Directorate for Mathematical and Physical Sciences

Background for the Discussion on Long-Range Planning at the MPSAC Meeting of April 3-4, 2003

Computational Science[1]

Over the past decade, scientific computing has evolved into a discovery tool for science and engineering. Computations are now as much part of the scientific toolkit as theory and experiment. Today, most research in the physical and biological sciences as well as in engineering is unthinkable without a strong computational component. Computational science---the aggregate of activities needed to advance the frontiers of science through computations---is emerging as a new discipline, which is already being recognized in several university programs and practiced on a routine basis by many researchers in the field.

Computational science is a distinct mode of scientific inquiry. It is driven by discipline-specific applications, but is also concerned with the discovery of general principles (models and algorithms) underlying the computational process. It introduces a paradigm shift comparable to Newton's introduction of calculus, unifying seemingly disparate practices in scientific computing and thus building the foundation for new discoveries through the application of advanced computational techniques.

Scientific computing has been recognized and encouraged in each MPS division for several years, and significant resources have been devoted to it. Yet, despite tremendous advances in the computational infrastructure, many challenging problems remain unsolved, either because the computational models are poorly understood or the existing algorithms lack the necessary structural stability. Multiscale phenomena in physics, chemistry, and materials science, as well as effects due to general relativity in astronomy, provide challenges that are well beyond current capabilities. A focused research program, involving disciplinary scientists, algorithm developers, and computational scientists, that addresses the fundamental computational issues (models and algorithms) common to the various disciplines would advance the state of the art of scientific computing and thus push the frontiers of science through computations.

Computational science crosses boundaries by its very nature. No part of MPS escapes involvement with computational science, and there are growing opportunities with biology, the geosciences, and engineering. Different disciplines face similar problems; Computational Science is the new discipline that addresses these problems. MPS has an opportunity to actively support and help shape the future of this new discipline. We therefore propose to make Computational Science a priority area within MPS.

Divisions within MPS have sponsored various workshops and reports addressing issues of computation in their respective disciplines. In the Spring of 2002, a Steering Committee on Computational Physics produced a report to the NSF on "Computation as a Tool for Discovery in Physics." Computational issues figure prominently in the Workshops on Opportunities in Materials Theory organized by DMR (the most recent workshop took place in October, 2002), as well as in the DMR Computational Review held in June, 2002, at UIUC. The CARGO program in DMS addresses computational issues in the recognition of geometric objects, and the division has sponsored workshops in the recent past on computational issues in Statistics and Algebra, Number Theory and Combinatorics, with reports forthcoming. A workshop on "Computational Science, Mathematics, and Engineering" is being organized by the Society for Industrial and Applied Mathematics (SIAM) under DMS sponsorship and scheduled for March 2003.

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[1] The term "Computational Science" is used as a shorthand notation for "Computational Science and Engineering."

Connecting Quarks to the Cosmos
(The Physics of the Universe)

INTRODUCTION

As the new century begins, science is confronted with a set of major questions at the intersection of physics and astronomy. The answers require combining observations of our universe to examine processes occurring on the largest length scales with fundamental physics, which addresses processes occurring on the smallest length scales (subatomic particles).

This observation about the interconnectedness of astronomy and physics contains a powerful insight, namely that the study of cosmic processes answers questions about the most fundamental particles and forces of nature, while the study of elementary particles can answer questions about the origin, evolution, and fate of the universe. This is the guiding principle of a recent National Academy of Sciences study[2], “Connecting Quarks to the Cosmos,” completed in 2002. The report identifies “eleven science questions for the new century.” This report, along with several related long-range plans and assessments published recently, forms the intellectual framework and community input for a possible coordinated interagency research plan.

THE COMING REVOLUTION IN THE PHYSICS OF THE UNIVERSE

As the 21st Century begins, one can confidently predict that our ideas about elementary physics and cosmology are about to undergo a radical transformation. This prediction rests on three extant circumstances. First, two of the great intellectual achievements of the 20th Century, the Standard Model of Particle Physics and the Standard Cosmological Model, together, provide a powerful and elegant framework for understanding the physics of the universe. Second, major questions, summarized below, make it clear that our present knowledge is still woefully inadequate to describe the physics of the universe. Third, experimental and theoretical approaches, driven by the tension between the first two observations have set the stage to provide the breakthrough discoveries that will revolutionize our understanding. Eleven questions that express the prospect for this revolution are:

What is Dark Matter? What is the nature of dark energy? How did the universe begin and how did its present large-scale structure come to be? Did Einstein have the last word on Gravity? What is the mass of the Neutrino and how have Neutrinos shaped the evolution of the Universe? How do cosmic accelerators work and what are they accelerating? Are Protons Unstable? Are there new states of matter at exceedingly high density and temperature? Are there additional space-time dimensions? How were the elements from iron to uranium made? Is a new theory of matter and light needed at the highest energies and electromagnetic fields?

