# Theoretical Science in the Mathematical and Physical Sciences Directorate

## Report of the Workshop of October 28-29, 2004

"There is nothing so practical as a good theory".

Kurt Lewin, 1940

## I. Introduction

If there is a single defining theme for the mathematical and physical sciences, it is the deep partnership between theory and experiment. Powerful experiments and observations lead to impressive advances and discoveries as they do in the life sciences. But in the mathematical and physical sciences, highly developed theoretical structures play an equal role. They provide an elegant and often simple understanding of the physical world and generate the questions that shape much of frontier research.

Theoretical research in the mathematical and physical sciences ranges from the fundamental constituents of matter to the molecules of life to the large-scale structure of the universe. It can reduce to the study of a single particle or expand to the description of emergent collective behavior. Its tools include abstract mathematical concepts, careful analysis, physical intuition, powerful computation, and the interpretation of large data sets. Theory is highly interdisciplinary, with common themes often playing out in many different physical arenas. An example appearing throughout this report is the challenge of understanding phenomena that span disparate length and time scales.

The Directorate for Mathematical and Physical Sciences (MPS) supports a rich array of theoretical science in each of its five divisions. This work takes place in university and college departments, national laboratories and facilities, and research centers throughout the country and beyond. Theorists work as individuals, in small groups, and as members of research teams and experimental collaborations.

The theoretical science supported by MPS represents an important resource for our nation and the world. Its excellence has been nurtured over the years by a strong partnership between the scientific community and the National Science Foundation. The scientific staff of MPS draws on community advice through reviews and panels, and broadly through the MPS Advisory Committee (MPSAC).

The MPSAC has often discussed issues of special concern to theory. At its Spring 2004 meeting, it considered a set of such issues, some of which had been brought to its attention by Assistant Director Michael Turner. Following these discussions, the MPSAC decided to establish a two-day Workshop on Theoretical Science in the Fall of 2004 at the National Science Foundation. A Steering Committee (Appendix A) was established to organize the Workshop and to choose a broad set of participants from each of the MPS Divisions (Appendix B). The invitation letter to the participants from Michael Turner (Appendix C) describes the charge to the Workshop.

The meeting began with a set of five science talks, one representing each of the five Divisions. It then broke into five parallel Divisional sessions, each organized around three broad areas: the science, modes of support, and education and outreach. Reports from these sessions were heard at the end of the first day. These were drawn on to organize a set of three MPS-wide topical breakout sessions on the morning of the second day, on the science, on modes of support, and on education and outreach. The Workshop concluded with a general discussion of all the observations and recommendations.

This report first samples some of the exciting theoretical science supported by MPS, highlighting open questions and challenges. It then presents the MPS-wide observations and recommendations emerging from the Workshop. Next, it describes a set of division-specific observations and recommendations. All of the **recommendations appear in bold face** throughout the report. The appendices include the membership of the Steering committee, a Workshop participant list, the invitation letter of Michael Turner, a set of questions provided to the participants in advance of the Workshop, and the agenda of the meeting.

## II. Frontier Theoretical Research

### A. Astrophysics and Cosmology

> "I ask you to look both ways. For the road to a knowledge of the stars leads through the atom; and important knowledge of the atom has been reached through the stars".
>
> Sir Arthur Eddington, 1928

Several decades have elapsed since the discovery of the X-ray and microwave backgrounds, neutron stars, black holes, and quasars. In the intervening period, the entire 70-octave electromagnetic spectrum, from Megahertz frequencies to TeV energies, has been opened up for study, and cosmic ray, neutrino and gravitational wave astronomy have begun. Theory has been at the core of this transformation in our understanding of the universe, and it is shaping the design of the next generation of instruments that will extend our knowledge even further.

Observations of microwave background fluctuations, supernova light curves and X-ray-emitting clusters of galaxies have revolutionized our understanding of cosmology, demonstrating that we inhabit a spatially flat, accelerating universe. However, these observations are intelligible only as a result of theory, which has furnished the framework for interpreting these data and for transforming accurate and reproducible measurements into a quantitative description. Many challenges remain: What is the nature of the ``dark matter'' that dominates the material content of the universe—is it made up of as yet undiscovered elementary particles? Why is it that there are more baryons than antibaryons in the universe? What is the physics of inflation? How did the first stars, galaxies and black holes form, ending the "dark ages" that prevailed after the universe recombined? The greatest challenge of all to cosmology is to divine the nature of the ``dark energy'' that has been invoked to account for the acceleration.

Another great advance in astronomy has been the discovery of extra-solar planetary systems in relative abundance, all of which (so far) differ significantly from the solar system. These systems present major challenges to theory. Their origin is tied to the formation of stars, a classical and as yet unsolved problem in astrophysics. Planets originate in disks of gas and dust around newly formed stars, and it is believed that magnetic fields control the dynamical behavior of these disks. Such disks control not only the formation and growth of planets, but also of moons, stars, black holes, and galaxies, and they are ultimately responsible for most of the non-thermal, high-energy phenomena that we observe. The greatest roadblocks to further understanding of disks and the stars they orbit involve nineteenth century physics operating over very large ranges of temporal and spatial scales—e.g., multifluid, compressible turbulence in shearing, magnetized, self-gravitating media in which the transfer of radiation is important. Twentieth century physics is also essential: Disks are partially or fully ionized, and plasma processes operating on small scales determine the non-thermal emission from disks and the evolution of the magnetic fields threading the disks. Nuclear and condensed matter physics is central to our understanding of neutron stars and planets. Distinctive spectra, outflows and oscillations are observed that are within the reach of theoretical explanation as computational astrophysicists achieve greater resolution and the capability to combine more of the relevant physical processes within a single simulation.

A third major development has been the discovery of the great prevalence of black holes in the universe. Essentially every large galaxy has a massive black hole at its center. How did these objects form, and how are they related to the formation of galaxies? Galaxies also contain stellar-mass black holes, some of which may form in gamma-ray bursts. Black holes of all sizes provide a laboratory in which we can test the laws of physics, particularly gravitational physics, under conditions that cannot be replicated on Earth. The most spectacular events involving black holes are believed to occur when they merge with other black holes or with stars, and it is an outstanding challenge to theorists to predict the gravitational wavetrains produced by such events.

## B. Atoms, Molecules and Materials Chemistry

> "Every natural science always involves three things: the sequence of phenomena on which the science is based; the abstract concepts which call these phenomena to mind; and the words in which the concepts are expressed. To call forth a concept, a word is needed; to portray a phenomenon, a concept is needed".
>
> Antoine Lavoisier, 1789

Chemists seek to understand, design, and control the properties of molecules and materials. Theory is at the very center of this enterprise, providing the framework for the atomic and molecular level description of chemical reactivity and structure. Theory is critical for the interpretation of experimental data, for the prediction of new behavior, and for the inspiration and guidance necessary for designing the next experiments. Great strides have been made in the development of accurate theories of atomic and molecular behavior for increasingly complex processes, in bulk states of matter as well as at interfaces. Moreover, theoretical chemists have adapted their tools for use in industry and by experimentalists. While chemists, physicists, and molecular biologists all seek to understand complex systems, many opportunities and challenges remain squarely in the domain of theoretical chemistry, including quantum mechanical treatment of complex molecular processes, transition path identification, multi-scale chemical phenomena, and design of molecules and materials from first principles.

