosystems are atomically precise assemblies of nanoscale components that combine to form some complete machine. Nanosystems can be so large as to be microscopic, or even visible to the naked eye[2].

One proposed implementation of molecular manufacturing is the nanofactory[3]. As input material, the nanofactory would take a set of feedstocks made up of carbon-rich substances, such as natural gas, and other common, inexpensive substances like urea, acetone, and silicone that provide the necessary atomic building blocks, such as nitrogen, oxygen, and silicon. The nanofactory would then extract the desired elements from the feedstock using sorting mechanisms[2] and assemble them into sub-components[4,5] that themselves get assembled into a final product[6]. This nanofactory could possibly be small enough to fit on a desk, yet be able to produce a wide variety of high quality, low-cost products, such as laptop computers with a billion CPUs or medical nanorobots.



This nanofactory mechanism takes cubes of diamond and assembles them into the sub-component at the top. As more and more layers are added to the sub-component, it slowly extrudes out of the surface of the mechanism.
(Image © 2006 John Burch, Lizard Fire Studios, www.lizardfire.com)



This is a closer view of the mechanized wheel that takes the diamond cubes from a conveyor belt to pass up to the sub-component being assembled inside a nanofactory.
(Image © 2006 John Burch, Lizard Fire Studios, www.lizardfire.com)

One such medical nanorobot could be the "respirocyte", an artificial red blood cell able to deliver 236 times more oxygen to the body than natural red blood cells. It would have several sensors and an onboard nanocomputer that physicians could program via acoustic signals. Applications of the respirocyte could include transfusable blood substitution, treatment of fetal and newborn child disorders, lung disorders, enhancement of cardiovascular procedures, and prevention of asphyxia[7].

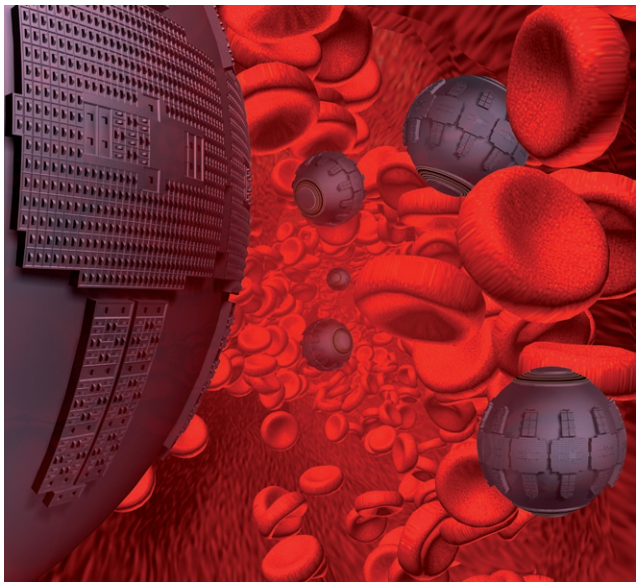
Accompanying the benefits of nanotechnology are potential risks. For example, there are concerns that the disposability of nanodevices would lead to "nano-litter" which could build up in the environment and become a health hazard. This emphasizes the importance of developing our understanding of nanoscale phenomenon so as to better reduce the potential risks.

Before we can productively orchestrate the assembly of molecular mechanisms and nanosystems, sufficient nanotechnology theory must be developed. Much of this theory will be validated, or even derived, from the virtual experimentation afforded by the computer simulation of nanospace. Simulation permits us to perform experiments with nanosystems that we cannot yet build nor probe, enabling the optimization of components and interactions before a single structure is actually fabricated in the laboratory. Also, simulation enables us to perform experiments that may be too expensive, or even hazardous, to perform otherwise. The accurate simulation of nanosystems is critical to the testing and exploration of our theories and ideas about nanotechnology.

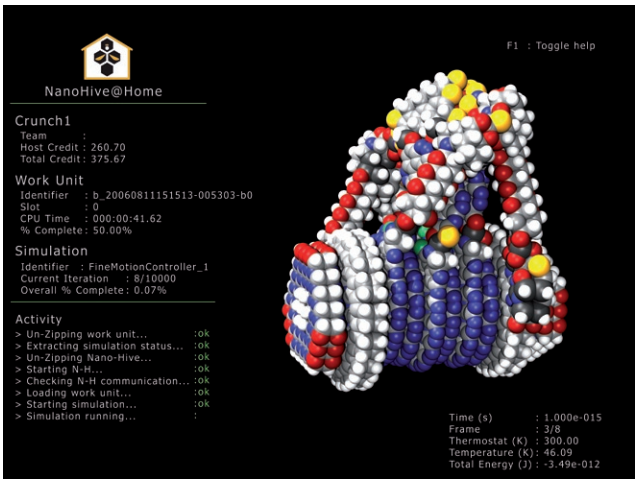
NanoHive@Home

Molecular simulation is based on mathematical models of atomic and molecular properties. Quantum mechanics is a mathematical representation that models atomic and subatomic systems, providing an accurate model for molecular simulation. The Schrödinger equation, which embodies the complete description of the space and time dependence of quantum mechanical systems[8], while utterly accurate, is prohibitively difficult to solve for all but very small molecules. Several computational approximations to the Schrödinger equation have been developed[9,10,11], each trading computation accuracy for speed, and therein lies the crux of molecular simulation. We can generate very accurate results, but the computation will take a long time. Alternatively, we can simplify the computation to speed things up, but at the expense of chemical accuracy of the system being simulated.