This is the right time to attack these science questions as a result of a confluence of recent advances in technology, discoveries made in the last few years, and advances in theoretical ideas.

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[2] Connecting Quarks with the Cosmos: eleven Science Questions for the New Century (National Academies Press, 2002)

New technologies have put us on the verge of measuring Einstein's gravity waves for the first time and make it possible to produce telescopes with adaptive optics and detector arrays with unprecedented resolution. Colliding beam accelerators are reaching deeper and deeper into the fundamental structure of matter; and heavy-ion colliders are being used in hopes of re-creating the quark-gluon plasma, predicted to exist immediately after the Big Bang. The nature of dark matter remains a stubborn mystery; but physicists and astronomers may be close to learning its nature. The recent discoveries that neutrinos have mass and that the expansion of the universe is accelerating have caused physicists and astronomers to revise basic doctrines of scientific faith. And new facilities that create ultra-high energy density plasmas offer a way to investigate extreme environments that exist throughout the various phases of the lifecycle of stars. Sometimes predicting and sometimes reacting to this progress, theoretical advances have created a host of new concepts to explain and guide the observational advances.

A joint NSF-NASA-DOE coordinated research plan is being assembled under OSTP leadership.

Cyberinfrastructure

Cyberinfrastructure involves high performance computing, databases, instrumentation and fabrication facilities, human interfaces, visualization and associated interconnecting distributed networks. Cyberinfrastructure encompasses developing a revolutionary new way to do science by harnessing the tremendous advances in information technology to forge a powerful and global tool for discovery, analysis, synthesis, collaboration, and education. The participation of disciplinary sciences, each of the mathematical and physical sciences prominent among them, is crucial in defining how cyberinfrastructure is realized. Owing to the often profound differences in research cultures, each discipline must determine how to effectively harness powerful IT resources for advances at scientific frontiers.

Cyberinfrastructure is a central factor to many research and education opportunities by MPS in the decades ahead. A few examples illustrate the potential: global GRID technology for management and execution of data intensive research; distributed networks of computers that will enable use of computational science as a discovery tool; online, remote operation of experimental resources located anywhere in the world; distributed human interfaces that will surmount barriers of geography and physical handicap enabling collaborative interactions; new concepts in education that bring the world's best activities to the desktop; and information resources that are a quantum leap beyond the WWW. A dream of cyberinfrastructure is the seamless integration of all such activities empowering a researcher to access experimental data, compute, and interchange ideas all in a digital environment.

Examples of the use of cyberinfrastructure in future research by MPS disciplines are numerous and growing rapidly. The global GRID will enable management of terabytes of data to be managed with distributed assets; and it will enable researchers and their students equal access to the discovery opportunities in huge data sets being generated in distant facilities, e.g., LIGO, LHC, SDDS, other observatories abroad and in space. This facility with remote assets extends to the use of remote experimental facilities by researchers located anywhere in the world. The federation of data archives, the development of analysis and visualization tools that share common protocols and ensure interoperability among distributed data sets, as is being done with the National Virtual Observatory, are essential to realizing the promise of research. The GRID will also focus-distributed supercomputers on frontier problems such as calculating the mechanical properties of materials starting from atoms and microstructure. The effective use of advanced computation as a discovery tool in all forms of research will require new paradigms from disciplinary sciences together with advances in computer science; the result will be a new generation of cyberinfrastructure.

Exploiting this emerging opportunity requires several forms of strategic planning, collaboration, and investment. The development of the global GRID needs to be done through collaboration between CISE and MPS programs. For example, GRID development at the present time is being driven by the needs of the LHC collaboration, with a collaboration involving PHY, CISE, DOE, CERN, and the European Union. This collaboration is well along in organizing and needs the resources to succeed. Similar examples show scientific disciplines across MPS are likewise involved in conceptualizing the GRID. Computational science requires sophisticated use of distributed resources, with the necessary hardware, software, security, dedicated IT staff, etc. Use of distributed facilities on all scales requires the infrastructure to enable scientists to become directly involved in the operation and use of facilities distributed across the country and beyond. Educational and collaborative systems are being planned and require substantial development.

