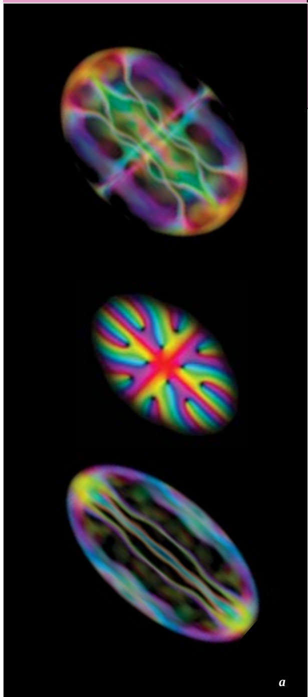
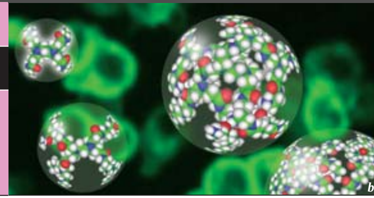
Foundations for SCIENTIFIC LEADERSHIP

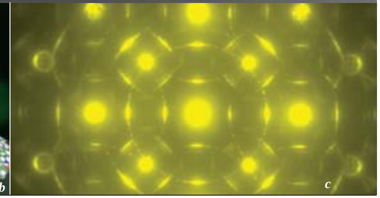
CROSSING BOUNDARIES – INTERDISCIPLINARY SCIENCE

Today the boundaries between all disciplines overlap and converge at an accelerating pace. Progress in one area seeds advances in another. New tools can serve many disciplines, and even accelerate interdisciplinary work.

Rita R. Colwell, Director, National Science Foundation, February 2003







Such disciplinary interconnections, many scientists believe, will shape the scientific enterprise for the rest of this century, with teams of investigators tackling complex problems whose solutions call for knowledge, methods, and technical skills from a variety of fields. One early indicator of the trend: In 1990, only 6 percent of 1,600 researchers using DOE's synchotron light sources to study atomic particles were from the life sciences; today more than 40 percent of the more than 6,000 researchers using these instruments are bioscientists.

Scientists traditionally have tried to understand Earth's environment by taking sample observational measurements – such as of water tables, rainfall, cloud cover, air flows and temperatures, ocean currents, vegetation and animal distributions, photosynthesis rates, polar ice thickness – and theorizing about how all these factors fit together. In this century, advanced information technologies will make it possible to see how such influences work together and to develop deeper knowledge of the environment as a complex system of systems interacting with and affected by humans.

Complexity in biological systems

A major NSF initiative, Biocomplexity in the Environment, is funding a wide range of multidisciplinary efforts to map biocomplexity systemically, from the genetic and submolecular scale to macroclimatic forces and effects of human activities. Researchers at the University of North Carolina, for example, have developed a real-time environmental scanning system that couples chemical-detection technologies with tomographic mapping capabilities to compute pollution maps covering large geographic areas. The maps can depict multiple chemicals at once, a significant factor in examining chemical constituents and dispersal of industrial and agricultural residues.

The emerging field called chemical genetics depends on IT capabilities for rapid discovery of microscopic research tools that will narrow the gap between what bioscientists are learning about human proteins and applications of these findings in clinical medicine. Chemical genetics aims to identify small molecules that either activate or deactivate protein functions. Researchers can use these "molecular probes" to more quickly analyze how proteins malfunction in such diseases as cancer, multiple sclerosis, and Parkinson's. Harvard University chemists sponsored by NIH's National Cancer Institute have created ChemBank, an online repository of small-molecule chemical structures and properties and accompanying IT analysis tools for biologists to contribute to and use. The Harvard lab is systematically identifying molecular probes in an automated screening process that uses imaging and software tools to capture data on the effects of various small molecules on protein behavior.

How the other half lives

In DOE/SC's Genomes to Life program, hundreds of Federal, industry, and university researchers from the biological, environmental, physical, and computing sciences are engaged in a long-term effort to extend IT-based genetic research methods to the world of microbes. These tiny organisms, which make up more than 50 percent of Earth's total biomass, control biogeochemical cycles and affect soil productivity, water quality, and global climate.

In that sophisticated biomachinery – which can use even toxic wastes as energy sources and can produce such diverse energy products as hydrogen and methane – scientists see means for developing clean energy, removing excess carbon dioxide from the atmosphere, and remediating contaminated environments left as a legacy of the Cold War. The research is applying "high-throughput" computational methods developed in the Human Genome Project to identify microbial proteins and their functions. But it will also require computing power and tools far beyond today's levels to develop data about and analyze the behavior of large microbial systems and colonies, as well as their multiscale, multidimensional interactions with the environment.

Scientists with multiple skill sets

Even the work of individual scientists – such as Surya Mallapragada, an Iowa State University researcher named one of the world's top 100 technical innovators for 2002 by *Technology Review* – highlights the multidisciplinary flow of contemporary science. In research supported by DOE and NSF, the materials chemist and chemical engineer is combining biomolecular chemistry, advanced IT capabilities, and nanotechnology in a technique to regenerate nerve cells, which are not amenable to methods used with other types of cells. On an ultrathin (a few thousandths of an inch) biodegradable polymer film that she and her team engineered, the researcher uses digitally controlled laser and ion-reactive etching instruments to make grooves a few microns (millionths of a meter) deep. The grooves are then coated with protein and Schwann cells (which in the body form nerve cells' myelin sheath) and peripheral nervous system axons are placed in each sheath-like groove. The axons have grown at a rate of three or four millimeters daily, and Mallapragada has successfully applied the technique to regenerate sciatic nerves in rats. She is examining how to extend the concept to central nervous system cells, such as those of the optic nerve, which pose even more difficult regeneration problems.

a) Bose-Einstein Condensate (BEC), a new form of matter demonstrated by NIST researcher Eric Cornell and colleagues, earning them a 2001 Nobel Prize in Physics. BEC is created when atoms are supercooled to an almost motionless state. Simulation images show unique vortical patterns formed by BEC (bright areas indicate lower atom density) in quantum trapping experiments.

b) University of Michigan researchers are experimenting with dendrimers – spherical polymer molecules with a uniquely consistent branching chemical structure – as vehicles for identifying diseased cells, reporting their location, and delivering targeted therapies. Details on page 53.

c) DOE/SC-funded work at the University of Illinois Center for Microanalysis of Materials aims to understand the electrical properties of nanoscale heterostructures such as layered oxide thin films for future electronics.