Quantum-based molecular theories describing combustion, atmospheric chemistry, and biochemistry are crucial for developing fossil fuel alternatives, for understanding global warming and ozone depletion, and for uncovering the molecular basis of life processes, including disease and aging. Solutions to such problems await accurate electronic structure methods for (i) excited electronic states of molecules (which play a crucial role in atmospheric chemistry and solar energy conversion); (ii) open-shell molecules (e.g. free radicals present in fuel combustion); (iii) large molecules (e.g. proteins that dictate disease evolution, and polymers found in fuel cells); and (iv) molecules with heavy elements (e.g. for extraction of heavy metals from the body and the environment).

The calculation of static molecular properties is a necessary beginning, but it is not sufficient. The time evolution of molecular behavior must be understood as well. We must be able to characterize quantitatively the dynamics of chemical reactions, which will require theoretical advances on many fronts. New approaches are needed for the treatment of nuclear dynamics, Born-Oppenheimer breakdown, and multiple potential energy surfaces. Quantum treatments of van der Waals forces are essential for describing polymers and biomolecules such as DNA; sufficiently quantitative theories have yet to be formulated. Accurate force fields describing interatomic interactions are critical for molecular simulations; both their derivation from quantum mechanics and well-founded analytic forms remain elusive. Biomolecules such as proteins inhabit potential energy landscapes with numerous pathways from initial to final states; theories for sampling such landscapes and characterizing transition paths are still in their infancy.

Many molecular and material phenomena are characterized by multiple length and time scales. Molecules vibrate in less than a pico-second while reactions often occur in greater than milliseconds. The length scales over which defects in solids affect material behavior range from nanometers to the macro-scale. Fully general analytical and numerical methods that seamlessly span such scales do not yet exist, while extraction of new phenomenological equations and concepts from such simulations has only just begun. Ultimately, multi-scale theories should be able to describe long time, macroscopic behavior, starting purely from quantum mechanics at the atomic level, accounting for critical rare events.

Finally, the ultimate grand challenge is to solve the inverse problem: given a desired macroscopic property, design from first principles the molecule or material possessing it. This last challenge remains an open frontier.

## C. Condensed Matter and Materials Physics

> "We often think when we have completed our study of one, we know all about two, because 'two' is 'one and one.' We forget that we have still to make a study of 'and'."
>
> Sir Arthur Eddington, 1930

The laws of quantum mechanics that govern the behavior of atoms are well understood. But when large collections of atoms are assembled to form matter, new and surprisingly complex behavior emerges. Coulomb correlations can take what appears to be a metal on short time and length scales and turn it at large scales into an insulator, or a broken-symmetry state such as a superconductor or magnet, or even an exotic phase with topological order but no local order parameter as in the fractional quantum Hall effect. Small changes in parameters can lead to quantum phase transitions among these novel phases. At some non-zero temperature, classical behavior ultimately emerges, but the essential degrees of freedom and the parameters in the effective theory are often determined by quantum mechanics at shorter scales. Even beyond the scale at which the behavior is classical, there are numerous other multi-scale phenomena at the frontier of theoretical research including turbulence, non-equilibrium pattern formation, crack initiation and propagation, and protein folding.

New concepts are therefore needed at successive length, time, and energy scales at which distinct, collective phenomena emerge. These concepts constitute the organizing principles of emergent matter that cannot easily be simplified or reduced to the well-understood first principles of quantum mechanics. Although theoretical advances in the study of emergent phenomena are crucial for the development of new materials and new technology, these studies are most often projects in pure theoretical physics.

Equilibrium statistical mechanics is an enormously successful theory capable of dealing with emergent phenomena. But no general theory exists for the many systems that are changed drastically by external influences and are never close to equilibrium. Recognition that classes of such systems often exhibit common (‘universal’) patterns of behavior is a key step in understanding the organizing principles. Many materials exhibit poorly understood non-equilibrium phenomena. For example, crack initiation and propagation is challenging because of the interplay of many length scales, and is very important in contexts ranging from aerospace to earthquakes.

Electron-electron correlations yield many unexpected phenomena . Examples include high-temperature superconductors, new ‘strange metal’ (non-Fermi liquid) phases, the fractional quantum Hall effect, and hitherto unexpected effects of disorder. Standard methods of electronic structure calculations based on density functional theory, unable to account for correlations, are inadequate to describe these new phenomena. Dynamical mean field theory (DMFT) is a new technique, which captures the quantum fluctuations associated with strong correlations and yields quantitative accuracy for the electronic structure and new insights into the physics of some of these strongly correlated materials. Other important new techniques involve Chern-Simons theory, Green’s-function Monte Carlo methods, and non-perturbative approaches to exotic ordered states such as spin liquids and topological superconductivity.

Quantum uncertainty, long thought to be only a limitation, is now understood also to be a resource for computation and secure communication in ways that are impossible classically. While the goal of creating a large-scale quantum computer remains remote, rapid experimental progress is now being made in a number of areas, with strong and growing interactions among the atomic, optical, condensed matter and NMR communities. An important offshoot is a host of new ideas in signal analysis and noise reduction in NMR and atomic clocks, and in quantum measurements.

The study of "soft" materials, such as liquid crystals, where entropy dominates the physics, continues to be vibrant, and has expanded to encompass biological matter. The constituents of cells, such as the cytoskeleton or the cell membrane, are soft materials, with mechanical and rheological properties akin to those of conventional soft matter, but are kept out of equilibrium by a constant input of energy via chemical or biochemical reactions.

## D. From Atoms to the Planck Scale

> "Nature has always looked like a horrible mess. But as we go along we see patterns and put theories together; a certain clarity comes and things get simpler".
>
> Richard Feynman, 1983

The past ten years have seen an exciting convergence of research interests in atomic, molecular and optical (AMO) physics and condensed matter physics. The exquisite experimental control available in the AMO arena makes this a fascinating field for theoreticians. Ideas developed over the past four decades in the study of driven, damped, open quantum systems in quantum optics, are now being applied to quantum coherence in condensed matter systems such as superconducting qubits. Conversely, the condensed matter language of quantum phase transitions, and exotic order parameters is being applied to new regimes of strongly correlated ultracold bosonic and fermionic gases. Additional forefront areas of AMO theory include ultrafast light pulses (now pushing into the attosecond regime) and their use as probes of electronic and nuclear dynamics in atomic and molecular systems at their natural time scales; and calculations of extraordinary precision essential to the interpretation of symmetry-violation tests and possible variations of the fundamental constants.

The strong interactions of the atomic nucleus have challenged theorists for decades, leading to some of the most elegant and broadly applicable tools of theoretical physics. In recent years, effective field theory methods have been refined to provide a beginning picture of the two- and three- nucleon interaction. Precise calculations of the properties of light nuclei have been carried out using Greens function Monte Carlo techniques. The underlying theory of the nuclear force, QCD, emerged in the 1970's, drawing on the advent of Yang-Mills gauge field theories. It was shown that these theories are "asymptotically free", the interaction strength weakening with decreasing distance. For QCD, the gauge theory of quarks and gluons, the weakening sets in at sub-nucleon distances. At the nucleon size itself, the interaction is strong, confining the quarks and gluons, and making analytic solutions enormously challenging. However, much progress is being made using sophisticated Monte-Carlo algorithms, on fine-grained space-time lattices. Among the current experimental studies of QCD, none are more fascinating than those at the Relativistic Heavy Ion Collider (RHIC). Large nuclei are compressed and heated, creating for an instant a plasma of unconfined quarks and gluons. Numerical simulations of QCD as well as new analytical techniques for the description of strongly interacting thermal media, are essential for the interpretation of these experiments.

