Directorate for Mathematical and Physical Sciences
Advisory Committee Meeting Minutes
May 30, 2007

Welcome and Introductions

The Directorate for Mathematical and Physical Science Advisory Committee (MPSAC) met via a teleconference. Present at the National Science Foundation were members of NSF staff. MPSAC members took part in the meeting via teleconference.

Dr. Michael Witherell, Chair, called the meeting of the Directorate for Mathematics and Physical Sciences Advisory Committee (MPSAC) to order at 1:30 PM. He noted that the reason the MPSAC was meeting via a teleconference was due to financial constraints imposed by the FY 2007 budget. He noted that there were now four subcommittees of the MPSAC.

- The American Competitiveness Initiative (ACI) MPSAC subcommittee, chaired by Dr. Cynthia Burrows, had finished a draft report that was discussed at the April 2007 meeting;
- The MPSAC subcommittee on the FY 2009 research opportunities, chaired by Mike Witherell, which had completed an early draft to be discussed at this meeting;
- The AC subcommittee on facilities, still being formed; and
- The AC subcommittee on centers/institutes, ready to be appointed.

In addition a subcommittee on NSF Stewardship of Light Sources is being formed from the community and will report to MPS through the MPSAC.

Dr. Tony Chan, Assistant Director for MPS, welcomed members of the MPSAC and thanked them for the work they had done.

Witherell briefly reviewed the April telecom, indicating that the MPSAC discussed the Continuing Resolution for FY 2007 funding, the Committee of Visitor Reports for the Division of Chemistry (CHE) and for the Division of Mathematical Sciences (DMS), and the formation of the subcommittees listed above.

He then briefly outlined the agenda for this meeting::

- Approval of the ACI subcommittee report;
- Discussion of ideas for the FY 2009 budget planning process;
- An opportunity for AC members to express any concerns they would like to air;
- Meeting with the NSF Director and Deputy Director; and
- Other topics.

After this introduction the Chair turned to the Assistant Director for MPS for his welcome and introductory remarks.

Remarks by MPS Assistant Director

Dr. Tony Chan, the MPS Assistant Director, introduced the NSF staff, both present and on the phone. He thanked the MPSAC for its two draft reports and indicated that the report on the FY 2009 budget had already been used in planning. Dr. Chan reiterated that, while the FY 2009 planning had entered the embargoed stage and the embargo would last until the President's Budget Request is submitted to Congress in February 2008, the MPSAC should be aware that their input was valuable and was being used. He also thanked the MPSAC for their enthusiasm and participation in MPS' activities at a level exceeding that of previous MPSACs.

Acceptance of the ACI Subcommittee Report

Witherell asked if the MPSAC had any additional remarks with respect to the ACI Report that had been presented to the MPSAC at the April 2007 meeting. Hearing none, he declared the present version final and transmitted by the MPSAC to MPS. The ACI Subcommittee Report is attached as Appendix II.

MPSAC Research Opportunities Subcommittee

Witherell noted that the subcommittee draft report had combined ideas from the divisional breakout groups into MPS themes. This synthesis from the MPS perspective is well suited for the AC. The six sections of the report were:

- Learning from Biology
- Beyond Moore's Law
- Complex Systems
- Massive Data Sets
- Workforce
- Outreach

The Chair called on AC members not on the subcommittee to comment,

Dr. Lars Bildsten asked what was the audience and the hoped for impact of the document would be. Witherell responded that it was input to MPS for 2009 budget planning and to help motivate and express the ideas in effective ways. He also noted that sections of the report were in priority order. Chan commented that he wanted to have a view from the community and would be using the report in preparing for the budget process. Witherell noted that this report did not replace divisional input that expresses MPS division-specific opportunities. Chan added that the topics in the report were cross-divisional and would help make a broader case for the budget request.

