RISE

REINVESTMENT INITIATIVE IN SCIENCE AND ENGINEERING

> ***"There is a single light of science,***
> ***and to brighten it anywhere***
> ***is to brighten it everywhere."***
> ***Isaac Asimov***

A Discussion Document of the *Advisory Committee of the Mathematical and Physical Sciences Directorate*
May, 2000

REINVESTMENT INITIATIVE IN SCIENCE AND ENGINEERING (RISE)

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REINVESTMENT INITIATIVE IN SCIENCE AND ENGINEERING (RISE)

> ***"The United States is living off historical assets that are not being renewed"***
>
> **Charles M. Vest**
> **President MIT**
> **(Congressional Joint Economic Committee Hearings**
> **May, 1999)**

I. CONTEXT

The United States of America (U.S.) will begin the 21st century as the world's leading economic, technological, and peacekeeping power. We are enjoying an unprecedented and prolonged period of prosperity. As many economists, scientific, technological, and political leaders have noted this prosperity of the U.S. can, in large measure, be traced to discoveries in basic research, which have spawned new industries creating both material and intellectual wealth. For example, the modern digital computer revolution is based on basic research in mathematics and quantum mechanics. This revolution has led to a tremendous increase in economic productivity. The current, rapidly evolving, field of medicine is and will continue to be based on basic research on the structure and functioning of DNA. The current globalization of market economies and the associated changes in human interaction are attributable to the worldwide network of computers. These development were made possible by basic research in materials, quantum optics, electronics, information, and networks.

The U.S. has led in basic research and the transformation of this knowledge into industry simply because it attracted some of the best minds in the U.S. and from all over the world, science was relatively well funded, and the research universities evolved into great centers of science and engineering and, frequently, the birthplace of entrepreneurs, who translated the research know-how into leading technologies and, sometimes, the creation of new industries.

Basic research may be considered to move in two streams. One is the stream of steady and measured progress, on a very broad front, of the sciences and engineering and the other, singular or very rapidly evolving, discoveries or developments that change the course of research and which lead to new industries. If the U.S. is to maintain its position in the world, both streams need to be supported by adequate funding , the latter, frequently, by specialized Initiatives.

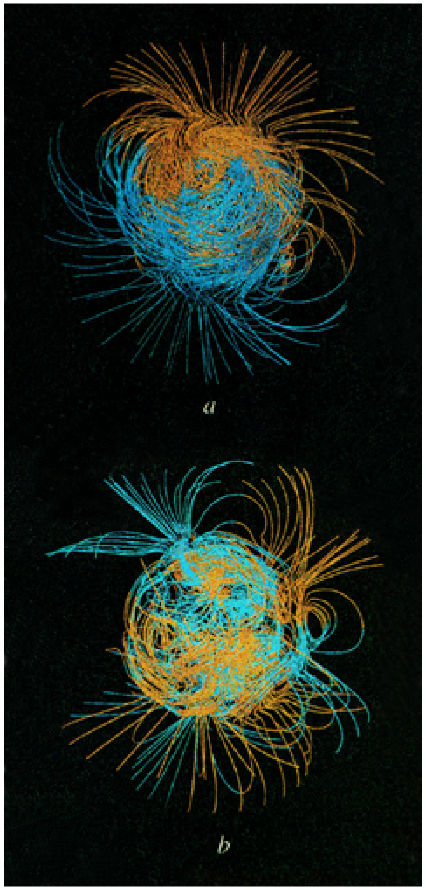
In this context, we laud the increase in support of the life sciences but believe, as many others have articulated, that the broad base of support for the rest of basic research needs to be increased in the U.S. from its almost stagnant value since 1970.

In this call, we argue, with the support of examples, that we are living through a period of very rapid changes in basic research that point to unprecedented opportunities to comprehend nature. These opportunities, if seized, will provide us with some of the answers that range from the ageless quest of mankind to understand what the universe is comprised of to the atom-by-atom synthesis of new materials and from the nature of consciousness to the large scale simulation of protein folding. If history is any guide, these opportunities in basic research will surely lead to new technologies, which, we believe, will further enhance the flourishing of the U.S.

Because this document originates from the Directorate of the Mathematical and Physical Sciences (MPS), the examples, which follow, reflect this bias. We believe that similar opportunities exist for the rest of the sciences and engineering. The forces driving these changes are the same. Therefore, a broad initiative is suggested. We tentatively name this initiative **RISE**– The **R**einvestment **I**nitiative in **S**cience and **E**ngineering. We propose to advance this initiative in four stages. First, we will create a model RISE in the context of MPS. Second, we would propose to extend the RISE concept across the NSF, through the use of the Advisory Committees. Third, and hopefully, a presidential study is commissioned to independently asses the need and priority of a RISE initiative. Fourth, if the presidential commission so recommends, a RISE would be established by all of the appropriate science and engineering agencies.

IDEAS

> ***"Every great advance in science has issued from a new audacity of the imagination."***
>
> ***John Dewey***



Computer model of earths changing magnetic fields through projected time spans.
Nature, Vol. 377, No. 6546

II. IDEAS

1. Fundamental and Interdisciplinary Mathematical Sciences

The mathematical sciences are a key component of current science and engineering. Even those sciences whose reliance on mathematics in the past has been slight, for example, certain areas of the biological sciences and economics, turn increasingly towards analysis and synthesis, and become increasingly mathematical. The MPS Directorate must advance the mathematical sciences, both in research and in training, as the foundation for the science of the 21st century.

The recent decades have seen extraordinary advances in the mathematical sciences and in their applications. Computational mathematics has made spectacular progress and powerful contributions across the spectrum of science. Number theory has solved some of its classical problems and contributed to encryption and internet security. Geometrical tools appear in mathematical physics and in data visualization. The success of biotechnology hinges to a great degree on mathematical tools. Mathemat-ical modeling is the key to understanding molecular structure and dynamics. Fundamental areas of mathematics have deepened their knowledge and move in the direction of new and fascinating questions posed by sophisticated applications in other disciplines.

