CROSSING BOUNDARIES – NANOSCALE SCIENCE AND TECHNOLOGY

> A biological system can be exceedingly small. Many of the cells are very tiny, but they are very active. They manufacture various substances, they walk around, they wiggle, and they do all kinds of marvelous things – all on a very small scale. Also, they store information. Consider the possibility that we, too, can make a thing very small which does what we want – that we can manufacture an object that maneuvers at that level.
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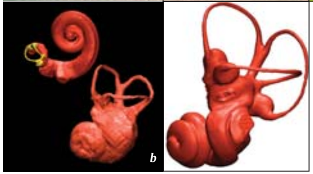
> **Richard Feynman, 1959 speech, "There's Plenty of Room at the Bottom"**



Interdisciplinary science is perhaps most dramatically displayed in the new field of nanotechnology, where, as OSTP Director John H. Marburger puts it, "the notion that everything is made of atoms finally becomes operational."

Nanotechnology, with IT as both a major driver and an enabler, is developing at the intersection of materials science, engineering, physics, chemistry, and biology. With dimensions of only a few billionths of a meter, nanoscale structures are typically investigated with advanced IT capabilities that enable scientists to see and manipulate individual atoms and molecules as well as simulate nanostructural dynamics with mathematical precision. The NITRD agencies, which pioneered tools for nanoscience through research on next-generation semiconducting and superconducting materials, chip architectures and microfabrication processes, MEMS devices, optoelectronic/photonic technologies, and visionary molecular computing concepts, remain at the forefront of nanoscale discovery. DARPA, DOE/SC, EPA, NIH, NIST, NSA, and NSF are core participants in the National Nanotechnology Initiative, an Administration R&D priority for FY 2004 as is the NITRD Program.

Nanotechnology research leads in many long-term directions, including custom-designed materials with properties unlike any we know today, revolutionary techniques for combating disease and maintaining health, and ultra-miniaturization of computing and other mechanical and electronic systems. But the nanoscale realm holds many mysteries. We do not yet understand, for example, how the laws of physics operate in nanoscale structures – their behavior cannot be predicted from physics at the macro scale. Even so, nanotechnology promises an extraordinarily diverse range of innovations ahead, as suggested in the following examples of current research advances.

In work awarded the top honor of the International Conference on Computational and Experimental Engineering and Sciences, a NASA computational nanoscientist and his team have engineered a process to fabricate carbon nanotubes – the strongest new material yet devised, with the ability to be either a semiconductor or a metal – and have successfully demonstrated nanotubes in semiconductor logic circuits. The goal of this and related research is nanoscale computing, sensing, telecommunications, and avionics components to radically reduce the weight and scale of spacecraft. The versatile nanotubes are also being used in strong lightweight polymer composites for structural applications. NASA studies indicate that replacing aluminum aircraft structure with carbon nanotube composites could reduce the dry weight of large commercial aircraft by 80 percent, with a 25 percent reduction in fuel use.

Biomolecular motors

One of the most astonishing areas of nanoscale discovery is molecular biology, where scientists, such as those in the Genomes to Life effort, are trying to understand how the work of life actually gets done at Feynman's "bottom" level. Like tiny vehicles, many types of protein physically move or transport subcellular material. Following on the new knowledge about proteins' complex shapes, investigators are examining "biomolecular motors," proteins that change shape to generate force, or torque, in order to carry out tasks.

In an elegant application of electron microscopy and IT-driven optical tweezer techniques, researchers funded by DOE, NIH, and NSF have not only measured in real time the power of a biomotor but demonstrated what may be a key mechanism of viral infection. The research showed that bacteriophage phi-29 – a virus that destroys soil bacteria – packs large amounts of its DNA into its external shell, called a capsid, a space about 6,000 times smaller than the DNA's normal volume. The packing action requires 57 to 60 piconewtons of force – which the researchers describe as the equivalent of lifting six aircraft carriers if scaled up to human dimensions. The internal pressure generated in the capsid is 60 atmospheres – about 10 times the pressure in a champagne bottle. The researchers propose that, like a champagne cork, the compressed viral DNA, which cannot replicate unless it enters a host cell, explodes into the healthy cell to which the virus has attached.