There are two general types of molecular simulation – molecular mechanics and *ab initio* – with several hybrids



The respirocyte is a nanomedical device by designer Robert Freitas that acts as an artificial red blood cell. This image shows respirocytes and red blood cells flowing through a blood vessel, most likely a small artery. In the foreground at left, we see a closeup of the respirocyte surface including the sensor apertures and the individual rotating disks (containing active binding sites) comprising each of the thousands of sorting rotors. At lower right, we see another nearby respirocyte with its pumping station geometry and polar barcodes clearly visible.
(Image (C) 2002 www.e-spaces.com AND rf@rfreitas.com)



The NHAH screensaver graphics. Participant statistics, information about the work unit being calculated, and information about the simulation are shown at the left. The center shows an animation of the nanosystem being simulated. Animation data, and some measurements from the simulation are shown at the lower right. (Image © 2006 Nanorex, Inc.)

of the two. *Ab initio*, or quantum mechanical simulation approximates the Schrödinger equation; molecular mechanics, on the other hand, may completely ignore quantum mechanical effects in adopting a force field approach. Force fields are formulas that describe the potential energy of a system of atoms, and may be parameterized based on empirical data, or quantum mechanical simulation. The force field approach provides for very fast calculations, at the expense of chemical accuracy. Hybrid approaches to molecular simulation use different techniques for different regions of a system[12]. Molecular mechanics is used where speed is more important than accuracy, such as, the large static housing of some molecular mechanism. Quantum mechanical simulation is used where accuracy is paramount to the purpose of the simulation; an example is the region where a chemical reaction (the breaking or formation of a chemical bond) is to take place.

Despite hybrid techniques, there are still limitations to the size of molecular systems that can be simulated. Small systems of hundreds or perhaps thousands of atoms can be simulated with a high level of quantum mechanical accuracy on single computing clusters, but systems of hundreds of thousands, or millions of atoms are prohibitively large for calculation with in-house computing hardware.

NanoHive@Home (NHAH) is a distributed computing system used to accurately simulate nanosystems too large to be calculated via conventional means, thereby enabling further scientific study in the field of nanotechnology. By distributing the computation of molecular simulations over tens of thousands, or hundreds of thousands of computers via the BOINC platform, NHAH is able to simulate nanosystems with sufficient quantum mechanical accuracy for scientific and engineering study.

NHAH is sponsored by Nanorex, Inc., which develops computational modeling tools made specifically for the design and analysis of productive nanosystems. Nanorex's management and scientific advisory board consists of several pioneers in nanotechnology, including Dr. K. Eric Drexler, often described as the "father of nanotechnology", and Dr. Ralph Merkle, co-recipient of the 1998 Feynman Prize for Nanotechnology. The NHAH team works with scientists and engineers developing large nanosystems to understand which simulations will result in publications that would have the biggest impact in the field. For example, some of the first simulations will be for the testing and development of a series of nanofactory mechanisms.

NHAH is completely open-source and free. It is a not-for-profit project with all results made available to the public domain, free and clear.

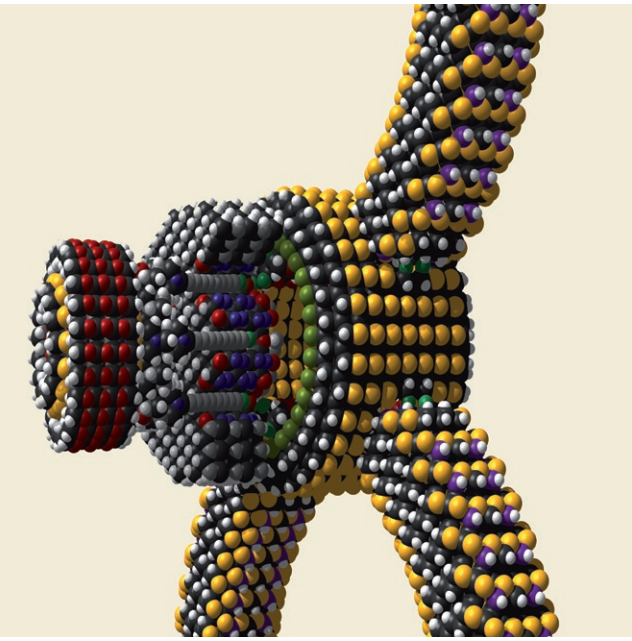
The simulation software that NHAH employs is Nanorex's NanoHive-1 Nanosystems Simulator (NH1). NH1 is a state-of-the-art simulation framework designed for scalability across distributed and parallel computing networks from the ground up. It has a unique and highly flexible plugin architecture that can incorporate the capabilities of any simulation engine. For example, one plugin wraps the capabilities of the quantum mechanics library developed by Sandia National Laboratories, the same library used in their Massively Parallel Quantum Chemistry program[13].