The mathematization of science will accelerate. The key role of computing will generate the need for developing new mathematical algorithms. New mathematical modeling will transform data into knowledge. The understanding of stochasticity and uncertainty, of large data sets and their uses, will become ever more important. The mathematical sciences will also provide the critical support for emerging areas in science. It will develop the combinatorial optimization and pattern recognition algorithms for bioinformatics, as well as the mathematical tools for the modeling, simulation, control and manufacturing of nano scale and quantum molecular devices. A golden opportunity now exists for MPS investment in mathematics, in algorithms to harness computer hardware, in geometrical tools for computer graphics and physics, in statistics and modeling across the science spectrum, and in branches of mathematics yet to be imagined.

The *1998 Report of the Senior Assessment Panel of the International Assessment of the U.S. Mathematical Sciences* warns that the U.S. leadership position in the mathematical sciences is at risk. At the current level of investments, it is doubtful that the US leadership position can be maintained. This is a call for action.

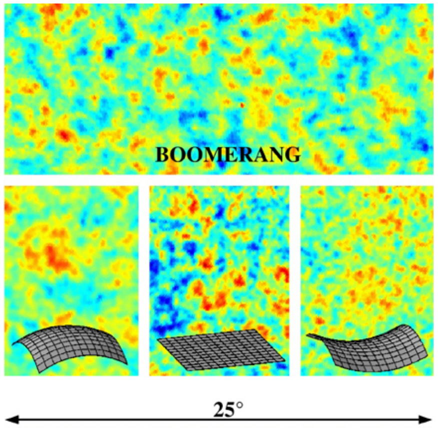
The mathematical profession must recruit some of the Nation's best talent, while contributing to the training of a large science and engineering workforce. The MPS Directorate has begun to act through the creation of new national institutes in multidisciplinary mathematical sciences with the explicit vision of strengthening the connection between mathematics and science and engineering. Increased funding would allow MPS to pursue vigorously a broad agenda: growing the next generation of deep thinkers, making possible breakthroughs in fundamental areas, enlarging innovative training programs in the mathematical sciences, strengthening links to science and engineering, funding mathematicians' involvement in other disciplines, supporting a new focused research groups initiative. Continued US prosperity and leadership in the mathematical sciences, as well as in the entire science and engineering enterprise, will depend upon the these and other initiatives.

2. Origins and Evolution of the Universe

Research on the 'Origins of the Universe' seeks to answer some of humankind's most compelling questions: How did the Universe begin, what is its structure, and what is its ultimate fate? How did matter, the chemical elements, planets, stars, and galaxies form? What is the nature of the dark matter and dark energy which fill the Universe and control its evolution? We are entering an era when great strides can be made in addressing these questions, but substantially increased levels and new modes of support from NSF will be essential. Answers to such basic questions about the fundamental properties of the building blocks of matter and the creation and fate of the Universe require next-generation facilities and bold new experimental and theoretical approaches from many disciplines. In particular, they will require melding of the techniques of modern observational and theoretical astrophysics with experimental and theoretical particle, nuclear, gravitational, atomic, plasma, and molecular physics; theoretical and laboratory chemistry; applied and computational mathematics; and advanced information technology and computing. Research in this area represents a growing collaboration among the physical sciences, which also has significant educational potential and public appeal. Major developments during the last century hinted at this future.

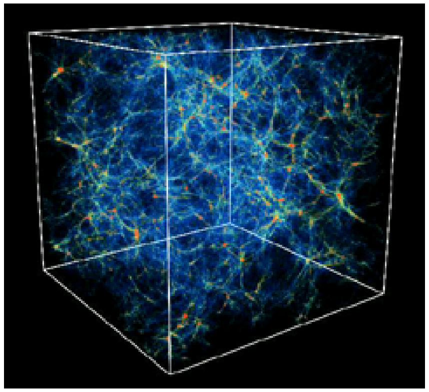
In 1915, Einstein derived his cosmological equation to describe the structure of space and time. The equation implied that the universe must be in motion. Einstein rejected that conclusion and introduced a new term into his equation, which he called the "cosmological constant". This constant represented a new, undiscovered form of energy that counteracted gravity and permitted a static universe. Soon after 1929, when Edwin Hubble discovered that the universe was indeed expanding, Einstein called the cosmological constant "the greatest blunder of my life".

In 1948, George Gamow and others combined Einstein's cosmological theory with the theory of nuclear reactions to describe the evolution of universe during the first few minutes after its beginning, the moment we call the "big bang". Gamow deduced that the universe at that time must have been filled with radiation at a temperature of billions of degrees. Otherwise, very little hydrogen would remain in the universe today, and stars as we know them would not exist. In 1964, physicists at Bell Laboratories discovered this radiation, which has now cooled to



The curvature of the universe can be inferred from measurements of the characteristic scale of the angular variations of the cosmic background radiation. A universe with positive curvature (lower left) will magnify the scale, while a universe with negative curvature (lower right) will de-magnify the scale. The observed fluctuations (top panel) have a characteristic scale in agreement with the prediction for a flat universe (lower center).

Source: www.physics.ucsb.edu/~boomerang/



Results of a simulation of the distribution of matter in a block of the universe 500 million light years on a side. The calculation starts from very slight initial density fluctuations such as those seen in the cosmic background radiation. As the universe expands, the fluctuations grow in amplitude until they resemble the density structure seen in the universe today.

Computing the Universe from the National Center for Supercomputing Applications

2.73 degrees above absolute zero as a result of the cosmic expansion. This cosmic background radiation carries a record of the structure of the universe when it was less than a million years old, long before any galaxies or stars existed.

Now, in the first year of this millennium, astronomers supported by NSF are observing the cosmic background radiation with instruments on balloons at the South Pole and on radio telescopes located on a high plateau in the Andes. These observations show that the early universe was almost, but not quite, perfectly smooth. We see tiny angular variations in the background radiation -- a few parts per hundred thousand -- that trace the initial density fluctuations of the universe that have condensed into the vast network of galaxies that populate the present universe. By measuring the statistical properties of these angular variations, astronomers can infer the curvature of the universe and several other quantities that determine its evolution.