Dr. Robert Kohn, a member of the subcommittee, commented that the subcommittee had eliminated ideas that were division specific. Dr. Douglas Arnold commented that he felt the reports were well written and represented a nice selection of cross-cutting topics. He had a question concerning the outreach section that involved both scale and motivation. Witherell responded that communication was important for NSF, and while this subject was not MPS specific, MPS should speak out on it. The point was less the specific ideas than that outreach be addressed. Arnold felt that this section required further work and Witherell agreed. Dr. Susan Coppersmith felt that what had been written was good, and was not sure it was a problem. Witherell said one could say that it was important to MPS but that the subcommittee was not providing a specific mechanism. A discussion ensued on the manner in which NASA and NSF develop press releases. Witherell asked the MPSAC to send him an email on whether to rewrite this topic in a more general manner and to send any editorial comments on the other topics.

Dr. Rhonda Hughes addressed the workforce topic and asked why it emphasized postdocs and young faculty and why undergraduate and graduate support was not addressed. Dr. Elizabeth Simmons commented that recent budget requests have focused on student transitions and this would be a complement to that. Dr. Dusa McDuff noted that no one was addressing the rentry issue and getting people back into the workforce. Could they be retrained and reentered into the academic workforce? Witherell commented that this had not come up in subcommittee discussions. He also noted that postdocs have been neglected.and the report emphasizes that individual investigator awards are the main support of postdocs. Kohn felt that a paragraph on reentry could be added and Witherell asked that McDuff draft such a paragraph and that Simmons incorporate it in the report.

Hughes commented that the success rate for new investigators was also related to this topic. There were different ways of supporting new investigators, including small grants or travel grants. These could have a large impact on the individuals receiving them as grants and fellowships are difficult to obtain and are very significant for young people. Chan commented that MPS was supporting ACI fellows, and there is an emphasis on transition into the academic environment. Simmons thought that Hughes might consider adding a paragraph on this topic. Kohn felt that one should simply describe the problem. Arnold noted that the American Mathematical Society provides a lot of small travel grants.

The discussion then turned to the section of the report on emergent behavior. Chan noted that "complex systems" is a common term, used in many ways in technical settings. What does it mean and how do we talk about it? Defining complexity is a challenge and he looked to the MPSAC for advice. Witherell stated that this section was longer than the others because it is more complicated. The subcommittee would include input from this discussion and continue to refine the section.

Bildsten was concerned that the subcommittee was picking winners. He wondered why MPS couldn't say that the sections are examples of the intellectual ferment in various fields. He would be concerned if these were considered initiatives. Chan responded that the subcommittee report were ideas that would be used by MPS if they aligned with what MPS wished to do, and Bildsten asked who determines what MPS wants to do. Dr. Judith Sunley responded that there were many sources of input – divisions, workshops, advisory committees, the National Academy. MPS tries to integrate all of these inputs into the MPS funding request. The MPSAC is an important source of advice, but there are also other important ones.

After some further discussion Witherell asked that all MPSAC members send comments on the draft report to him. Witherell subsequently sent a letter (Appendix III) and a final version of the report – Appendix IV -- to Chan on June 27. A document on MPS outreach was also included (Appendix V).

General Discussion

Witherell asked if there were general comments from members of the MPSAC. Bilsten wondered how MPS maintains focus on the disciplines. Chan responded that while MPS was focusing on MPS-NSF wide initiatives, division-specific initiatives are strongly encouraged. However, division specific arguments were not necessarily compelling at OMB or on the Hill. Gruner asked how one would know if NSF funds the best science. This is an investment process, and investment principles should be applied to the funding process. Witherell responded that in principle, that is the role of the MPSAC. Both Dehmer and Aizenman referred to the role the COVs play in this process. Hughes noted that COVs might be reluctant to give honest assessment due to an inherent conflict. There was some discussion of this, including the concept of a two panel review. Bildsten asked whether the Intellectual Merit review criterion was given major weight in the review of a proposal. Sunley responded that the two criteria were given equal weight.