QCD and the electroweak theory comprise the successful Standard Model of particle physics. But the large masses of the W and Z bosons show that the electroweak gauge symmetry is somehow broken. How this happens remains one of the most important questions in particle physics. Every idea, from a single Higgs boson, to the appearance of supersymmetry, to the existence of extra spatial dimensions, involves new symmetries and new phenomena. Theory assures us that the new phenomena will be observable at the next generation of high energy colliders, in particular the Large Hadron Collider. And somewhere in the array of new heavy particles are those that make up the dark matter dominating the mass density of the universe.

There are many other mysteries. Why are there three families of quarks and leptons and why do their masses differ so dramatically? And can the electroweak and strong forces be unified at some high-energy scale? The neutrinos are especially intriguing. The significance of their tiny masses, revealed in the neutrino-oscillation experiments of the past decade, continues to elude theorists. But these masses may be our most direct window on grand unification. Finally, there is CP symmetry, the combination of space reflection and the reversal of sign of a particle's charge. Its small breaking, observed only in rare meson decays, is unexplained so far, and its consequences are profound. It is essential for understanding why the universe contains so much more matter than anti-matter.

Gravity is weak in laboratory experiments, but strong and surprising in astrophysical environments such as black holes. It is described by general relativity out to cosmological distances, where it appears to be coupled to a mysterious dark energy. But will general relativity persist to all scales? Further, the gravitational coupling grows with energy, becoming comparable to the other forces of nature at the Planck scale of 10^19 GeV, not far beyond the energy scale of strong and electroweak unification. There, a complete unification of the forces of nature may emerge. The most promising idea is string theory, which proposes that at the smallest distances all matter is composed of tiny loops, or strings. Shaped by compelling ideas of consistency and symmetry, including supersymmetry, it incorporates gravity and quantum mechanics, and could provide the answers to many of the deepest questions posed by the Standard Model.

## E. Theory in Biology

> "The fact of evolution is the backbone of biology, and biology is thus in the peculiar position of being a science founded on an improved theory."
>
> Charles Darwin, 1876

The scientific study of living systems is undergoing a major transformation. Genetic technology is providing vast amounts of data regarding the components underlying life, and high-resolution real-time imaging of living matter has become commonplace. The challenge for physicists and chemists, in partnership with biologists, computer scientists and mathematicians, is nothing less than to elucidate the principles whereby the microscopic parts self-organize and work together to accomplish the task of survival.

The role of theory in this new era is to develop new concepts and methodologies for non-equilibrium complex systems such as living systems and eco-systems. There must be a two-way flow of ideas between theorists focused on the new physics and mathematics, and theorists applying these insights to a broadening array of biological processes. A difficulty is that living systems do not break up into subsystems at different spatiotemporal scales that can be individually tackled. Instead, information seems to pass back and forth readily between the microscopic scale of individual bio-molecules and genes and the macroscopic level of single cell and single organism functionality. Thus the foldings of prion-type proteins (of mad-cow fame) have been implicated in such large-scale processes as Darwinian evolution (in yeast) and neural memory (in Aplysia).

There are many questions whose answers require advances in the theory of complex systems. Starting from evolution, we need conceptual guidance as to how biological information is stored and processed in a way that makes it functional and yet conducive to adaptive change. We need a theory of biological network functioning that will go beyond static graph theory and deal with actual task performance. We need to understand how the cell uses molecular interactions, spatial compartmentalization, and multiple levels of feedback to respond accurately to differing environmental cues. Even at the molecular level, there are mysteries. How do bio-molecules reliably perform their tasks in the crowded cellular milieu without aggregation and non-specific (incorrect) binding? At the multi-cellular scale, cells communicate and cooperate using an alien language of chemical signals, direct contact interactions, and forces mediated by the extra-cellular medium; we need to learn this language. The grandest challenge is the physical basis for human cognition, where even our most complex models seem like inadequate cartoons of a bewilderingly complex multi-faceted system.

What theoretical constructs will be needed for this new era? Although it is difficult to make predictions, some hints seem to be emerging. The notion of a special landscape in protein folding is perhaps more generally applicable, for example to signal transduction networks such as those that control the cell cycle. Ideas from dynamical pattern formation in non-equilibrium physics seem to be necessary to explain how cells process spatially varying input information. Information theory approaches are spreading, from sensing in the brain to cell-cell communication. Will all these trends somehow merge to form a coherent set of principles for a theoretical biology? Are these principles different for different levels of the biology hierarchy? Will we be able to use this to synthesize more powerful "bio-mimetic" technology? Opportunities abound for theoretical physical scientists to participate in the generation of a whole new approach to the biological world.

## F. Mathematics and Computation

> "The enormous usefulness of mathematics in the natural sciences is something bordering on the mysterious."
>
> Eugene Wigner, 1960

Modern research in pure and applied mathematics and statistics ranges over a vast landscape, much of it shaped by interactions with the physical sciences. Work in high-energy theoretical physics, in particular string theory, has led to entirely new developments in geometry and topology. Computational simulation is an important tool across all the natural sciences. The analysis of massive data sets has become crucial as the scale and sophistication of experiments has grown. And some of the most exciting current theoretical research has evolved from problems purely internal to mathematics.

The formulas of high-school algebra for solving polynomial equations are actually rare. We can't solve most systems of algebraic equations by concrete formulas. But spectacular progress has been made at understanding the qualitative nature of the solutions: how many there are, and what geometrical and topological properties they have. While these techniques are helping to provide the theoretical underpinnings for modern string theories, the influence travels in both directions: correlation formulas from string theory and quantum field theories have stimulated vigorous geometric developments in mathematics. One recent development: a new use of the topological tool known as K-theory, originally developed by pure mathematicians from purely internal motivations, but later encountered by physicists in the study of anomalies, and now appearing in a brand new form.

Computation has become an important tool throughout the physical sciences. Computer simulations can bridge intellectual gaps, such as the relationship between quantum-scale models and continuum-scale models of a physical process or material; moreover, computer simulations can be the most convenient channel for communications from theory to the design of experiments. Mathematical scientists are confronted by deep problems in the study of theoretical models that span disparate scales of length, time, or energy. Numerical methods for reliable computation at multiple length or time scales are extremely challenging to design, since the passage from small to large scales by summing many small changes enacts the numericist's nightmare by adding many small errors that may compound into a large one.

The nature of experimental data is changing rapidly. Astronomers, particle physicists, meteorologists, neuroscientists, and geneticists, are all blessed and cursed with data-gathering techniques that can put terabytes of information on record in short periods. These data have features that confound traditional statistical methodology: signals may be tiny compared to noise, features to be identified may be rare and unknown in shape, statistical properties of noise and signal may be non-stationary in time and unknown in distribution, and the data sampled in a single instant may have enormous apparent dimension. Ongoing work by statistical scientists addresses problems of pattern discovery and description, dimension reduction, and compression by applying methods of topology, computer science, and approximation theory.