The overarching needs in development and exploitation of cyberinfrastructure require two main elements, namely (1) collaboration with the IT community and (2) investment in the disciplinary programs to support their particular needs, which vary among fields and are rapidly evolving.

Facility Stewardship Initiative

STRATEGIC GOALS AND ISSUES FOR FACILITIES

The purpose of major facilities and infrastructure in the NSF context is to enable the scientific community to address important questions at the intellectual frontiers of science. This is expressed in the NSF strategic goals: "People, Ideas, Tools." Furthermore, the process of pushing the technical frontiers in the process of developing tools with unprecedented capabilities contributes to the development of technology and an advanced workforce. Thus facilities, indeed, address all three strategic goals. The decisions to produce such facilities, the successful oversight and management required, the need to ensure that these investments are fully exploited, and the orderly phase out after the primary goals are met are all receiving intense scrutiny now, as the NSF expands its role in producing major projects. Consideration of facility stewardship is an important part of strategic planning because they involve substantial costs, complexity, and risk. Moreover, they have great impact on the community, both because they usually lead to an increased need for PI support and because, if not adequately budgeted for, can actually divert resources away from PI support. These two implications for PI support have opposite signs and can have large magnitudes, creating the potential for serious unintended consequences and, thus, the need for rigorous up-front planning.

LONG-RANGE PLANNING ISSUES FOR MAJOR FACILITIES

The central issue in planning for major facilities is to quantify and plan for life-cycle costs. This sounds self-evident; however this perspective is seldom adopted early enough. A typical approach is to take an estimate of the construction costs as the costs of the project. This can underestimate the total project costs by a factor of two, leading to unacceptable impacts on future budgets and on support of PIs, most of which are unrelated to the project. What should life-cycle costs include? A typical life-cycle cost analysis should include preconstruction R&D, design and engineering, acquisition of long lead time components, construction, commissioning, operations and maintenance, IT infrastructure, research costs, and upgrades. The total project cost (TPC), viewed in this way, greatly exceeds the construction costs; and it is necessary to make formal plans for budgeting for the TPC at the time a decision is made to proceed with the project. The benefits are that the true costs are known and provided for, enabling a successful project execution; and costs of increased research activity and upgrades are recognized. The consequence is that fewer projects are undertaken, assuming slowly growing budgets.

POSSIBLE ACTIONS

A possible action is to promote the idea of a facilities initiative, which would provide the funding levels needed to both provide for full funding for exploitation of major facilities. There is precedent for such an idea, because OMB provided a $50M step for full exploitation of DOE facilities a few years ago, when it was recognized that an increased level of support was needed to fulfill the promise of these investments. This would be an NSF-wide action, accompanying the increased facility planning procedures, and it would formally address the operations and research needs of present and future MREFC construction projects.

High-Dimensional Massive Data

Data have always been essential to advancement throughout science and engineering, whether through experimental validation of new theoretical insight, or through new hypothesis arising from the study of existing data. With the almost incredible amounts of data now being amassed, the 21st century promises to propel scientific advances to hitherto undreamed-of levels. In order to fulfill this promise we need tools to extract the relevant information from high-dimensional massive data sets, tools for a better understanding of the underlying science, tools based on sound scientific insight, tools that account realistically for uncertainty and ignore spurious distractions. Focused and interdisciplinary efforts are absolutely critical to developing these tools.

Technological advances in instrumentation development and the exponential growth of computing power have made it feasible to collect massive amounts of data, often with many variables being measured (which is what makes the data high-dimensional). The development of appropriate and efficient tools that enable the extraction of features and patterns that are linked to and provide insight into the underlying scientific process will offer a unique opportunity to revolutionize the advancement of science. While computer scientists have developed some nifty and efficient algorithms for looking at certain features of massive data, these are almost always deterministic and fail to make the necessary links to the underlying scientific process. Thereby they often fail to provide a sound scientific basis for the conclusions drawn and can too often lead to incorrect conclusions.