Astronomers are also using ground-based optical and infrared telescopes to map the distribution of galaxies in the universe. The Sloan Digital Sky Survey is observing the locations and motions of millions of galaxies in the nearby universe. Larger telescopes at the Kitt Peak National Observatory and the Cerro Tololo InterAmerican Observatory and the new 8-meter Gemini telescopes will measure the distributions of galaxies so distant that we can see them as they were when the universe was only 5 - 10% of its present age.
From such observations, we know that the matter in universe must have evolved from a nearly formless gas into the seething mass of galaxies, stars, and planets that we see today. Astrophysicists can understand this evolution in increasing detail. To do this, they solve the equations describing the dynamics of the matter in the universe. These simulations tax the capabilities of our most powerful computers.

Future surveys supported by the NSF will map the universe at optical, infrared, and radio wavelengths; producing three-dimensional maps of the distribution of galaxies. The huge data bases produced by these surveys constitute a vast treasure of information, not only about the structure of the universe itself, but also about the properties of a great variety of normal and exotic stars, galaxies, and interstellar matter. Through its Knowledge and Distributed Intelligence initiative, the NSF is making these data available for analysis by the entire world scientific community.

Both the observations and the theoretical simulations point to a startling result: more than 80% of the matter in the universe must reside in a form that has not been identified up to now. We see compelling evidence of this "dark matter" by observing the influence of its gravity on the motions of galaxies, which we measure with spectra taken with ground-based optical and radio telescopes, and through the distortion of their images by "gravitational lensing". Without dark matter, the universe today would have no stars and galaxies. Recently, astronomers using Cerro Tololo InterAmerican Observatory have discovered 'cosmic shear', the gravitational lens imprint of large-scale dark matter. Weak gravitational lensing is a unique new probe of the mass in the Universe. What is the dark matter? The dark matter is not composed of the elementary particles that have been identified by physicists up to now. NSF is supporting experiments of unprecedented sensitivity to detect new kinds of exotic particles that might account for the dark matter.

Recently, astronomers at the Cerro Tololo InterAmerican Observatory discovered that the luminosity of a certain kind of exploding star, called a Type Ia supernova, could be calibrated very accurately from the decay rate of its light. Today, NSF is supporting two programs to observe distant supernovae. The results are astonishing: it appears that the expansion of the universe is not slowing down, but that it is speeding up! To explain these results, cosmologists must introduce a new kind of "dark energy" that counteracts the deceleration of the universe due to the gravity of the dark matter. The new observations of the fluctuations of microwave background confirm the existence of this dark energy. The term that accounts for dark energy in the cosmological equations is the same cosmological constant that Einstein invented in 1915 and later discarded.

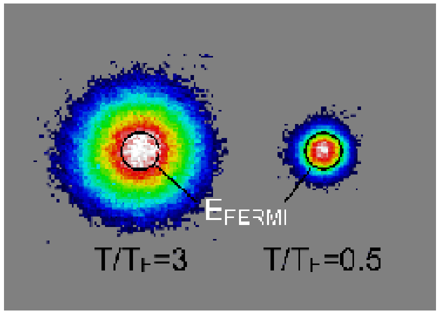
Dark matter and dark energy not only control the motion of the universe today; they also control its evolution immediately after the moment of creation. At that time, the entire universe was smaller than a single atom and the subatomic forces involved were greater than those that can be achieved with the most powerful particle accelerators on earth. Thus, the quest to understand the fundamental nature of space, time, and matter links astronomical measurements spanning billions of light years with measurements of high-energy particle interactions at scales much smaller than the atomic nucleus.

Today, astronomers are seeing their first glimpses of the universe when it was less than ten per cent of its present age, as the first galaxies were forming. Because the cosmic expansion shifts the light of these galaxies to longer wavelengths, astronomers must employ telescopes operating at infrared and submillimeter wavelengths to observe galaxies in the process of formation. The Gemini telescopes will observe newly forming galaxies with instruments sensitive to infrared wavelengths, and the Atacama Large Millimeter Array (ALMA) will observe them in greater detail through their radiation at millimeter and sub-millimeter wavelengths. The ALMA will be the culmination of a sustained effort by NSF to develop and support new technologies and telescopes to observe the formation of stars and galaxies through long-wavelength radiation.

The cosmological studies described above are only a part of the rich variety of astronomical science supported by NSF. Just in the past few years, NSF-sponsored researchers have discovered planets orbiting some 30 nearby stars. Indeed, at the end of 1999, astronomers made the first measurement of the diameter of a planet as it passed in front of its central star. As astronomers strive to understand the origin and fate of the universe, they are inevitably

“the Pod”
Arecibo
Observatory

photo courtesy of the NAIC,
Arecibo Obsrvatory,
a facility of the NSF
photographer: Tony Acevedo



Cold Fermions Demonstrating Degeneracy.

led to study the origin of stars and planets. Ultimately, these efforts will merge with the efforts by biologists to understand the origin of life on Earth and possibly elsewhere. As T.S. Eliot wrote,

> *"We shall not cease from exploration*
> *And the end of all our exploring*
> *Will be to arrive where we started*
> *And know the place for the first time."*
>
> *(from Little Giddings)*

The Initiative. As we enter the 21st century, the United States leads the world in Origins of the Universe research. Our leadership is now threatened, however. At current budget levels, the base of individual investigators and the capabilities at our national facilities are eroding. At the same time, Europe and Japan are making investments in research that in many respects match or exceed those of the U.S.

To adequately address these fundamental questions and to meet the challenge to U.S. leadership, we must increase the resources available to the individual investigators and stop the erosion – and then selectively enhance – the capabilities at our national facilities. While ensuring that the Gemini Observatories and LIGO are adequately instrumented, we must also proceed without delay on constructing and bringing into operation the new facilities that have been strongly endorsed by the community, such as the Giant Segmented Mirror Telescope, the 8-meter Synoptic Survey Telescope, and the Large Hadron Collider detectors. These investments will allow us to probe deep into the clouds of interstellar matter from which stars form, to study the processes that occurred in the early Universe including early formation of galaxies, to probe dark matter over vast reaches, detect Earth-threatening asteroids, and to understand conditions early in the Big Bang from which our Universe originated. Terascale data management and mining, joining ground-based and space observations, will lead to a National Virtual Observatory. The creation of such large facilities is increasingly being coordinated with other agencies to optimize the U.S. investment.

