Research and Education Opportunities in Mathematical and Physical Sciences

Learning from Biology

Lessons drawn from biological systems provide insight into physics, chemistry, materials science and mathematics. A single cell is capable of synthesizing thousands of molecules. The brain stores and processes information more efficiently than any computer. Biomechanical systems are lightweight yet survive abuse and can climb a jumble of rocks. A bird can fly ten thousand miles on the energy content of several ounces of fat.

An important challenge for the physical sciences is to turn these lessons from the biological world into solutions for some of the most important technological problems facing society. Can we develop artificial catalysts capable of inexpensively making drugs and other chemicals without toxic waste? What new paradigms of information storage and computing will allow us to go beyond Moore's law? How can we devise materials and mechanical systems capable of operating with minimal environmental impact in rugged, hostile terrain or under the ocean? How do we maintain a high standard of living using less energy from sustainable sources?

Learning how biological systems work has already inspired new technology. The composite protein-mineral structure that makes it possible for sea shells and bone to resist fracture has been mimicked to make very tough plastic, metal, and ceramic composites. By applying the mathematics of spin glasses to model the behavior of the nervous system physicists have developed neural networks capable of solving pattern recognition problems very efficiently.

The physical and biological sciences often nourish each other. For example, the mathematics and physics of x-ray crystallography, originally devised to understand the structure of simple chemicals, has provided much of our understanding of molecular biology. Crystallography has, in turn, been advanced by the difficulties of understanding the structure of viruses.

Because of advances in our understanding of both biological and physical sciences, we are in an unprecedented position to take advantage of these lessons from the biological realm. The interaction between the physical and biological sciences raises both to higher levels, and in doing so serves the intellectual and physical needs of modern society.

Beyond Moore's Law

The central goal behind this research initiative was articulated in the FY 2008 budget request for MPS: "To go beyond Moore's Law will require entirely new science and technologies, as well as new algorithms and new conceptual frameworks for computing." It is imperative that this remain a central focus for MPS research next year and beyond.

To design hardware capable of computing performance well beyond the next generation of computers will require one or more new technologies based on fundamentally new science. The change will be as dramatic as that achieved when the vacuum tube was replaced by the transistor. The physical science programs at the NSF will focus on developing several possible scientific approaches, including quantum control, carbon-based systems, molecular electronics, spintronics, and single electron transistors. It is not yet clear which of these approaches will end up in commercially competitive products. For this reason, it is essential that the NSF support a diverse set of possible breakthrough technologies. As was the case with silicon-based computing, the nation that leads in these efforts will have substantial economic advantages in the world economy.

Tomorrow's computers will be more capable and faster. But 50 years from now computers will be DIFFERENT. New approaches are beginning to be explored, including quantum computing (whose basic operations are Hermitian rather than Boolean) and DNA computing (whose essence is the vast parallelism achievable in molecular systems). The design and manufacture of such computers poses many challenging problems in materials science, physics, chemistry, and biology. And the efficient use of such computers poses huge challenges to mathematics and computer science in the design of new algorithms and software.

Alternative models of computing will not replace silicon, just as video-on-demand has not replaced broadcast TV. But different models have different strengths. New approaches like quantum or DNA-based computing have the potential, if successful, to solve problems presently far beyond the realm of possibility. Indeed they would change the very nature of the questions we ask.

Understanding and Controlling Emergent Behavior in Complex Systems

Nature abounds with examples of complex systems in which new behavior emerges on large scales. In biological systems emergent behavior has developed through evolution: insects cooperate, hearts beat, and brains think. Emergent behavior also arises from general physical laws: atoms form crystals, storms form tornadoes, galaxies form spiral arms. Emergent behavior is also manifest in social and economic systems, e.g. in crime statistics and the stock market.

One of the grandest challenges facing science today is to understand and model such emergent behavior. Learning to predict emergent events such as earthquakes, hurricanes, and massive solar flares has important social and economic implications. Improved understanding of feedback in complex networks will lead to better control of epidemics. Techniques based on self-assembly and self-repair will lead to the design and manufacture of new materials and devices -- such as artificial skin and self-optimizing fuel cells. Since emergent behavior is ubiquitous, improved understanding will have far-reaching consequences across the entire spectrum of science and engineering.

While each complex system is different, many characteristics that recur across disparate fields are amenable to numerical modeling and simulation. Large-scale numerical modeling has become a key technique in essentially all fields involving complex systems, and provides results ranging from local weekly weather forecasts to the history and future of the Universe on giga-light-year scales. The increasing success of large-scale simulation is due not only to dramatic improvements in computer memory and speed, but also – perhaps even more – to the development of better algorithms. Algorithm development of this kind is extremely active across many disciplines at NSF.

Simulation is an essential tool for studying complex systems, but it is rarely adequate by itself. For many systems, even the development of an adequate numerical model is a major challenge. It is rarely possible to simulate all macroscopic and macroscopic length and time scales simultaneously. Development of "subgrid" models, or other methods of averaging over microscopic scales, is required to complete the systems of equations for a macroscopic system. In all fields, new methods and fresh understanding will be important for the efficient targeting of our computational resources.

The study of complex systems requires cross-disciplinary approaches. To give some examples: methods from statistical physics are beginning to have impact in neuroscience; nonlinear-dynamics-based models of synchronization, developed for applications in biology, can explain oscillations in physical systems as well; and insights from biological networks are suggesting techniques for the design of robust chemical reaction systems. The cross-cutting nature of this field makes it a natural candidate for an NSF-wide initiative.