Data sets in astronomy, as an example, have grown enormously, both in size and complexity. Critical astrophysical questions, such as the estimation of cosmological parameters from observations as disparate as galaxy clustering and the cosmic microwave background, and the study of galaxy formation and evolution from very large but low signal-to-noise samples, depend on the development and interpretation of sophisticated statistical techniques, and especially on a proper accounting for uncertainty when data are plentiful but poor quality.

There are numerous examples like this: massive data from experiments in accelerators and nuclear reactors; massive data from remote sensing; massive internet traffic data; massive genomic data; massive data for climate prediction; massive financial data; massive data to represent and compare images; and so on.

The underlying scientific processes can be widely different. The structure of the data can be widely different as well, including its noisiness. But massive data is ubiquitous in science and represents the door we must open for the advancement of science at an entirely new level at the beginning of the 21st century. MPS is uniquely positioned to open this door since it represents both “tool makers” and “science makers”.

Increasing core support in the Mathematical and Physical Sciences

From the X-ray luggage scanner at an airport to the Magnetic Resonance Imager in the local medical facility, from modern synthetic techniques for manufacturing cheap pharmaceuticals to the neutron scattering facilities used to develop new materials and unravel the molecular basis for disease, and from the data encryption algorithms that safeguard electronic funds transfers to the wondrous discoveries that we have made about the world inside the atom and within the universe at large, we are surrounded by the fruits of research into mathematical and physical science in our everyday, economic, and cultural lives. As well as seeking a fundamental understanding of nature, research in the MPS disciplines provides the foundation of our technological society and the basis of our national defense. And research and training in MPS disciplines has repeatedly led to the emergence of new fields of science and technology. Scientists trained in MPS disciplines were key players in the revolutionary development of molecular biology and computer science in the 20th century, and research in mathematics and the physical sciences has proven to be an engine for economic growth including, especially recently, growth in the biomedical, communications and information sectors.

The pace of discovery in basic mathematical and physical sciences will be even higher in the 21st century than it was in the 20th. While it is important to support broad efforts in areas that build on the previous discoveries, the need to invest in mathematical and physical science research – to replace the seed corn – has never been greater than it is today and yet, by most indicators, this investment has lagged and we are now seeing the consequences. Our premier research laboratories are not as well equipped as needed. Our brightest young people, who might once have devoted their lives to the discipline of a research career, are being lured away by easier and more lucrative alternatives. Perhaps most damaging of all, the appreciation of mathematics and physical science and the confident understanding of its most basic principles have been seriously eroded in the population at large, from those who rely on technology to carry out their work to politicians charged with making difficult economic choices. A major reinvestment in the MPS core is absolutely essential in order to create the knowledge and develop the physical and human resources needed for the nation's economic well-being and security in the 21st century.

The field of mathematical and physical science encompasses a vast collection of strongly linked, active subfields. Although some areas of rapid growth, such as nano-technology, can be identified, the majority of the most significant discoveries – the next lasers, transistors and imaging devices – will continue to arise in an unscripted manner from the core program. This is the very nature of research. The National Science Foundation has an enviable record of success in identifying and fostering promising investigations out of the core research program in addition to supporting its more concentrated and programmatic research. There is now an historic opportunity to re-energize the mathematical and physical sciences and usher a new age of achievement in their service to society: the **MPSAC recommends a re-investment in the nation's future by increasing the financial support of the MPS core research program. This recommendation adds to identical calls for such an increase in support for the physical sciences by PCAST and the authorization and appropriations bills for FY 2003.**

Molecular Science and Technology (MOST)

Civilizations are often defined by their capabilities: The Iron Age and Bronze Age, for example, reflected society's extensive use of those materials thousands of years ago. Today, atoms and bits define our civilization. Our exquisite control of bits has led to the Information Age, which has profoundly affected how we communicate and how we collect, manipulate, transmit, and store data.

By comparison, our control of atoms is still, in many respects, at a primitive stage. The last century saw scientists and engineers develop a firm understanding of the covalent and ionic bonds that link atoms into molecules and materials, representing the sharing and transfer of the electrons that comprise these bonds. As a result of advances in instrumentation, we can now image and manipulate single molecules and atoms, and we can follow reactions in real time. These advances have brought us to the beginning of what might be called the Molecular Age, an era in which complex chemical and materials structures can be created with predictable properties and in which the nature of multitudinous coupled chemical reactions in living cells can be studied and analyzed. To launch the Molecular Age, however, will require mastering a formidable challenge: understanding the myriad weaker, non-covalent interactions between collections of atoms and molecules that control their connectivity, architecture, reactivity, and emergent behavior. Investment in a basic research agenda for the Molecular Age that supports structure-reactivity investigations will pay enormous dividends for our society in such diverse areas as manufacturing, environmental quality, health and medicine, and information technology. Investment in molecular studies of complexity phenomena will enable us to address two of the grandest of challenges: What is the molecular origin of life and what is the molecular basis of consciousness?