Hughes felt that a major topic interest involves pipeline issues. There does not appear to be, after all these years, much progress in gender and diversity issues, and asked why this was the case. It was essential that within the MPS disciplines this had to be addressed. Dehmer responded that there had been considerable progress on the gender issue but not on racial diversity. He referred to the recent workshop the Division of Chemistry had on this topic, and noted that the Divisions of Materials Research, Astronomical Sciences, and Physics would be holding a similar workshop.

The discussion then turned to cross-disciplinary efforts. Johnstone suggested that a matrix showing division to division interactions would be a good way of displaying such efforts, and if a pattern of non-zero activities showed up in such an analysis it would be quite interesting. Ostriker commented that she would like to see cross-disciplinary efforts used to support disciplines rather then such efforts becoming a prescription of what MPS should be doing. She wished to commend the Division of Astronnomical Sciences on carrying out the Senior Review and for beginning to implement it.

The meeting then turned to preparing for the visit by the Director and Deputy Director of NSF.

Meeting with NSF Director Dr. Arden Bement Jr. and NSF Deputy Director Dr. Kathie Olsen

Witherell welcomed Dr. Arden Bement Jr, NSF Director, and Dr. Kathie Olsen, NSF Deputy Director to the meeting. After thanking them for taking the time from their busy schedules to join the meeting, Dr. Witherell referenced a February 2007 teleconference with advisory committee (AC) members where they discussed the Research and Related activities increase for MPS and the flat funding for NSF Salaries and Expenses (S&E). The S&E funding for FY 2007 had led to the need for a MPSAC spring meeting by teleconference. He noted the formation and enthusiastic participation of MPSAC members in the following four sub-committees:

- American Competitiveness Initiative (ACI);
- FY2009 Research Opportunities;
- Major Facilities (not yet convened); and
- Centers & Institutes (not yet convened).

Witherell referred to FY 2008 budget request language that aligns MPS to ACI, and gave as an example “Beyond Moore’s Law.” Witherell said that the MPSAC was interested in any comments Dr. Bement had with respect to the position of Congress on the NSF’s role in the ACI and how that will play in the future.

Bement responded that there was a need for the development of metrics, both quantitative and qualitative in nature, to assess how well NSF efforts align with ACI. Bement suggested that MPS should pay special attention to areas where NSF has a unique role with respect to other federal agencies (especially NIST and DOE). He stated that communicating NSF’s contributions was important. Additionally, it is important to look at cross-directorate activities that MPS can be involved with, especially with respect to the biological sciences.

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Bement noted that efforts in supporting ACI long-term goals in K-12 education were important and that it was important that classrooms have cyber-enabled connectivity. Connectivity was a key matter that had to be addressed. Witherell responded that the MPSAC document “Research Opportunities in the Mathematical and Physical Sciences” would be completed shortly and would address some of these issues.

Witherell informed Bement that the MPSAC was looking at the proposed FY 2008 budget request for MPS and had discussed whether there should be increased investment across all NSF programs or whether the focus should be on competitive areas related to ACI. The MPSAC felt that a balance should prevail between the two. Bement noted that NSF is in competition with NIST and DOE and stressed the need for NSF to to have competitive arguments for support of its activities. In asking for increased funding from OMB it was necessary to argue for research that is compelling in its nature, research that addresses important national needs, and research at new frontiers

Witherell asked about the role of MPS in implementing Cyber Discovery and Innovation. Bement stated that the NSF Cyberinfrastructure Council (CIC) established in July 2005 is the governing body for cyberinfrastructure. Membership on the Council includes Assistant Directors and Office Directors. Bement and Olsen serve as Chair and Vice-Chair of the Council. The CIC’s responsibilities include contributing to cyberinfrastructure strategic planning, the development and review of NSF-wide cyberinfrastructure budget recommendations, and oversight of cyberinfrastructure assessment and evaluation activities. The CIC sets priorities and focus areas and determines where synergies exist. Witherell pointed out that the FY 2009 budget priorities include cyber modeling for the study of complex systems and emergent behavior. Bement noted the dramatic shift in science during the past 10 years and the resulting increase of data to be managed. Data analysis and synthesis are now on equal footing with reductionist physics. He went on to say that cyberinfrastructure refers to data storage, data mining, and analysis; it does not refer simply to new hardware. Bement urged the group to think of how to utilize cyberinfrastructure to address complex problems. Olsen described the upcoming solicitation on the interoperability of data, a cross-foundation program.