Some of the most striking recent discoveries concern problems that originate from within mathematics. Thirty years ago, Robert Langlands proposed a series of ideas that, if true, would unify highly disparate areas in mathematics: number theory, representation theory, algebraic geometry, and analysis. After much effort, great progress in this direction has finally begun to emerge and there is now hope that Langlands' "program" may come to fruition within the next decade. A similar story concerns Poincaré's conjecture from 1904 concerning manifolds that can be deformed into spheres. Smale's spectacular solution (in 1961) for spheres of dimension 7 or more led to a revolution in topology. This was followed by special proofs for spheres of dimensions 6, 5, and 4, but the three dimensional case (which was Poincaré's original goal) seemed to defy all attempts. There now appears to be a proof in the three dimensional case, and it involves a host of radical new techniques that will continue to affect the subject long after interest in the original problem has dissipated.

## III. MPS-Wide Observations and Recommendations

Many of the issues of concern to theory are important for experiment and observation as well. The discussions of the Workshop often ranged beyond theory, as did the observations and recommendations emerging from the divisional and topical breakout sessions. This is reflected in the MPS-wide observations and recommendations of this section. Some are broad, but they are especially critical for theory since so much of it relies on NSF for support.

### A. The Science and its Support:

The best ideas for basic scientific research emerge from the scientific community itself. In many cases, this inquiry-driven research is supported in response to unsolicited proposals. It can be found in established or emerging disciplines, and frequently involves the pursuit of risky ideas.

In theoretical science, inquiry-driven research by individuals and small groups is the central, key component. Individual investigators, working with students and postdoctoral fellows, produce much of the most exciting science. Collaborating in larger groups can also be very effective in theory. The advantages include solving complex problems involving multiple disciplines and skill sets, the presence of critical mass to spark ideas, the leveraging of resources, and the shared mentorship of young scientists.

Grants for the support of individuals and collaborative groups are extremely important, as are grants to groups of theorists with related interests. In addition, grants to experimental groups can provide support for theorists, who can often be important members of experimental collaborations.

**Recommendation A1. MPS should preserve inquiry-driven theoretical research at the frontiers. The support of unsolicited proposals from the scientific community should remain a very high priority.**

**Recommendation A2. MPS should foster a breadth of effort in theoretical science, and be responsive and flexible to new and sometimes risky opportunities and emerging disciplines.**

For theorists, as well as experimentalists and observers, there is a natural tension between the support for individuals and smaller groups on the one hand and for larger groups and centers on the other. This is mirrored in the tension between the support of unsolicited proposals and solicited ones. Both are important, and establishing the right balance is a continuing challenge for MPS. It is also a Division-specific challenge, which has been considered by each Committee of Visitors (COV) in recent years. It is important to note that MPS centers that focus on theory, or that include theory as a component, have played a very valuable role in the scientific community.

**Recommendation A3. Each Division of MPS should continue to monitor carefully the mix of center support, group support, and the support of individual investigators in theoretical science. The Divisions should develop metrics to determine the appropriate balance among these modes of support, for the advancement of science and for educating the next generation of scientists.**

Grant duration and magnitude are of great concern across MPS. They are critical issues for theoretical scientists, many of whom must rely solely on the National Science Foundation for support. It is the current policy of the National Science Board to increase the duration and magnitude of principal investigator grants.

**Recommendation A4. The Divisions of MPS should work to increase the duration of individual and group grants to theoretical scientists in response to unsolicited proposals. MPS is urged to secure the incremental funding to increase the magnitude of grants in theory. These steps should be taken even in times of budgetary stringency.**

Frontier theoretical research often evolves rapidly and in surprising directions. There will always be important opportunities that do not fit comfortably into any one of the established disciplines around which the programs of MPS are structured. The work can be inter-divisional, inter-directorate, and even inter-agency. Program Officers look for these opportunities, and the Office of Multidisciplinary Affairs (OMA) provides start-up support, although it generally does not participate in individual or small group awards. There is a perception among theoretical scientists that research proposals at disciplinary boundaries sometimes “fall through the cracks”.

**Recommendation A5. MPS should ensure that adequate mechanisms are in place for the review and support of proposals for theoretical**

**research at the boundaries of the established disciplines, as well as theoretical research that combines several disciplines. The success rate for such proposals should be the same as for disciplinary proposals of comparable quality. The Office of Multidisciplinary Affairs (OMA) should play a more active role at the individual and small-group levels.**

Major and moderate initiatives at the NSF, including those associated with large facilities, often do not include support for important, related theory. This can be short sighted, since theory is crucial for the interpretation of frontier experiments, and can set new experimental agendas. Furthermore, modern instruments and experiments require broad theoretical understanding for their proper design.

**Recommendation A6. Support for theory, including grants to individual investigators, should be a part of major or moderate programs in each of the Divisions of MPS.**

Computation is a fundamental part of theoretical science. It is essential for exploring theoretical structures themselves, for simulating the behavior of complex, non-linear systems, and for the interpretation of precision experiments and observations. State-of-the-art computational facilities of all sizes, and their support, are critical for theoretical research. Algorithmic development, often interdisciplinary, is also a very important component of theory.

**Recommendation A7. MPS should provide strong support for computational facilities, for the development of publicly available, professional quality code, and for algorithm development.**

MPS-supported theoretical research, some funded through the Information Technology Research (ITR) initiative, has played a vital role in advances in computational science.

**Recommendation A8: New resources should be sought to ensure that outstanding research that has been initiated using Information Technology Research (ITR) funds can be sustained throughout the theoretical programs of MPS.**

Biologically related research is increasing throughout the Divisions of MPS. Theoretical concepts from the physical sciences and mathematics are being applied to biological systems, biologically-inspired principles are being used to design new materials, and experimental advances are enabling new probes of living systems. The trend towards doing biologically relevant and related research is also occurring in other NSF Directorates, and is likely to continue and even accelerate over the next decade.

**Recommendation A9: As biologically-related theoretical research becomes more and more pervasive, it is increasingly important to coordinate the support of this research across all the Divisions and Directorates of NSF.**

Program Officers play a key role in developing and sustaining theoretical research. The demands on them have grown substantially in recent years, with new programs and initiatives, increasing international collaboration, and the mounting scale of much of modern science.

**Recommendation A10. Program Officers responsible for theoretical science are over-committed throughout MPS, and need additional help. Permanent Program Officers are especially important for the health of the theoretical programs of each Division.**

## B. Education and Training

The health of theoretical science relies critically on the education and training of young scientists. From the advanced undergraduate level on, promising students with an interest and talent for theoretical research must be encouraged and supported. The nurturing of talented students must begin even at the high school level. Mentoring plays a key role at every stage, and it is important to insure that faculty members and senior research scientists in theory are engaged and effective at mentoring.

NSF-supported workshops on professional development and teaching for faculty are oversubscribed. They have high impact and are of relatively low cost.

**Recommendation B1. MPS should encourage the Division of Undergraduate Education in the Education and Human Resources**

**Directorate to expand workshops on professional development and teaching for faculty.**

The CAREER program for young faculty has been very successful. In the MPS theoretical science community, however, there is a perceived excessive emphasis on innovative teaching proposals, especially at the K-12 level. Teaching and mentoring at the undergraduate, graduate, and postdoctoral levels are also very important.

**Recommendation B2. MPS should be flexible about the innovative teaching component in the CAREER program. A set of best practices and existing K-12 opportunities for investigators should be communicated to applicants, reviewers, and panels.**

Summer schools for the advanced training of graduate students in theory are highly valuable. They provide opportunities for students to broaden and deepen their knowledge of specialized topics, and to become acquainted with their peers at other universities and senior scientists from the U.S. and abroad.