Expected Outcomes. With the required investments in people, tools, and ideas, over the next decade MPS supported investigators will be able to exploit fully these scientific opportunities:

- Physics during the Big Bang, and evolution of the early Universe,
- How galaxies originated from quantum fluctuations in the early Universe,
- The nature of dark matter and dark energy,
- The chemical evolution of galaxies,
- How stars and planetary systems form, and possibly
- Discovering habitats for biological processes beyond Earth.

New tools and technologies open new windows and lead to unexpected discoveries. Our goals for the next five years are aimed at ensuring U.S. leadership in research on the 'Origins of the Universe'. Our challenge is clear.

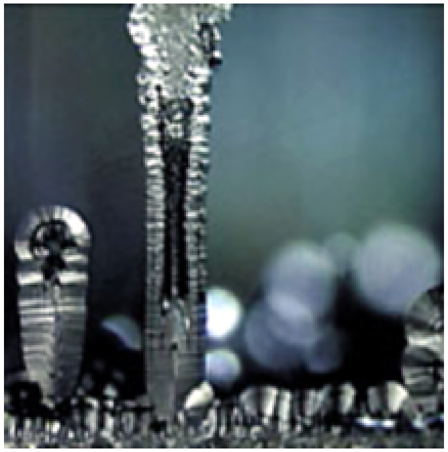
3. Quantum Science and Engineering

Over the last one hundred years, there have been stunning advances in our understanding of the microscopic world. We have learnt that the microscopic world is described by quantum mechanics. The rules by which this mechanics operates are different from classical mechanics and their elucidation has profoundly changed our concepts of nature, that had been developed over many centuries of thought and experimentation. Within the last fifteen years, we have gone beyond the historical reductionist approach to explaining phenomena by examination on the most rduced scale to one of synthesis, in which control and manipulation of nano-scale entities such as atoms and molecules have become the ‘Quantum Legos’ of scientists. We are witnessing the growth of the embryonic field of quantum science and engineering.

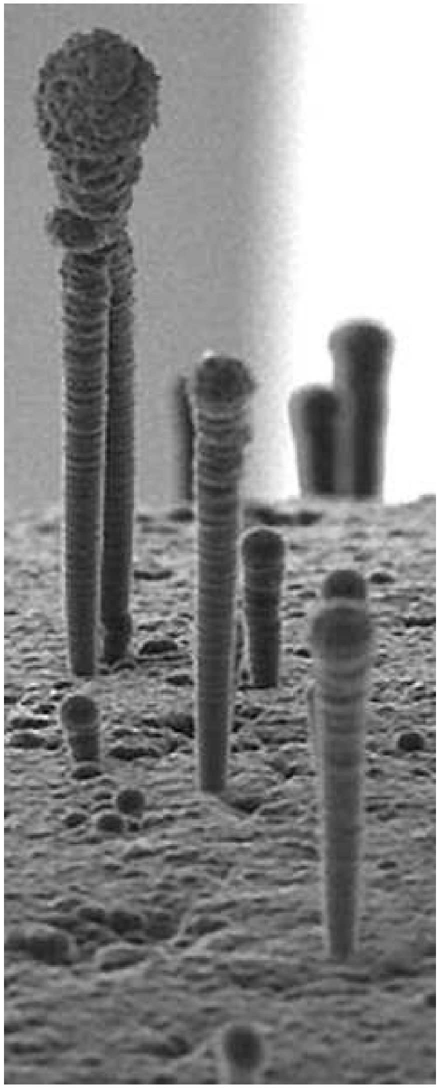
These developments are changing not just the kind of science that is done but also the sociology of science. The latter arise from a blurring of the boundaries between discipline oriented academic departments; atoms are common to all materials whether they be of interst to the life sciences or the physical sciences. We believe that the scientists of tomorrow will increasingly view manipulation and control of the arrangement of individual atoms or molecules as the unifying theme and functionality a predicatable consequence of what they synthesize. This shift is expected to have a prfound impact on science of the future and on technologies that arise from it.

The excitement of research and discovery and the enormous opportunities that are there for the taking in quantum science and engineering can just barely be conveyed by the printed word. In the following, we present some examples taken from research done within the last five to ten years. These include the manipulation of single atoms by scanning probe microscopies, atom cooling and trapping in controlled electromagnetic fields, single-atom control of chemical reactions, quantum optics and electronics in nanoscale systems of one, two, and three dimensions, atom lasers, quantum coherence and non-classical electron behavior, and quantum computers.

New techniques from atomic force microscopy to high-intensity X-ray sources to sophisticated electron microscopy, make it possible to observe crystal surfaces with atomic resolution, to image individual molecules, and manipulate individual atoms. Researchers recently produced the first experimental images of electron orbitals in a crystal, and in a succession of remarkable experiments, scientists have coaxed first bosons and now fermions into low temperature quantum states, forming a new kind of matter. Using ultrafast laser pulses and magnetic fields, the Bose-Einstein Condensate electron-hole pairs in semiconductors can be carefully manipulated, and electron spin states can be preserved over surprisingly long distances. Quantum chemistry has reached the point where it is now possible to calculate energy levels and structures of moderately complex molecules. Techniques of laser-based quantum control make it possible to engineer predetermined wavefunctions, and laser cooling has made it possible, for the first time, to control the translational motion



Carbon "trees" on graphite electrodes, grown autocatalytically through restructuring of newly deposited carbon surfaces. The tallest tree is about 300 microns in height.



Different aspect of the surface of carbon"trees" shown on page 10.

of a single atom, isolating the atom for fundamental quantum mechanical measurements or harnessing it to be used as a tool in surface science, biophysics and physical chemistry. 'Artificial atoms' or 'quantum dots' can be produced singly and in ordered arrays by exquisitely sensitive control of deposition techniques such as molecular beam epitaxy or even by molecular self-assembly. The economic potential of quantum-realm technology is considerable. For example, thin-film 'giant magnetoresistance' (GMR) materials grown as alternating nanoscale layers of iron and chromium used in computer hard drives amounted to $34 billion in 1998.