Discovery from Massive Datasets

We have entered the Age of Information. In almost every area of science, technology, and commerce we face the task of organizing, analyzing, visualizing and interpreting huge quantities of data. At present, much of this information is used inefficiently, is stored in obsolescing forms, or ends up being discarded for lack of adequate tools. We need improved approaches and algorithms for both extracting insight from data and preserving data for future use. This is a fundamental scientific challenge, with far-reaching practical consequences.

Why do we have so much data? In some areas (for example astronomy, high-energy physics and genomics) automated processes are designed to collect, process, and archive huge amounts of information. In other areas (for example climate models, protein folding, cosmology, crystal growth, and turbulent combustion) simulations of complex physical systems generate huge, time-structured datasets, which include -- if we can extract it -- crucial information about their large-scale behavior. In still other areas (for example communications and sensor networks, electronic financial exchanges, and web-based surveys) the very sources of the data are themselves products of the information age.

What do we want to achieve? One goal is the detection and extraction of weak signals or rare events from noisy and high-volume datasets; this task is central, for example, to astronomy and homeland security. In some settings the signal will follow a template drawn from a large but well-defined set of known patterns; in other settings the class of signal patterns must be learned from the data itself. Another goal is the synergistic merging of diverse datasets; applications of this type abound for example in geosciences, ecology, astronomy, medical imaging, and economics. Combining datasets from different eras requires archiving techniques that keep data broadly accessible as systems change. High-frequency data pose special challenges; for example, the detection of credit-card fraud entails efficient real-time processing of streaming information. Dimension-reduction is a recurring theme: in weather prediction, genomics, cognition, and other complex systems, we can detect previously-unknown relationships between observables by finding low-dimensional approximations of high-dimensional datasets. The processing need not all be done by computers; improved visualization techniques will permit both professional scientists and trained technicians to assimilate more information and use it more effectively. Finally, new algorithms developed within individual scientific disciplines need to be analyzed to decide whether they might be effectively deployed in other domains.

Can we achieve these goals? The answer is yes, provided we invest now in the underlying science. The successful development of web search technology provides a hint of what is possible -- and of the intricate link between algorithms and applications. When we marvel at the ability of Google to sort quickly through petabytes of data to match keywords and phrases, we should also marvel at the recent algorithmic developments that make such searches possible. The sorting and pattern-matching techniques involved are only one example of the many types of algorithms that are needed to mine information and distill insight from oceans of archived raw data.

What science is required? Though the applications are diverse, there are many cross-cutting themes. Often they involve fundamental issues from statistics, computer science, or mathematics. For example: when should we use stochastic models to separate "signal" from "noise"? Can sparse representations like those used in data compression also be useful for extracting information from large data sets? Can dimension reduction tools be improved by using methods from geometry or topology? How can new approaches to and standards for data storage, sharing and confidentiality provide improved persistence of diverse datasets as hardware, operating systems, and algorithms evolve?

When will we achieve these goals? Research is unpredictable, but some things are certain. The Age of Information is already upon us. Its diverse challenges are driving new science. And our success in meeting these challenges will dramatically influence the pace of progress in almost every area of science and technology.

Developing the Scientific Workforce

Developing a diverse, globally engaged STEM workforce is an issue of paramount importance to NSF. In recent years, NSF has made progress on bridging critical junctures in STEM education pathways and on broadening participation in STEM disciplines. Further progress requires attention to the postdoctoral years and to the system of individual investigator grants, the main source of support for training young researchers.

One critical need is the development, implementation, and dissemination of best practices for the postdoctoral years, which form an extended transitional period between graduate education and establishment of an independent scientific career. The diversity of the STEM cohort tends to decrease during the postdoctoral period, as members of under-represented groups leave in disproproportionate numbers. At present, the career guidance postdoctoral fellows receive depends on local conditions and varies greatly in quality. Fellows are often unsure about what they should to do maximize their potential for staying active in STEM fields in the long term. Should they focus exclusively on acquiring more independent research experience? on demonstrating their ability to obtain grant funding? on acquiring teaching experience and proficiency? After the typically intense and narrowly focused Ph.D. experience, how can they broaden their knowledge base to gain entry to newly developing fields?

NSF should support individuals, institutes, and professional organizations as developers and providers of regional or national networking activities and professional development opportunities for postdocs. It is crucial to keep young scientists in the pipeline, facilitate their re-entry into STEM disciplines or re-training into new STEM fields and generally maximize the impact of the national investment in their education.

The system of Individual investigator grants, the primary vehicle for supporting the training of postdoctoral fellows and graduate students, is widely perceived to be less healthy than in the past. Success rates for single-investigator proposals in several divisions have dropped to 20%, and award amounts are frequently insufficient to sustain productive research programs. Severe and long-term consequences will develop if this situation is not improved. Because individual investigator grants are made to many scientists at diverse institutions, maintaining adequate levels of support improves the chances for success of the entire scientific enterprise.

Higher success rates, adequate funding levels, and greater stability of funding are very important to enhancing diversity in the scientific workforce, and enabling intellectual mobility. Many studies have shown that high-achieving and ambitious individuals from less-advantaged social backgrounds preferentially select non-STEM professional careers because of the perception of financial risks involved. The low success rates for proposals will also become increasingly damaging to overall recruiting if it is not corrected soon. Reduction of financial risk is important in capturing and retaining the best researchers of the next generation, among both traditional and under-represented populations.