**Recommendation B3. The Divisions of MPS, possibly together with other agencies, should support focused summer schools for advanced training of graduate students in theoretical science.**

The NSF has little statistical information specifically identifying theory graduate students and their support patterns, which can be very different from experimental students. Since theory grants are typically smaller than experimental grants, many students in theory rely more on teaching assistantships and other forms of university support. Readily available information on these patterns would be very helpful in assessing their impact on the education of theorists and in suggesting possible actions by universities and by MPS.

**Recommendation B4. Statistical information on theory graduate students in MPS should be collected routinely and maintained by the NSF.**

Summer programs for gifted high school students, which have been supported in the past by NSF, have been very successful in attracting young people into careers in science.

**Recommendation B5. MPS should support summer programs for gifted high school science and mathematics students.**

## C. Broadening Participation

Despite the progress of recent years, there is much work to be done to increase diversity in theoretical science. The proportion of women entering the field has increased some, but the number of under-represented minorities remains as tiny as ever. The effort to increase diversity must begin at the K-12 level and continue through college, graduate school, postdoctoral training, and the early stages of academic and scientific careers. Retention is a problem at every stage. The NSF takes diversity very seriously, with many approaches being brought to bear. The discussions of the Workshop did not identify issues specific to theory, but several observations and recommendations emerged that were of particular concern to the participants.

The competing demands of child care and professional responsibilities can be a major impediment for women pursuing scientific careers. Indeed, many women opt out of the pipeline after graduate school simply because they cannot envision means by which both family and career can be balanced.

**Recommendation C1. NSF should expand the definition of allowable expenses to grants to permit the charging of child-care expenses during periods of professional travel. In addition, MPS should explore ways to create incentives to universities and other institutions to provide sufficient, high quality child-care facilities.**

The availability of exciting research opportunities and mentoring by faculty members and senior scientists plays a very important role in attracting women and under-represented minorities at the undergraduate level to careers in science. Partnerships among universities, industry, and national laboratories can be especially effective, introducing students to the breadth, flexibility and teamwork in such venues.

**Recommendation C2. MPS should expand undergraduate research programs in theoretical science that place an emphasis on recruiting under-represented minorities and women, including programs involving partnerships with industry and national laboratories.**

Diversity must be encouraged strongly in the theoretical science research community beginning at the graduate–student and postdoctoral levels where retention is critical.

**Recommendation C3. MPS should develop a mechanism, such as supplements to research grants, for the support of members of under-represented groups and women at the graduate-student and postdoctoral levels in theoretical science.**

**Recommendation C4. MPS should regularly examine the diversity of speakers and organizing committees at meetings that it supports involving theoretical scientists. It should do the same for the advisory panels for the facilities and centers that it supports. MPS should identify, promulgate and reward best practices. It should take into account recent practice in making funding decisions for all meetings and workshops.**

## D. Outreach

The scientific advances of recent years have captured the interest of people everywhere, and the benefits of science are widely appreciated. The theoretical research community can take pride in this, but it also has a responsibility to continue to educate the general public. The funding of scientific research by the NSF and other government agencies, so essential for its continuing progress, depends finally on the support of an informed and supportive citizenry.

Federal science agencies such as the NSF can play an especially important role in this effort. They can do so directly and by their support of individuals, centers, and laboratories across the country. The NSF, through its Office of Legislative and Public Affairs (OLPA), is now strengthening its outreach efforts in a variety of ways. This is to be commended, but the resources should be provided to do more, including the education of the general public on exciting advances in theoretical science.

**Recommendation D1. MPS together with the Office of Legislative and Public Affairs (OLPA), should take greater responsibility for**

**– Publicizing and taking credit for MPS-supported theoretical research. This can be done through NSF publications themselves and**

**by working with the private-sector media. NSF can learn from the best practices of other agencies.**

**– Educating and helping theoretical scientists to communicate with the general public.**

**– Educating journalists on the wide variety of theoretical science supported by MPS. A summer school for journalists could be helpful.**

**Recommendation D2. MPS should establish a program for outreach grant supplements to theoretical scientists who are especially effective at representing science to the public.**

## IV. Division-Specific Observations and Recommendations

The recommendations in this section emerged principally from the breakout sessions centered around each of the five Divisions of MPS. They were discussed by the Steering committee and the participants, but not necessarily endorsed broadly by these groups.

### A. Astronomy (AST)

In Astronomy, the funding balance of theory and observation within the grants program is appropriate and the review of theory proposals is being well handled with the current organization.

**AST Recommendation 1: The Astronomy Division should maintain the current structure of its grants program. It should continue to form review panels in response to the proposals received so as to maximize the ability to compare proposals on similar topics. Each review panel should include both theorists and observers, with a balance that approximates the nature of the proposals in that panel.**

**AST Recommendation 2: In the AST Postdoctoral Program (AAPF),**
**– Letters of recommendation should be made available to reviewers in making their decisions on whom to select.**
**– Non-citizens based at US institutions should be eligible; the Hubble Fellowship program shows one way to do this.**
**– It is important that the AAPF program reflect the range of activities supported by AST, and this is best ensured by having the review panels reflect this range. Theory is a critical component of astronomical research, and AST should strive to ensure that theorists are represented on the AAPF review panel in proportion to the number of theorists applying for fellowships.**

**AST Recommendation 3: The Senior Review of facilities planned by AST should include a review of the balance between the grants program and support of facilities.**

**AST Recommendation 4: The scientific staff at AST-supported centers such as NOAO and NRAO should be strong in theory as well as in observation and instrumentation, subject to the condition that staff theorists would share equally in carrying out service for the centers.**

**AST Recommendation 5: Review panels should be informed that AST supports the concept of group grants for theorists that provide collective support for items such as computer personnel, computers, group postdocs, and visitors that the group feels are best supported at the group level.**

**AST Recommendation 6: Theory Challenges should be a budgeted part of any major or moderate initiative in AST, as recommended in the Decadal Survey.**

## B. Chemistry (CHE)

Due to the successful development of software by theoretical chemists, computational chemistry research has increased dramatically, with funding from the Theoretical and Computational Chemistry program (TCC), as well as other programs within the Chemistry Division (CHE) and elsewhere in NSF (e.g., the Information Technology Research initiative). The use of these theoretical tools is growing, by theorists and also by experimentalists, in academe, industry, and national laboratories. The most recent budget allocations for TCC do not reflect this success. Over the past 5 years, growth in budgets for experimental CHE programs has exceeded that for theory, even though TCC is the primary steward for research in this sub-discipline.

**CHE Recommendation 1: CHE should ensure adequate budget allocations in the Theoretical and Computational Chemistry program and other CHE programs for development of new theoretical methods and associated software, as well as simplified analytic models that provide new insight.**

Solutions to complex problems often require a diversity of expertise beyond that held by the typical single principal investigator. A particular phenomenon may be explored optimally by an all-theoretical team consisting of, e.g., a quantum chemist, a dynamicist, and a statistical mechanician, rather than any one of them alone.

**CHE Recommendation 2: CHE should encourage proposals to the Collaborative Research in Chemistry (CRC) program from small groups of theory-only investigators, as described above.**

Encouraging interdisciplinary collaborations to probe complex processes will require still larger endeavors. The remarkable success of theory institutes supported by PHY, DMR, and DMS in bringing scientists together is one that could be emulated in other disciplines. Theoretical chemistry has no analog to these institutes. Funding of one or two national centers for theoretical chemistry, in different geographic locations, could provide a resource to develop new collaborations, facilitate cross-fertilization, and introduce students and postdoctoral fellows to a wide array of sub-disciplines.