While 'roadmaps' for electronic device miniaturization and many other critical areas are important, they will no longer suffice as technology enters the quantum realm. New paradigms will be needed for technological advance, and these will come only through scientific understanding of the underlying phenomena. Mysteries abound. For example, quantum mechanics has been plagued by what seems to be 'action at a distance' but what is, in reality, a manifestation of the concept of entangled states. These in turn arise as a consequence of quantum coherence. Transmission of quantum information over a distance, or 'quantum communication', relies on the existence of such states, but before this can be exploited we must understand how such states are generated and what kinds of systems will best retain coherence over a distance. A better understanding is needed of how to couple the macroscopic world with systems that are inherently quantum mechanical in nature. How do quantum mechanical systems interact over long time intervals and how can these interactions be used to develop systems for quantum computing, for example? More generally, how can we make use of multiple quantum systems in a controlled manner? Such questions extend from the quantum wave functional character of individual atoms and molecules to that of complex systems such as superconducting materials and superfluids. Instead of classical conductors carrying macroscopic quantities of charge, in the quantum realm individual electrons are manipulated.

Addressing such issues will lead to new science and new phenomena with enormous potential for practical application. Coherent sources of atoms may make the 'atom laser' a tool with as much impact for physicists, chemists, materials scientists and biologists as the photon laser - but the step from 'where and what light can do' to 'where and what atoms can do' is in its infancy. Wavefunction engineering and quantum control will form the basis for investigating the fundamental limits imposed by the 'rules' of quantum mechanics and will pervade all attempts to realize technology at the quantum limit - for example in quantum computing, which may (or may not!) be the breakthrough that drives profound technological and ultimately societal changes in the new century.

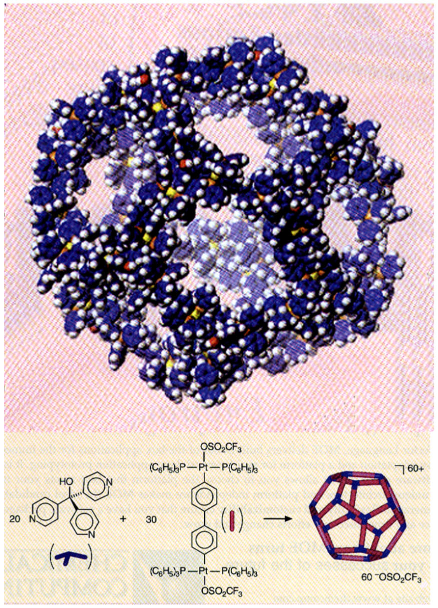
The marriage of theoretical advances with computational materials science will ultimately revolutionize our ability to design functional materials from first principles, and in the shorter term, quantum chemical calculations will be developed to the point where the structure of complex proteins can be predicted. As scientists and engineers learn to fabricate complex one, two and three-dimensional structures on a nanometer scale, new phenomena will emerge and be exploited. In condensed matter physics, challenges to both fundamental understanding and technological exploitation over the next few years include the behavior of strongly-correlated electron systems (key to high temperature superconductors and the quantum Hall effect, for example), low-dimensional systems such as carbon nanotubes and macromolecular assemblies (often complex materials with unique properties), and a renaissance in magnetic materials research (including for example 'spintronics' in which the integration of semiconductors with magnetic materials provides the potential for functional exploitation of electron spin).

The pace and excitement of scientific and technological advances in this 'quantum realm' are accelerating not only in the U.S., but worldwide, and the potential of these advances for societal change through the coupling of scientific understanding, engineering development and technological opportunity is unprecedented. With these continuing advances, the next five to ten years will see the emergence of the quantum realm as the key to 21st-century technology.

4. Molecular Connections

When complemented by recent advances in physics and in mathematical and computational modeling, the disciplines of chemistry and materials science offer a powerful and varied arsenal for uncovering nature’s secrets and creating future technologies critical to environmental, medical, and technological advances. It is a near certainty that improved electronic and optical components, coatings, chemicals, and pharmaceuticals will result from research in molecular science and engineering. Importantly, understanding phenomena at the molecular level has much broader implications: Such understanding is also critical to continued progress in genetics, neurobiology, ecosystem dynamics, climate studies, novel materials development, and smart manufacturing. Interaction with other disciplines is also a source of inspiration, and will become the norm as we move from a reductionist to an integrative period in scientific inquiry. For example, biological processes may suggest materials design strategies and fundamental research in areas such as complex fluids and soft condensed matter. The connections that MPS makes will lead to a wide range of benefits, including materials for artificial organs and methods for drug and gene delivery. These outcomes and many others will be by-products of the continuing search by molecular scientists to observe, understand, and control molecular, cellular, and nanoscale processes in real time.

On September 7, 1999, *Nature* (1999, *401*, 49) reported an NSF-supported discovery that provides



Fifty molecules assemble to form supramolecular dodecahedron. The structure, assembled by Peter J. Stang at the University of Utah and building on previous work by Leo A Paquette at Ohio State University, is believed to be the first supramolecular dodecahedron.
Chemical and Engineering News, Vol. 77, No. 46

a metaphor for current work and future opportunities in molecular science and engineering. Researchers at Arizona State University used X-rays and electron diffraction techniques to capture direct images of the electronic bonds that keep together the atoms of oxygen and copper in a compound called cuprite. This result opens the way to investigation of the details of copper-oxygen binding in related cuprate compounds. Some cuprates conduct electricity without resistance at temperatures about 140 degrees Fahrenheit above that of conventional superconductors, which can only function near the absolute zero of temperature. Since some scientists predict that high temperature superconductors will underlie much of the technology of the 21st century, this new imaging technique and the detailed visualization of bonding it provides may speed the answers to questions about the source and requirements for superconductivity and suggest design strategies for new materials.

Synergy between instrumentation and synthesis is the fulcrum upon which we must leverage our current technological capabilities while building the refined molecular foundation required to achieve future opportunities, both those conceivable and those not yet imagined. Recent instrumentation breakthroughs in scanning probe microscopy, single-atom spectroscopy, and other techniques like the one described above are providing finer level detail and improved understanding of relationships between synthesis, structure, properties, and processing of chemicals and materials. Heralded by elucidation of the structure-function relationships operative in DNA, RNA, and various enzymes as well as discovery of a new form of carbon, C60, modern instrumentation is opening the door to a new era of development of complex materials, variously described as “macromolecular”, “supramolecular” or “nanoscale.” What is needed is expanded research directed toward molecular design from the atomic and molecular scale to complicated architectures at the scale of thin films and nanodevices. This requires development of even more advanced instrumentation for characterization and manipulation of structures and devices at the nanoscale and more clever and comprehensive synthetic strategies. Some synthetic strategies may involve self-assembly, self-replication, biocatalysis, and mimicry of biological systems, none of which are currently well understood, and complementary enhancements of theory, modeling and simulation methodologies.