Getting themselves together

Another facet of nanoscale molecular research examines how both organic and inorganic atoms and molecules organize themselves into larger structures. Understanding what scientists call "self-assembly" is a critical step toward the ability to custom-design novel materials for such uses as targeted delivery of drugs and therapies inside the body, protective coating and encapsulating, imaging, and automated microfabrication. Advanced IT techniques have confirmed the fantastically intricate lattice structures formed by inorganic atoms and molecules such as in metal alloys. But self-assembly processes in organic matter, governed by genetic instructions, are less well understood. NSF-supported researchers in February 2003 reported a milestone in such work, achieving a self-assembled liquid crystal lattice of 255,240 atoms in branching molecules called dendrons, which make up the protein coat around viruses. The result, published on the Web site of the journal *Science,* was not only the most complex organic structure yet created via self-assembly, but also the first organic compound to assume an intricate structural form previously seen only in metals.

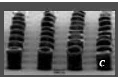
Revolutionary computing devices

Just as IT is critical to the future of nanotechnology, nanoscale science is seen as the means of surmounting IT's "red brick wall" – the approaching physical limit to the miniaturization of chip architectures, and thus to advances in computing speeds. The NITRD Program encompasses research in biomolecular chemistry and quantum physics as potential sources of revolutionary computation and data-storage technologies. One gram of DNA, for example, stores the equivalent of 10^8 terabytes of digital data – about ten thousand times the capacity of today's largest mass storage systems. In 2002, University of Southern California researchers funded by DARPA, NASA, NSF, and the Office of Naval Research achieved a notable biocomputing success, using DNA molecules to reach the correct answer to a computational problem with 20 variables and more than a million possible solutions. Previous DNA experiments had solved problems with a maximum of nine variables. "This landmark study," said *Science,* "proves that molecular computation is not a far-fetched possibility but a quickly evolving discipline that may have major impact on more established disciplines such as biotechnology."

Quantum IT research begins with the fact that subatomic particles (atomic nuclei, photons, electrons, etc.), which follow the unique laws of quantum mechanics, exist – in computing terms – partly in both the binary 0 and 1 states at the same time. In theory, a particle's superposed quantum states, called "qubits," could provide the basis for exponentially higher calculation speeds than are possible in the binary world.

In 2001, NIST researcher Eric A. Cornell and two other Americans shared the Nobel Prize in Physics for proving the existence of a near-motionless atomic state – the Bose-Einstein Condensate – that had long been theorized but not achieved empirically. Since the evanescence of quantum states (they disappear in quadrillionths of a second as atoms spin and move) is a fundamental barrier to quantum computing, the ability to generate the low-energy Bose-Einstein state marked a significant advance. NIST and Massachusetts Institute of Technology researchers have proposed a quantum computer design based on this work. DARPA, DOE/SC, NASA, NSA, and NSF researchers also are exploring ways to exploit nanoscale phenomena in quantum information systems.

a) *Elaborate lab technologies and data mining enabled NSF-supported researchers to identify a protein – glucose-6-phosphate isomerase, necessary to initiate pregnancy in ferrets – that also plays a role in cancer metastasis.* ***b)*** *An international team, using visualization software developed for NIH's "Visible Human" data, has discovered a secret of whales' and dolphins' swimming skill – 3-D image reconstructions from CT scans of early and contemporary skulls show even the earliest cetaceans had mammals' tiniest semicircular canals for their size. Left to right, dolphin, early whale, bushbaby.*



c) *Carbon nanotubes, made with NASA fabrication technique. Each tube is about 100 nanometers wide.* ***d)*** *In biomolecular motor built by Cornell University researchers, adenosine triphosphate (ATP) enzyme powers nickel propeller at 8 revolutions per second. Post is 200 nanometers tall, propellers about 750 nanometers long.*