**CHE Recommendation 3: CHE should encourage proposals for one or two theoretical chemistry institutes, but they should not be initiated at the expense of single investigator grants in the Theoretical and Computational Chemistry (TCC) program.**

The single-investigator mode of research will continue to play the primary role in chemical advances for the next decade. A mismatch exists between the cost of personnel and the size of the average CHE grant. There is a similar mismatch between the normal duration of a research appointment (postdoc or graduate student) and the typical duration of a CHE grant. This problem is particularly acute in theoretical chemistry because TCC has primary national stewardship for the support of fundamental research in this area. While the average TCC grant provides adequate support for graduate students plus PI summer salary for three years, there is insufficient support for post-docs at a reasonable salary level.

**CHE Recommendation 4: CHE should develop a funding model for the Theoretical and Computation Chemistry (TCC) program that provides:**

- **Support for "full" people, as opposed to fractions (1 postdoc, and 1 or 2 graduate students for their research lifetime)**
- **A humane postdoctoral fellow salary**
- **A minimum of 1 month of summer salary per PI**
- **Base support for supplies, travel, and computation**

**This model should not be implemented at the expense of lowering the current success rate of TCC proposals.**

### C. Materials Research (DMR)

Condensed Matter Physics is a vibrant and broad subfield of physics, one of its essential strengths being the close coupling of theory and experiment.

Although it often has important consequences for technology, frontier theoretical condensed matter physics research, as in other areas of theoretical physics, is most often curiosity-driven, rather than application-driven.

**DMR Recommendation 1: DMR should continue to recognize the value of projects in pure theoretical physics, independent of their technological implications.**

**DMR Recommendation 2: The name of the theory program in DMR should be changed to Condensed Matter and Materials Theory.**

The breadth of condensed matter and materials theory makes communication of the excitement of the field particularly challenging. It is important for the field that this challenge be met in the form of public lectures, reports, and elegant popular books.

**DMR Recommendation 3: The Division of Materials Research should coordinate its outreach activities with groups such as the Solid State Sciences Committee of the National Research Council and the American Physical Society. DMR should assist the condensed matter community in articulating the excitement of the field. Mechanisms include the support of community collaborations leading to reports written for a variety of lay and scientific audiences.**

Condensed matter physicists attending the Workshop expressed much concern over the possible loss of important research in computational science that has been supported by the Information and Technology Research (ITR) initiative. This led to strong support for

**MPS-Wide Recommendation A8.**

Discussions among the condensed matter physicists at the Workshop also led to strong support for the careful coordination of the stewardship of biologically related theoretical research throughout the NSF:

**MPS-Wide Recommendation A9.**

## D. Mathematical Sciences (DMS)

The dichotomy in the mathematical sciences that is parallel to the distinction between theory and experiment in the other Divisions of MPS, is the distinction between core, disciplinary mathematics ("theory") and interdisciplinary ("applied") work. The relationship and balance between the two varies among different areas. In statistics or in optimization, for example, theoretical and applied aspects of the field are closely related.

By participating in the NSF “initiatives” and by launching a number of new research institutes, the DMS has significantly enhanced its support for interdisciplinary research. The available data on how the DMS budget is divided between core disciplinary support and interdisciplinary work indicates that the mix is now appropriate, although opportunities remain for further collaborative efforts between DMS and other Divisions. A number of organizations and entities fund scientific research in the U.S., but the NSF has a special responsibility as the primary steward for the mathematical sciences.

**DMS Recommendation 1: DMS should continue to monitor the balance between its support for theory and for interdisciplinary work, and it should seek to support the highest quality work without regard to the field.**

There was much discussion during the Workshop about ways to provide support for the large number of active researchers without existing research grants. DMS has implemented a number of creative solutions to this problem, including the development of Mathematical Sciences Research Institutes (which function as national user facilities and represent a variety of core and interdisciplinary interests) and the introduction of the Focused Research Groups program. Participants of the Workshop felt these programs were highly successful, and similar programs may be adopted by other Divisions of the NSF. A possible program of international travel grants was also discussed.

**DMS Recommendation 2: DMS should continue its support of programs that benefit the many active researchers who do not have research grants.**

There are excellent opportunities for mathematical outreach, particularly at the undergraduate level and K-12 levels that are critical period for recruiting young people to mathematics and science, and a number of examples of successful outreach were discussed at the Workshop. Summer schools for graduate students were also identified as a valuable investment:

**MPS-Wide Recommendation B3.**

DMS invests in graduate and postdoctoral training through a variety of mechanisms, including department-wide Vertical Integration of Graduate Research and Education (VIGRE) grants, research training groups, student and postdoctoral funding in individual investigator awards, and directly awarded mathematical sciences postdoctoral research fellowships. The VIGRE program, in particular, has become a prominent part of the DMS portfolio. It was originated with the idea that additional investment in fellowships and attention to the ways that mathematics and statistics departments recruit and train students should increase the number of U.S. students receiving PhDs, which had fallen substantially over 20 years or so.

**DMS Recommendation 3: DMS should conduct a review of the effectiveness of the VIGRE program relative to other forms of graduate and postdoctoral support.**

## E. Physics (PHY)

The Physics Frontier Centers have now been in existence for 10 years. Some include theory as a component and others focus completely on theory. There was a consensus among the physicists at the Workshop in favor of evaluating the success of these PFC's and the impact that their support has had on the support of other theory in the Physics Division. The Kavli Institute for Theoretical Physics is a uniquely broad center. It has just celebrated its 25$^{th}$ anniversary and is widely viewed as being highly successful. The Physics Division plans to review this center in 2006.

**PHY Recommendation 1: The Physics Division should continue to monitor the appropriate balance in theoretical physics among individual investigator support, group support and support through the Physics Frontier Centers.**

The duration and size of principal-investigator grants is of much concern in the theoretical physics community. The theory Program Officers in the Physics Division have had to work with very small budgets, and have been forced to under-fund, or not fund, many excellent researchers, especially new young principal investigators. The discussion of this issue among the physicists at the Workshop led to a strong endorsement of

**MPS-Wide Recommendation A4.**

The support of interdisciplinary research is another area of concern in the theoretical physics community. Discussions at the Workshop elicited strong support for

**MPS-Wide Recommendation A5**.

In the Physics Division, as in other Divisions, new initiatives often do not include support for essential, related theory. An example of this is the funding now being provided for high-energy physics associated with the Large Hadron Collider in Geneva, Switzerland. The physicists at the Workshop strongly supported

**MPS-Wide Recommendation A6.**

# V. Appendices

## A. Steering Committee

| | |
|---|---|
| Elihu Abrahams | Rutgers University |
| Morris Aizenman | National Science Foundation |
| Thomas Appelquist (Chair) | Yale University |
| Beverly Berger | National Science Foundation |
| Roger Blandford | Stanford University |
| Emily Carter | Princeton University |
| Susan Coppersmith | University of Wisconsin |
| Steven M. Girvin | Yale University |
| Frances Hellman | University of California, Berkeley |
| John Huchra | Harvard University |
| W. Carl Lineberger | JILA, Boulder |
| Christopher McKee | University of California, Berkeley |
| David R. Morrison | Duke University |
| Venky Narayanamurti | Harvard University |
| Vernon Pankonin | National Science Foundation |
| Jeanne Pemberton | University of Arizona |
| Celeste Rohlfing | National Science Foundation |
| Christopher Stark | National Science Foundation |
| Bruce Taggart | National Science Foundation |