Some critically important, but previously intractable, molecular-level problems are now becoming intellectually and technologically accessible, but require capabilities beyond those of the single investigator. Research efforts increasingly require not just a single investigator but teams of investigators with cross-disciplinary expertise in synthesis, analysis, computation, and engineering. Unfortunately, advanced instrumentation and personnel support requirements for such integrated research efforts are growing while commitment to core research in these areas has been eroding. Because the very near future holds exciting opportunities, MPS must undertake a major initiative to invest funding for basic research focused on:

- Synthesis and design strategies that link molecular scale understanding with functional properties of materials

- Instrumentation development for real-time and real-world characterization of reactions at the molecular scale.

This initiative would produce the following outcomes:

Creation of new synthetic methods, which will be economically efficient and environmentally beneficial

Characterization of new molecules and materials with exquisitely fine molecular resolution via improved and/or revolutionary instrumentation, which will become critically useful in biological, medical, geological, and manufacturing research and development

The ability to combine synthesis and characterization to tailor a wide range of valuable fine chemicals and sophisticated materials for use in medicine, electronics, optics, and imaging applications; and further product manufacturing

Creation of expanded pools of trained scientists and enhanced professional interconnections between scientists with complementary expertise to allow ever more rapid mobilization of effective, interdisciplinary teams to tackle the kind of complex opportunities certain to arise.

PEOPLE

"An invasion of armies can be resisted, but not an idea whose time has come."

Victor Hugo

Current achievements are built on a fragile personnel basis. More than half of the mathematical scientists joining the profession today in the U.S. began their scientific studies abroad.

II. PEOPLE

RISE—Reinvestment **I**nitiative in **S**cience and **E**ngineering—might serve equally as the acronym for "Reinvestment in Science Education" or "Research in Service to Education" for it is quite clear that technological leadership of the United States in the 21st century will **RISE** (or fall) depending on the quality of the education in science and engineering that it provides to its youth. Though there have been questions about the dependence of the economic and technological competitiveness of the United States on World leadership in academic science, there is little question that the quality of the science and engineering education, at all levels, is a key factor in sustaining its leadership position in science-based technologies.

A major challenge to the programs of the MPS Directorate is the translation of the remarkable discoveries and excitement of the research community into analogous and substantive outcomes in the education community. In its current state, the science and engineering education that is provided to U.S. citizens may not sustain its leadership into the 21st Century. The remarkable achievements of research funded by the MPS Directorate have been based on increasing percentage of work by graduate students who did not receive their early education in the U.S. The U.S. and the World have benefitted from the participation of foreign nationals in its research and training programs in science and engineering. Such participation must continue. However, it must not insulate the faculty from the inescapable obligation to bring the benefits of the research enterprise to the education and training at all levels of the educational system of the U.S. citizenry.

Current Portfolio: The MPS Directorate is a research directorate; and while, it can and must speak to education broadly, its unique contribution in establishing the U.S. as a leader in science education will come when it speaks from the perspective of the research that it supports in its various divisions. It has been argued that "Doubling Research, Doubles Education", and the rigorous education of scientists and engineers that take place in the MPS funded programs is a dividend above and beyond the creation of new knowledge. The MPS Directorate funds directly through graduate student and post-doctoral stipends the education of scientists engineers at a level of $250,000,000 annually. Beyond the knowledge created, society continues to benefit from this research-based education over the life of the scientist or engineer through his or her skills in working in interdisciplinary teams at the forefront with a broad spectrum of disciplines. This has been the traditional route by which the MPS Directorate has contributed to science education and its achievements are unrivalled. This contribution to all levels of education, but mainly at the graduate level, is inadequate to meet the challenges of the 21st Century. New ways of and an appropriate context for leveraging the Research Investment of the Directorate for the preparation of a globally competitive, diverse American work-force must be developed.

IGERT and VIGRE are initiatives that would allow the Directorate to explore the limits of developing workforce sensitive programs with a minimum perturbation of the tradition of funding the education of scientists and engineers through support of research projects. These traineeship programs are platforms for exploring the broadening of the graduate education experience, for shortening the time to degree and for the systematic identification and control of those factors limiting the scope of and increasing the matriculation time for graduate science and engineering degrees.

Enhancing the global perspective of U.S. scientists and engineers is being pursued through the joint Directorate MPS-SBE International Postdoctoral Fellowhip which support the work of postdoctoral scientists at leading laboratory facilities throughout the world.

These efforts have grown out of sharply focused needs that have commanded the attention of the graduate education community for some time. Their effective implementation and further refinement will substantially improve the quality and responsiveness of graduate science and engineering education to national priorities.

The Initiative: U.S. graduate science, mathematics, and engineering education is limited by the scope, quality and perspective of science and mathematics education in the Kindergarten-to-Baccalaureate (K-16) education community. Of those students crossing the portals of undergraduate institutions with aspirations for pursuing careers in science, mathematics or engineering fields, 60% will not earn a science, mathematics or engineering degree. This high attrition rate occurs in the face of numerous demonstrations in many different settings that the ability to do science and mathematics is not limited to a small pool of students. It has been argued that effective science and mathematics education would provide students with the following:

- Factual Knowledge
- Technical Skills
- Critical Judgement
- Capacity for Discovery

The latter two pose the greatest challenge in their implementation by the K-12 community. Quite remarkably, these are the two factors on which the work and traditions of the MPS Directorate can have the greatest effect. The nuturing of critical judgment and the capacity for discovery require students and scholars coming together in authentic research settings.

Researchers best understand authentic research settings; it is, therefore, incumbent upon those researchers funded by the MPS Directorate to involve themselves and their work as integral parts of the K-12 education community. The context of this involvement is clear: to stem the high attrition rate among SME students in recognition of the evidence that the ability to do science and mathematics is not limited to a small fraction of the population. This aspect of RISE will place the greatest demands on

High school students have discovered a previously unidentified celestial object in the Kuiper Belt using images from the National Science Foundation's 4-meter Blanco Telescope in Chile.