The timeliness of this Molecular Science and Technology (MOST) initiative reflects the breathtaking advances in synthetic, instrumental, and computational tools of the past few years, and the cross-fertilization of expertise across traditional disciplines. Many of these advances are described in the recently released NRC report, "Beyond the Molecular Frontier." Some examples include: new preparative methods based on atom economy that lead to more environmentally benign manufacturing; developments in computational methods that permit more efficient and effective drug design; modeling and simulation studies that provide greater accuracy in descriptions of molecular speciation and transport in atmospheric, terrestrial and oceanic environments; and molecular and material structures and assemblies that have been designed to perform simple logic operations. Molecular systems have also been identified that exhibit characteristic nonlinear, chaotic behavior that is amenable to mathematical and computational modeling.

Among the tools that would be created through the MOST initiative is a suite of chemical imaging methods. In principle, single molecule detection methods can be developed to track large collections of molecules in space and time. Application of these chemical imaging methods to cells would revolutionize our understanding of metabolomics (the study of the multiple, coupled chemical reactions that govern the life of a cell) and its connections to proteomics and genomics. Application of these tools to surface-molecule interactions could be used to link cells to computer or sensor hardware surfaces; to prepare artificial tissue, bones, and teeth for human repair; and to self-assemble materials possessing a range of functionalities.

Advances in molecular science and technology that would be enabled by this MOST initiative will build upon and are complementary to existing NSF investments in nanotechnology, quantum science and technology, information technology, biocomplexity, and mathematics. With its emphasis on molecular interactions, the MOST initiative will produce a holistic view of bonding that can be applied across the full spectrum of science and technology. Support of the MOST initiative will provide the basic research infrastructure needed to place molecules in service to society in ways that were inconceivable just a few years ago. The Molecular Age that will be created will have considerable synergy with our current Information Age and will enable us to make optimal use of atoms and bits.

Quantitative Biology

In the post-genomic era, the biological sciences are experiencing a major change in the scientific approaches that are needed to advance the science in a major way. The largely descriptive methods that have served the biological sciences so well in the past are rapidly being complemented and in many cases replaced by more quantitative models, concepts, and techniques. In this evolutionary process the connections between the biological sciences and the mathematical and physical sciences are becoming critically important. This need has been clearly stated in the recent National Academy study *BIO2010 - Transforming Undergraduate Education for Future Research Biologists*. This study concludes that "life science majors must acquire a much stronger foundation in the physical sciences…and mathematics than they now get." The demand for such quantitative tools, together with the intellectual ferment that currently characterizes the biological sciences, is creating major opportunities for MPS investment. The payoffs on such an investment extend from understanding the living world at the most fundamental level to service to society in the health benefits that will invariably follow from an enhanced understanding of life processes.

Until recent years, the complexity of biological systems has prevented the more quantitative experimental and theoretical approaches that have defined the mathematical and physical sciences from being broadly applied to the biological sciences. However, with the advent of advanced experimental and data analysis techniques, this situation is rapidly changing. Theorists from the mathematics, chemistry, physics and materials research communities are developing models and approaches adapted to the analysis of complex systems. New experimental techniques, bolstered with new instrumentation and access to national user facilities for synchrotron radiation, neutron scattering and high magnetic fields, are making it possible to study biological processes at a level of detail that allows direct comparison between theory and experiment. Chemists and physicists are now able to observe and manipulate single biological molecules. Massively parallel experimental techniques such as combinatorial chemistry and gene chip technologies are making it possible to analyze thousands of biological samples simultaneously. The vast amount of information about biological systems that has accumulated as a result of these experimental advances over the past decades is stimulating new thinking in the search for unifying principles.