## B. Participant List

### Division of Astronomical Sciences (AST)

| | |
|---|---|
| Aizennman, Morris | National Science Foundation |
| Begelman, Mitchel | University of Colorado |
| Bildsten, Lars | University of California, Santa Barbara |
| Blandford, Roger | Stanford University |
| Deustua, Susana | American Astronomical Society |
| Frogel, Jay | AURA |
| Hernquist, Lars | Harvard University |
| Huchra, John | Harvard University |
| Kamionkowski, Marc | California Institute of Technology |
| Lin, Douglas | University of California, Santa Cruz |
| McKee, Christopher | University of California, Berkeley |
| Norman, Michael | University of California, San Diego |
| Olinto, Angela | University of Chicago |
| Ostriker, Eve | University of Maryland |
| Pankonin, Vernon | National Science Foundation |
| Salamon, Michael | NASA |
| Stone, James | Princeton University |
| Tegmark, Max | University of Pennsylvania |
| Tohline, Joel | Louisiana State University |
| Wheeler, Craig | University of Texas |
| Zweibel, Ellen | University of Wisconsin |

**Division of Chemistry (CHE)**

| | |
|---|---|
| Andersen, Hans | Stanford University |
| Cave, Bob | Harvey Mudd College |
| Carter, Emily | Princeton University |
| Futrell, Jean H. | Pacific Northwest National Laboratory |
| Hernandez, Rig | Georgia Institute of Technology |
| Hilderbrandt, Dick | U.S. Department of Energy |
| Hynes, Casey | University of Colorado |
| Ladanyi, Branka | Colorado State University |
| Lineberger, W. Carl | University of Colorado |
| McCoy, Anne | Ohio State University |
| Redondo, Tony | Los Alamos National Laboratory |
| Rohlfing, Celeste | National Science Foundation |
| Rossky, Peter | University of Texas |
| Schmidt, Peter | Office of Naval Research |
| Swope, Bill | IBM |
| Tuckerman, Mark | New York University |
| Tully, John | Yale University |

**Division of Materials Research (DMR)**

| | |
|---|---|
| Abrahams, Elihu | Rutgers University |
| Balazs, Anna | University of Pittsburgh |
| Chakraborty, Bulbul | Brandeis University |
| Chelikowsky, James | University of Minnesota/Exxon |
| Coppersmith, Susan | University of Wisconsin |
| Girvin, Steve | Yale University |
| Johnson, Duane | University of Illinois, Urbana-Champaign |
| Kivelson, Steven A. | Stanford University / University of California at Los Angeles |
| Koelling, Dale | U.S. Department of Energy |
| Kotliar, Gabriel | Rutgers University |
| Levin, Kathy | University of Chicago |
| Louie, Steve | University of California at Berkeley |
| Lubensky, Thomas | University of Pennsylvania |
| Marchetti, Cristina | Syracuse University |
| Narayanamurti, Venkatesh | Harvard University |
| Olvera, Monica | Northwestern University |
| Reynolds, Peter | Army Research Office |
| Rikvold, Per | Florida State University |
| Taggart, G. Bruce | National Science Foundation |
| Tesanovic, Zlatko | Johns Hopkins University |

**Division of Mathematical Sciences (DMS)**

| | |
|---|---|
| Conrey, Brian | American Institute of Mathematics |
| Damon, James | University of North Carolina at Chapel Hill |
| Devadoss, Satyan | Williams College |
| Goresky, Mark | Institute for Advanced Study |
| Isenberg, James | University of Oregon |
| Johnson, Raymond L. | University of Maryland |
| Kettenring, Jon R. | Telcordia Technologies |
| Mann, Ben | DARPA |
| Morgan, John | Columbia University |

| | |
|---|---|
| Morrison, David | Duke University |
| Rosenberger, James | Pennsylvania State University |
| Stark, Christopher | National Science Foundation |
| Wheeler, Mary | University of Texas, Austin |

**Division of Physics (PHY)**

| | |
|---|---|
| Appelquist, Thomas | Yale University |
| Bagger, Jonathan | Johns Hopkins University |
| Baym, Gordon | University of Illinois |
| Berger, Beverly | National Science Foundation |
| Bialek, William | Princeton University |
| Chivukula, R. Sekhar | Michigan State University |
| Coon, Sid | U.S. Department of Energy |
| Friedman, John | University of Wisconsin at Milwaukee |
| Goity, Jose | Jefferson Laboratory, Hampton University |
| Goodman, Jordan | University of Maryland |
| Gross, David | University of California at Santa Barbara |
| Hogan, Craig | University of Washington |
| Kirby, Kate | Harvard University (SAO) |
| Levine, Herb | University of California at San Diego |
| Mandula, Jeffrey | U.S. Department of Energy |
| Meystre, Pierre | University of Arizona |
| Mueller, Berndt | Duke University |
| Randall, Lisa | Harvard University |
| Rosen, Peter | U.S. Department of Energy |
| Pullin, Jorge | Louisiana State University |
| Quinn, Helen | Stanford Linear Accelerator Laboratory |

## C. Michael Turner Invitation Letter

Dear MPSAC Members and Theory Workshop Steering Group Members,

I would like to invite you to the October 28-29, 2004 workshop "Theoretical Science in the Mathematical and Physical Sciences Directorate." This workshop is intended to identify, to the National Science Foundation's Mathematical and Physical Sciences Directorate (NSF/MPS), approaches on how best to support and nurture theoretical research in the 21st Century. The changing landscape of scientific opportunities, the emergence of exciting opportunities at discipline boundaries, and the increasing prominence of computational science provide new challenges to the support of theory. What remains unchanged is the transformative power of advances in theory.

Scientists representing each of the five MPS divisions (Chemistry, Astronomy, Mathematics, Materials Research, and Physics), NSF scientific staff members, and observers from other agencies and organizations will attend the workshop.

The workshop will begin Thursday morning, October 28 with a set of five scientific talks (including yours) to provide a sampling of some of the exciting theoretical research currently being supported in each of the divisions of MPS. In subsequent sessions, the workshop will focus on the opportunities and challenges that theoretical science presents to the MPS Directorate. We expect the workshop to provide recommendations to MPS in three broad areas:

1) Important scientific opportunities for theory within the mathematical and physical sciences;
2) Modes of support for theory across MPS; and
3) The education and training of young theorists.

On Thursday afternoon we will have five breakout sessions organized along divisional lines that will meet with the staff of the five MPS Divisions (Astronomical Sciences, Chemistry, Materials Research, Mathematical Sciences, and Physics) to discuss and formulate the views of that discipline with respect to these three areas. A plenary session will then follow, in which reports will be presented from each of the divisional breakout sessions.

To frame the discussion in each session, a set of common issues and questions will be prepared in advance and circulated to all participants. In addition, I have attached a list of documents you can access on that web that provide some background for the workshop. Please be sure to look at this material prior the workshop.

During the evening of October 28, the workshop steering committee will meet to refine the set of questions to be discussed at interdisciplinary issue-oriented breakout sessions on the morning of Friday, October 29. The results of these breakout sessions will then be presented to the entire workshop.

We will conclude the workshop Friday afternoon with a discussion of the recommendations the workshop wishes to make to MPS.