NHAH takes advantage of the BOINC screensaver graphics feature to show an animation of the simulation results from the initial conditions to whatever point the simulation is currently at – so participants will see more and more of the result as they compute more and more NHAH work units. The animations are essentially schematics of the molecular systems with balls of different size and color representing the atoms of different types. The participants will be able to rotate, pan, and zoom the animations, and switch between different molecular representations. This interactive feature, combined with explanations of the simulation from the NHAH website, can help participants to get a clear sense of what is going on with the simulation they are helping to compute.

Planned Simulations

Nanofactory

Some components of the design for the nanofactory, described in the introduction above, have already been designed in atomic detail. NHAH will be used to test and further develop the proposed designs in simulated nanospace.



This image shows the molecular structure of some of the inside components of the sorting pump for the nanofactory. The cutaway shows the flourine-tipped carbon rods used to sort the various stock molecules from the adjacent chamber. Molecular ducts channel feedstock in, and sorted molecules out of the chamber. (Image © 2006 Nanorex, Inc.)

The simulations will be conducted in coordination with Dr. Damian Allis, who is a theorist in residence at the Center for Science and Technology, Syracuse University, and Research Scientist at Nanorex, Inc. The simulations will focus on the following mechanisms:

- Sorting pump – sorts specific molecules from a mixed feedstock
- Delivery wheel – captures and delivers the stock molecules into the assembly process
- Abstraction – pulling select atoms off a molecule to prepare it for deposition
- Deposition – depositing the prepared molecule onto the product

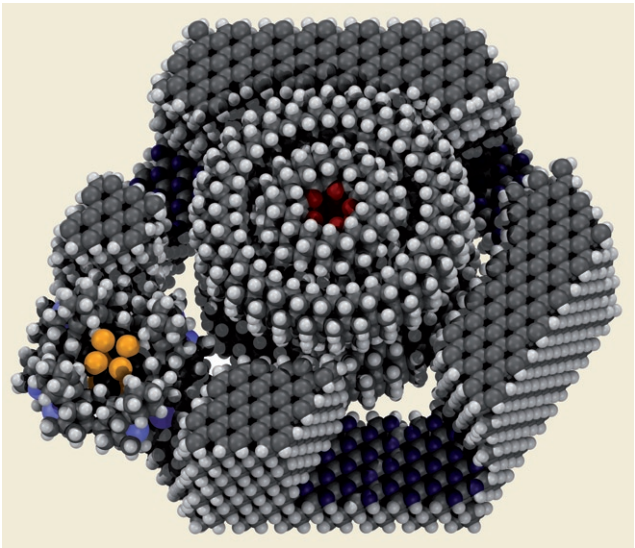
HiveArena

With HiveArena, contestants enter their nanodevices into the NHAH simulation space, and compete against each other to achieve some specific goal. The purpose of HiveArena is to leverage the ingenuity of scientists, engineers, inventors, and students to accelerate research and development in nanotechnology.

This image shows the molecular structure of a sorting rotor found downstream of the sorting pump (the top of the housing has been removed to show the inner mechanisms. The larger rotor in the center sorts acetylene molecules from larger hydrocarbons such as benzene, and delivers them to the smaller wheel at the lower left, where they are transferred to the tooltips that perform the actual assembly. (Image © 2006 D. G. Allis, www.somewhereville.com)

There will be two event types in HiveArena, the contest event and the challenge event. The contest event is designed such that its goals are known to be achievable, albeit with state-of-the-art nanotechnology engineering skills. Contestants will be supplied with an example of a nanodevice capable of achieving the basic goal, and the winner will be the team that produces the nanodevice that best achieves the contest goal. For example, one contest event will be the sprint – contestants will be supplied with a constant magnitude of energy for the duration of the race, and the winning nandevice will have traversed a surface from point A to point B in the shortest time. Another contest event will be a long distance race – contestants will be supplied with a finite amount of energy with which to race to point B.

The challenge event goals are designed to be at the cusp of our nanotechnology engineering knowledge. There will be no known example device capable of achieving the goal; to win, teams must produce a nanodevice that is able to complete a task that tests all of the requirements of the challenge. Winning teams will have pushed the envelope of our knowledge to achieve remarkable nanodevices. Some examples of these challenges may initially include nanoscale power sources, motors, or inter-device communications systems. Later challenges may be nanobots, or swarms of nanobots, capable of seeking out HiveArena-supplied virus



nanobots, identified with special molecular signatures, and eliminating them. Challenge events that have been won may then turn into contest events to further help drive research and development.

NHAH participants will, of course, get to see the contests and challenges un-fold before anyone else via the screensaver animations. And since the visual part of the simulation results are quite like movies, the teams that crunched work units towards the simulation could appear in the credits at the end, listed in order from most work units crunched to least. Additionally, winning teams could get to decide which songs to put in a simulation video soundtrack.

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