> ***"The students' discovery has shown that all students from a broad range of backgrounds can make solid, exciting and inspiring scientific contributions."***
>
> **Carl Pennypacker**
> **Founder, Hands-On Universe, and Astrophysicist**
> **Lawrence Berkeley National Lab and The Lawrence Hall of Science**

“Great discoveries and improvements invariably involve the cooperation of many minds.”

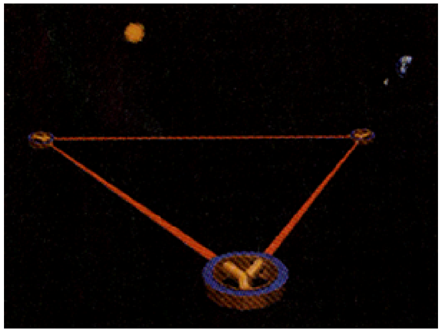
Alexander Graham Bell
Scientist/Inventor (1847-1922)

the creativity and administrative abilities of the staff of the MPS Directorate. First, the current portfolio of activities at the K-12 level serve well-defined needs of infrastructure development, informal and enhancement activites and must be continued; these are legitimate interface activities for the MPS Directorate in the K-12 community and are not to be mediated by the individual investigator. Second, there must be paradigm shift in the configuration of grant award, performance expectation and the appropriate outcomes of a successful investigation.

TOOLS

"He that invents a machine
augments the power of a man
and the well-being of
mankind."

Henry Ward Beecher
Author (1813-1887



Computer simulation of LISA - Laser Interferometer Space Antenna. LISA, the space counterpart of LIGO - the Laser Interferometer Gravitational-Wave Observatory, would find sources of long-period gravitational waves.

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III. TOOLS

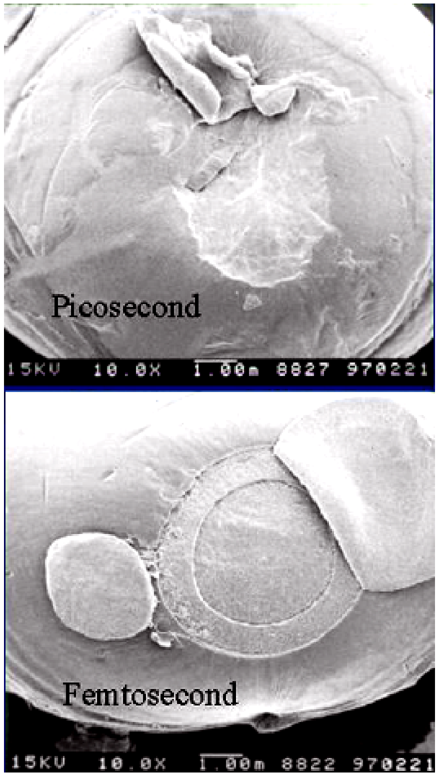
Today, we are in an era of exploding scientific opportunity enabled by numerous revolutions in tools for science. Tools have allowed a stunning view into nature that has captured the imagination of the world -- from the far reaches of the universe and the beginnings of time to the fundamental makeup of matter and the workings of life. These new tools are spread across the breadth of science and engineering. Discovery is expanding at an accelerating pace and the U.S. needs to be central to this process or it will cede leadership to others. Without forefront facilities and tools, our leadership in forefront science will disappear. Investment in instrumentation has many payoffs; perhaps the most powerful relates to the training of the next generation of leaders in science and engineering. Instruments and their supporting infrastructures are becoming more costly and complex. The scientific problems we face today involve complex phenomena and these can only be studied with new generations of empirical tools and computers.

The university community relies on the NSF for funding and support of frontier facilities, and increasingly industry is coming to rely on the NSF sponsored fundamental research programs in universities to sustain them. Critical to modern commercial competitiveness, the tools of science are rapidly transformed into the tools and technologies of industry. The MPS currently invests 25% of its total budget in facilities. With the advent of networking and emerging information, computing and communications technologies, we are entering an era of remote and universal access to frontier instruments and infrastructure.

The strength and world leadership of U.S. science in each of the MPS disciplines is based on access to state-of-the-art advanced instrumentation, ranging from tabletop instrumentation to large facilities, and on adequate technical infrastructure to provide researchers the flexibility to move in new directions as new ideas and opportunities arise. Sophisticated facilities are not an optional part of the research enterprise; they are the drivers of fundamental research and technological innovation. Facilities serve entire communities, from large groups to single investigators. Without forefront facilities, our leadership in forefront science will disappear. The same is true at the 'table-top' limit. The power of smaller instrumentation has grown to the point where single investigators working together with their students can change how we think about the world and, indeed, provide windows on future technologies that will impact all our lives. For example, think of the new medical imaging techniques based on polarized noble gases that emerged from groups working on understanding polarization processes in atomic collisions. While a balance between the two extremes of investment -- facilities and tabletop instrumentation -- must be struck, the underlying guiding principle should be to support high-quality, innovative people and provide them with the resources to think expansively. By providing access to new regimes of complexity and understanding, we are educating new scientists in the latest technologies needed to expand the scientific and technological boundaries. These are the people who will guide the development of the next generation instrumentation and who will contribute the new drivers for economic growth in this country.

The promise of advanced instrumentation can be best understood by looking at current objectives and opportunities. Intense synchrotron light and neutron facilities are essential to make advances in understanding high-T_C materials (and designing new materials) and the molecular structure of biological systems. Studies of such materials using neutrons is an area of particular promise, providing a unique window on structure and organization, yet, as evidenced by a recent Academy study, there is a dearth of facilities and related instrumentation. New instruments have provided the means by which researchers have been able to explore regimes of time and space unimagined just a few years ago. Higher energy and intensity accelerators and new observatories with adaptive optics are planned that will probe the universe at extremes ranging from 10-18 cm to 10+28 cm. Researchers are now using femtosecond lasers to examine the making and breaking of specific chemical bonds; and new microscopies, such as scanning tunneling microscopy, are opening up the viewing of individual atoms and molecules. Advanced lasers, adaptive optics, new imaging techniques, and molecular-level manipulation techniques show enormous promise for applications in medicine and in biological research. New nano- and atom-level manipulation and fabrication techniques are being developed that have the potential to revolutionize communications and computational technologies. Such applications and the associated new technologies derive from investments in advanced instrumentation and instrumentation development tools that the country and the next generation will need to sustain our technological edge.