I have attached information concerning hotel reservations and background reading information. You will be receiving information for making travel reservations for the workshop (airline reservations must be made through the NSF contractor). Also, you will be receiving information concerning the agenda and additional background materials.

Please let Morris Aizenman (maizenman@nsf.gov, 703-292-8807) know as soon as possible whether you intend to participate at the workshop

Sincerely yours,

Michael Turner
Assistant Director

## D. Questions Provided in Advance of the Workshop

## A. The Science

**What are the most exciting frontiers of theoretical science in astronomy, chemistry, materials research, the mathematical sciences, and physics?**

A1. What is the breadth of theoretical science being supported in each division of MPS?
A2. What are the different approaches to theoretical research being supported in each division – basic, computational, phenomenological, *etc*.?
A3. Are the relations and distinctions between theory and experiment changing with time in each division? How discipline specific is this?
A4. In the theoretical sciences, what are the advantages provided by groups (often multi-institutional or multi-disciplinary) working on a common effort? These can be theoretical/experimental, theoretical/computational, only theoretical, etc.
A5. Do the divisions of MPS support all the theoretical science that they should, and that they are capable of supporting?

## B. Modes of Support

**Are the modes of support and the organizational structures within each division and within MPS as a whole appropriate for the theoretical science that is being supported and that should be supported?**

B1. What are the needs for different types of theoretical research – basic, computational, phenomenological (for example, stability, duration, institutional support, environment)?

B2. Among the different modes of support (individual investigator, group grants, centers), should some be further encouraged or discouraged by each division?

B3. Is there a need for more interdisciplinary research, crossing programs, divisions, or directorates? How should this be encouraged in each division?

B4. Within funding agencies, major initiatives are issued occasionally. Are initiatives needed in theory? When would it work and when would it not work? Can theory take advantage of this mode of support?

B5. What are the expectations for theory within predominantly experimental centers and facility modes of support?

B6. How do the modes of support in each division compare and inter-relate with other federal science agencies? How important is cooperation with other agencies?

C. **Education and Outreach**

**What should each division do in support of the education and training of the next generation of theoretical scientists – at the undergraduate, graduate, and postdoctoral levels? What should each division and the theoretical scientists it supports do to transmit the excitement of scientific discovery and increase scientific literacy among the general public?**

C1. For graduate students working in theory, support is provided by the NSF and by other sources (university fellowships and teaching assistantships, other non-federal sources, etc.). Post-PhD employment patterns are varied, with limited opportunities available in many areas. How can one judge the appropriate balance among the modes of NSF support and the appropriate number of graduate students to be trained?

C2. How can students be attracted to theoretical research? How can exposure to and participation in theoretical research by undergraduate students be encouraged and nurtured? Can this be achieved through REUs or other mechanisms? With respect to underrepresented groups, what should be done to encourage their participation?

C3. Divisional efforts in the education and training of theorists include support for summer schools, workshops, conferences, travel grants, postdoctoral fellowships, etc. How can the effectiveness of these efforts be judged, and are there other mechanisms that should be considered?

C4. How can each division further encourage and support scientific outreach by theoretical scientists – to K-12 students and to the general public?

**E. Agenda of the Meeting**

**Thursday, October 28**

| | |
|---|---|
| **7:00 – 8:00** | **Transfer from Sheraton National Hotel to NSF, Sign in** |
| **8:00 – 8:30** | **Coffee** |
| **8:30 – 8:45** | **Welcome Room 375**<br>**Dr. Michael Turner, National Science Foundation**<br>**Dr. Carl Lineberger, University of Colorado**<br>**Dr. Thomas Appelquist, Yale University** |
| **8:45 – 12:10** | **Plenary Session: Invited Science Talks Room 375** |
| **8:45 – 9:20** | **Dr. John Morgan, Columbia University, *"Using heat-type flow to understand the topology of three-dimensional manifolds"* (Mathematics)** |
| **9:20 – 9:55** | **Dr. Casey Hynes, University of Colorado, *"Theory of Chemical Reactions: Current Insights and Future Opportunities"* (Chemistry)** |
| **9:55 – 10:25** | **Break** |
| **10:25 - 11:00** | **Dr. Lisa Randall, Harvard University, *"Physics in Warped Space-time: Extra-Dimensional Possibilities"* (Physics)** |
| **11:00 – 11:35** | **Dr. Roger Blandford, Stanford University, *"Coming of Age in Theoretical Astrophysics"* (Astronomy)** |
| **11:35 – 12:10** | **Dr. Steven Kivelson, Stanford University, *"Fundamental Issues in Materials Theory"*(Materials Research) 12:00 –** |
| **13:30** | **Lunch** |
| **13:30 – 13:45** | **Plenary Session: Breakout Session Instructions**<br>**Dr. Thomas Appelquist, Room 375 13:45 – 16:45**<br>**Divisional Breakout Sessions for Discussion of Questions on *Science* (A), *Modalities of Support* (B), and *Education and Outreach* (C)** |
| | **Division of Astronomical Sciences (AST) Room 375** |
| | **Division of Chemistry (CHE) Room 430** |
| | **Division of Materials Research (DMR) Room 1060** |
| | **Division of Mathematical Sciences (DMS) Room 1020** |
| | **Division of Physics (PHY) Room 575 SII** |
| **16:45 – 17:00** | **Break** |

| | |
|---|---|
| **17:00 – 18:15** | **Plenary Session: Divisional Breakout Session Summary Discussions, Room 375** |
| **17:00 – 17:15** | **PHY: Dr. Thomas Appelquist, Yale University** |
| **17:15 – 17:30** | **CHE: Dr. Emily Carter, Princeton University** |
| **17:30 – 17:45** | **DMR: Dr. Susan Coppersmith, University of Wisconsin** |
| **17:45 – 18:00** | **AST: Dr. Christopher McKee, University of California, Berkele** |
| **18:00 – 18:15** | **DMS: Dr. David Morrison, Duke University** |
| **18:15 – 19:00** | **General Discussion** |
| **19:00** | **Adjourn** |

## Friday, October 29

| | |
|---|---|
| **7:00 – 8:00** | **Transfer from Sheraton National Hotel to NSF - Sign in** |
| **8:00 – 8:30** | **Coffee** |
| **8:30 – 9:15** | **Plenary Session: Discussion and Questions**<br>**Dr. Thomas Appelquist - Room 375** |
| **9:15 – 11:45** | **Interdisciplinary Breakout Sessions on Science (A), Modalities of Support (B), and Education and Outreach (C)**<br><br>**Interdisciplinary Breakout Sessions on Science - Room 375**<br>**Interdisciplinary Breakout Sessions on Modalities of Support - Room 1295**<br>**Interdisciplinary Breakout Sessions on Education and Outreach - Room 595 SII** |
| **11:45 – 13:00** | **Lunch** |
| **13:00 – 15:00** | **Plenary Session: Interdisciplinary Breakout Session Reports and Discussion - Room 375** |
| **13:00 – 13:15** | **Science: Dr. John Huchra, Center for Astrophysics** |
| **13:15 – 13:30** | **Modalities of Support: Dr. Steve Girvin, Yale University** |
| **13:30 – 13:45** | **Education and Outreach: Dr. Jeanne Pemberton, University of Arizona** |
| **13:45 – 15:00** | **General Discussion of Outcomes of MPS Theory Workshop Room 375** |
| **15:00** | **Adjourn** |