In a recent memorandum from the OSTP and OMB, John Marburger and Mitchell Daniels took note of the importance of this emerging new area and identified "Molecular-level Understanding of Life Processes" as one of the major scientific priorities of the present administration. They noted that the "sequence and structure data, coupled to modern computational power and to our ability to manipulate biological systems at the molecular level, will yield new experimental approaches that have the potential to unravel the complexity of life at the molecular-, cellular-, and organismal levels." As the biological sciences become more quantitative, the disciplines comprising MPS have a key role to play within this theme. MPS should step forth and assume a leadership role in what might be called "quantitative biology." Given the traditional NSF approach of supporting highly innovative science, and because NSF, unlike the NIH, does not have a mission beyond support for basic science, MPS is in an excellent position to foster this new direction. Moreover, MPS-supported investigators are already discovering for themselves the intellectual richness of quantitative biology.

The role of MPS in this theme is multifold. Foremost among these is the education and training of scientists to work at the interface between the mathematical and physical and biological sciences. This is best achieved through mechanisms that establish partnerships between MPS scientists and biologists. Postdoctoral research fellowships that foster this link and mid-career sabbatical exchanges are approaches that should be considered. MPS should also seek to strengthen existing connections with other funding organizations, such as the NSF Directorate for Biological Sciences, the NIH, and the Howard Hughes Medical Institute for co-funding of individual and group research projects that stress new quantitative approaches to biological problems.

Research and Innovation Sites for College Students (RISCS)

As noted in the President's FY04 Budget, it is critically important to the long-term health of our nation that it invests in basic research in the mathematical and physical sciences (MPS) and in the sustainable development of a strong MPS workforce. To achieve this objective, our nation requires an educational MPS infrastructure that is fully integrated with its MPS research infrastructure. Undergraduate MPS education plays a pivotal role in student decisions regarding whether to pursue careers in MPS disciplines. As Elaine Seymour documents in "Talking about Leaving", many students intending to pursue careers in MPS disciplines, or receptive to this possibility, are dissuaded from doing so by introductory college MPS courses that do not engage them. In many cases, these courses and associated laboratory experiences are repetitions of high school courses that provide little exposure to the exciting frontiers of MPS research or to the creative process of conducting scientific research. Not surprisingly, many students opt for what they perceive as more intellectually rewarding opportunities elsewhere.

To address these issues, the MPS Directorate proposes, in partnership with the EHR Directorate, a bold new initiative, Research and Innovation Sites for College Students (RISCS). These campus sites will bring the excitement of cutting-edge MPS and associated interdisciplinary research into introductory college courses across the full spectrum of postsecondary institutions. The RISCS initiative will create a network of sites that span the country at an annual cost initially of about $50M.

The model for RISCS is based on the teams of scientists, mathematicians, and engineers who currently participate in undergraduate research projects. The limited number of students who find their way into MPS majors are well nurtured in upper-level undergraduate courses and often provided with opportunities for conducting original research with faculty, postdoctoral, and/or graduate student mentor teams. Exposure to contemporary MPS tools - scanning probe microscopes, large telescopes, particle accelerators, nuclear magnetic resonance instruments, and huge databases, for example - and to concepts associated with exciting interdisciplinary areas like nanotechnology, astrochemistry, and bioinformatics lead many students to graduate training and careers in MPS and allied fields. In order to adapt this model for use in introductory courses, where a far larger and more diverse college student population will participate, the academic community will need substantial resources. Funding will be needed to customize MPS and associated interdisciplinary research problems so as to include large numbers of students. Resources will also be directed to the development and acquisition of widely accessible, modern instrumentation that can be used to conduct the research.

Research conducted through RISCS can lead to publishable archival research; to community-oriented service learning that provides information on, for example, air, water and soil quality; and to new curricular materials based on current research that can be used to update the curriculum continuously. The principal RISCS contribution, however, will be to provide MPS researchers with the infrastructure to infuse the curriculum with research experiences that reach far more students than are currently served. The sites will provide professional development not only for researchers, but also for in-service and pre-service teachers. Motivated high school students wishing to engage in research could do so through the sites, as well.

The RISCS initiative can integrate MPS research and education in ways that are unprecedented, but demanded by our increasingly rapid rate of discovery, and by our society's pressing economic, environmental, health, and security needs. The RISCS initiative will create a culture in which research and education are truly integrated in real time and contribute substantially to sustainable development of our MPS technical workforce and to science literacy.