MPS stewardship responsibilities lie primarily with the university community, which provides much of the intellectual leadership and is the source of future generation scientists – the people who will make the scientific advances and become the next-generation leaders. The prime university role should be to define how we will do science decades from now. In an earlier era, universities designed and built the new observatories, accelerators, computers, networks, and many of the technologies used in modern science. In order to provide mechanisms for universities to continue to participate actively in the creative process, they must be part of conceiving, designing, constructing, and operating facilities and infrastructure projects on a national lab scale. What are the new areas, basic technology developments, and expertise that we need to support this vital mission? Universities will provide the vision and the roadmap to answer these questions. Our responsibility is to provide (i) support for the needed new researchers, postdocs, and students to spawn the development of revolutionary new tools, (ii) the support needed to realize these new instruments, and then (iii) the support for their exploitation -- new science and sophisticated technical training.



Comparison of Picosecond and Femtosecond Lamellar cutting.
Journal of Refractive Surgery, 1998

> ***“There is one thing even more vital to science than intelligent methods; and that is, the sincere desire to find out the truth, whatever it may be.”***
>
> **Charles Sanders Pierce**

The MPS investment in facilities is approximately 25% of its total budget. Among the major current investments are the new GEMINI observatories, the NHMFL, CESR, LIGO, CUOS, the MSU/NSCL, and CHESS. Each of these facilities provides world-leading research opportunities. They provide central resources to user groups, large and small, from colleges and universities around the country. To provide for continued forefront science opportunities, new facilities have been regularly identified by their respective scientific communities. Each MPS facility represents a new intellectual thrust, and each is 'one-of-a-kind'. They are generally risky undertakings, because in order to make order-of-magnitude increases in science reach, new and innovative technologies are generally involved. In this regard, and in other ways, each facility is an engine of technological innovation. Science facilities have the institutional resources and infrastructure -- shops, computers, engineers, and engineering support -- to conceptualize and devise new tools, to develop new techniques, to build new instrumentation, and to implement new ideas, things that haven't been done before and that will advance the field. The advances realized by these new facilities rest on technology development that often appears later in commercial applications.

An important challenge is networking of facilities and remote distributed access so that they can be fully exploited. Because of the large capital investment, many of these facilities require multiple agency support and international partnerships. GEMINI and LHC are excellent models of such partnerships, GEMINI involving six countries, and LHC involving DOE and the CERN member states. The scientific community has learned to conduct research as visitors to such national facilities. Today, the NSF shares responsibility for constructing and operating national facilities with DOE, NASA, and NIH. The agencies complement one another in this regard. NSF should not shy away from leadership responsibility, even though the capital costs may be high. The science payoffs are often much greater than anticipated at the outset. Undergraduates, graduate students, postdoctoral researchers and faculty, in large groups and small, have benefited from access to such user facilities. Students' involvement in building instrumentation for these facilities helps to develop an advanced technical workforce.

The establishment of effective data archives and mining tools will be a key factor in exploiting the new science opportunities across MPS. Indeed, this opportunity applies across all of NSF. The usefulness of these national data banks will be increased by collaboration with other federal agencies and private organizations. A particularly good example is the 'national virtual observatory' Data -- several terabytes per day from ground-based and space observatories will be intelligently archived and cataloged, with enabling data mining and visualization tools. Such a national data facility could also include the output of huge simulations carried out on terascale machines. More important than the increase in efficiency are the unique opportunities for new science arising from creative use of such a national data facility.

Over the past 10 years, the investment in construction of MPS' large-scale infrastructure projects (MRE and MRE-class projects) totaled more than $600M. For the next 10 years, the university community has identified a number of projects that are central to continued advances in the core MPS sciences, calling for funding totaling $2.8B. Without a change in the paradigm of support for large-scale facilities and instrumentation, NSF will lose many of these opportunities, and at the same time lose the scientific momentum and drive to move into new areas. The existing paradigm is flat funding. In order to build a new facility, one has to shut down another. The story is similar for general instrumentation, where MPS invested more than $600M over the past 10 years. The tension resulting from the constant mismatch between science opportunities and support level for new instrumentation is destructive to the enthusiasm of young people driven by the prospect of discovery. Often, in order to balance new opportunities against exploitation of existing instrumentation, we are forced into less than optimal utilization of existing investments. As an example of the magnitude of this stress, the investment in construction of AST's large-scale infrastructure projects (MRE projects) totaled $110M over the past 10 years. The accelerated pace of discovery, fueled by rapidly advancing technological capability, demands an increased investment totaling over $860M (Atacama Large Millimeter Array, a national virtual observatory, Advanced Solar Telescope, 8-Meter Deep Sky Survey, 30-Meter Telescope, Square Kilometer Array) over the next 10 years. Other nations have taken bold steps in innovative instrumentation. In the field of ground-based optical astronomy, for example, Europe and Japan have invested far more than the U.S. in recent years. If we fail to move to a new cost curve, we will lose first rate science opportunities, not simply forgo lower priority projects. What is needed is at least a quadrupling of the present investment in small- and large-scale instrumentation projects.

The outcome of increased investment in advanced instrumentation and facilities will be world leadership in science. World leadership in science strongly impacts many sectors of our society -- from national security to a strong economy to our quality of life, from health to a clean environment to imparting the joy and excitement of discovery to our citizens. Such investments already have an enormous impact on students. Many of these investments can be further leveraged by new outreach activities. For example, outreach centers associated with facilities can reach out to K-12 students and influence the teaching of science as well. Investment in instrumentation is thus an investment in education and our future, because education in a discovery-rich society provides the feedback mechanism to sustain and guide the discovery process itself. Similarly, the public's direct participation in advanced visualization access to national data facilities, such as the national virtual observatory, will open a much needed avenue for public involvement in the excitement of scientific discovery.