Scientific Discovery in the Face of Uncertainty

Uncertainty has always been a fact of life, both in daily life and in scientific research. During the revolution in scientific thought, research, and understanding of the 17th, 18th, and 19th centuries, many (and probably most) people believed that a better understanding of physical, chemical, and biological processes would eliminate this uncertainty. However, beginning (primarily) in the 20th century, scientists began to recognize that better and better models for these processes did not lead to a reduction or elimination of uncertainty. Rather, the complexity of the uncertainty increased as the complexity of the model increased.

While there may still be scientists who believe better models will eliminate uncertainty, a growing number are recognizing that uncertainty is a part of the processes and needs to be built in to our models. While some researchers have been able to do this (e.g., statistical mechanical models, such as the Ising model), more often than not, uncertainty is simply treated as an "add-on" at the end to try to get the data to fit. While this may have been a reasonable approach when the models were fairly crude, it is not working now that models have become very complex. Uncertainty must be included in model building and not simply added as an afterthought.

Now is the time to support a concerted effort to understand and use uncertainty in scientific research. Continued efforts to try to eliminate it are futile. Microscopic models that incorporate uncertainty do not lead to arbitrary randomness. These models (which are often fairly simple at the microscopic level) can have macroscopic behavior consistent with the processes they are modeling (such as phase transitions in statistical mechanics). Models that do not incorporate this uncertainty have difficulty demonstrating some of this behavior.

Concurrent with this need to model uncertainty is the need to understand and compare data to these models. Whether data come from computer models, experiments, or observation of physical processes, recognizing where uncertainty occurs will be important in analysis, understanding, and comparison. Treating this uncertainty as an "add-on" will lead to poor results.

The understanding of uncertainty is an important research area. Development of models that incorporate uncertainty at the microscopic level will lead to a better understanding of physical, chemical, and biological processes. But, development of the models will not be sufficient. Simultaneously, we must develop and understand the tools for comparing data to these models. Recognizing how deterministic laws and random events fit together to form a complete process is a major challenge for scientific research of the 21st century.

Science Partnerships with Developing Countries

"Science and engineering research is now a global enterprise. Science and engineering have changed in ways that make international cooperation in research and education essential for the advancement of knowledge. We must find new ways for scientists and engineers around the world to work together."

- Rita Colwell

MPS has led the way in many aspects of building research partnerships between US scientists and educators and their international colleagues. Examples include the development of large-scale facilities such as GEMINI and the LHC as well as smaller-scale but highly effective collaborations in fields such as materials research. These activities have been highly successful, but for the most part they have focused on building partnerships and collaborations between US investigators and their colleagues in the developed countries of Europe and the Americas.

The potential advantages to be gained on both sides from collaboration in research and education in the MPS disciplines with partners in the developing countries of Africa, the Middle East, and parts of Asia, for example, remain largely unrealized. Yet the potential gains are considerable in all MPS disciplines including astronomy (examples include educational partnerships, southern hemisphere access, longitude coverage, access to good infrared and sub-millimeter conditions, radio-quiet and dark-sky sites) chemistry (e.g. water quality and environmental protection), materials science (e.g. 'green' materials, energy sources and distribution, structural materials, communications), physics (international facilities), and mathematics (e.g. international outreach through mathematical sciences research institutes, international exchanges and workshops).

In building such partnerships it will be critically important to identify topical areas of common interest where the scientific exchange and collaboration can be balanced in terms of intellectual contribution and level of effort on both sides, rather than exacerbating a one-way flow of scientific and engineering talent to the US from the partner countries. Some 'economically developing' countries such as India and China, for example, are 'scientifically developed' in many ways, with a substantial body of scientists making significant contributions to the scientific knowledge base, but this is not the case for all developing countries. The development of 'symmetrical' partnerships is therefore likely to proceed by different paths in different parts of the world.

MPS and INT will jointly develop a new area of emphasis to foster international collaboration in the physical sciences between US researchers and educators and their counterparts in developing countries. Awards will include one-to-one collaboration between individual investigators as well as collaborations between groups of investigators and center-to-center collaboration.

(NOTE: It may be a major challenge to find sources of support for the partners in the developing country. In developed countries NSF expects a 'counterpart agency' in the partner country or region to support an equivalent level of effort – this may not always be feasible in developing countries. NSF may need to develop partnerships with the State Department and/or other institutions addressing international issues in order to address this challenge.)