Witherell asked about international collaborations. Bement stated that international partnerships are critically important. He explained NSF’s position as the most interconnected research entity in the United States with respect to international relationships. He noted that principal investigators typically choose partnering scientists from around the globe and that NSF facilitates the process. The nature of the partnership should be such that each party gains positive outcomes (*quid pro quo)*. The role of developing collaborations essentially rests with scientists in our communities advising us about areas of synergy where an outcome cannot be achieved without the international partnership. Olsen also noted the role of programs like Division of Materials Research’s Materials World Network, the Integrative Graduate Education and Research Traineeship (IGERT), and the role of OISE to support international collaborations. Young people are a priority of NSF’s Office of International Science and Engineering (OISE). Overall, NSF relies on NSF Directorates to develop the programs based on feedback from their respective communities.

Witherell asked about additional areas for MPSAC to study. Bement remarked that the MPSAC has done a great job thus far. He commented that budget plans will be reviewed and revised several times prior to reaching the President. Bement urged Witherell to continue working with Chan to coordinate activities and focus areas. Olsen said that while the MPSAC is focusing on the FY 2009 budget plans, FY 2008 must not be forgotten. Budget planning is a year-round process and NSF will soon engage in the appropriations cycle for FY2008. Bement concluded his remarks by expressing his appreciation to all MPSAC members.

General Discussion

In the general discussion that followed Dr. Bement and Olsen's meeting with the MPSAC, it was noted that the teleconference format was better suited for subcommittee level meetings. Metrics for ACI were extremely important and the MPSAC has to think about how to apply them. Metrics can have enormous impact on programs and need to be discussed further. A problem with metrics for ACI is that it is difficult to predict what the goals and timelines for ACI should be. Perhaps one should set metrics after successes in this area were clear. Chan suggested adding division director presentations to future MPSAC meetings with respect to budget planning.

Witherell summarized proceedings from the meeting, noting that the MPSAC had accepted the Subcommittee Report on ACI, discussion had been held on the Research Opportunities in MPS draft document and that edits should be sent to him via email, that the subcommittee on major facilities and centers would be convened shortly, and that there will be a subcommittee on light sources that will be initiated shortly. Members were asked to send him suggestions for names of new members of the MPSAC via email with copies to Chan, Sunley, and Aizenman.

Adjournment

The meeting was adjourned at 4:30 p.m.

Appendices

APPENDIX I

ATTENDEES

MPSAC Members Present at NSF
Michael Witherell, University of California, Santa Barbara

MPSAC Members Present via Telephone
Douglas Arnold, University of Minnesota
Lars Bildsten
Susan Coppersmith, University of Wisconsin
Sol Gruner, Cornell University
Rhonda Hughes, Bryn Mawr College
Robert Kohn, New York University
Theresa A. Maldonado, Texas A&M University
Dusa M. McDuff,, SUNY-Stony Brook
Eve Ostriker, University of Maryland
Ian M. Robertson, University of Illinois at Urbana-Champaign
Elizabeth Simmons, Michigan State University

MPSAC Members Absent
Cynthia Burrows, University of Utah
Claude Canizares, Massachusetts Institute of Technology
Larry Dalton, University of Washington
Iain M. Johnstone, Stanford University
William L. Jorgensen, Yale University
Steve Koonin, British Petroleum, Inc.
Monica Olvera de la Cruz, Northwestern University
Jose Onuchic, University of California, San Diego
David Oxtoby, Pomona College
Marcia Rieke, University of Arizona
Winston Soboyejo, Princeton University
Robert Williams, Space Telescope Science Institute

MPS Staff
Morris Aizenman, Senior Science Associate, MPS
Tony Chan, Assistant Director, MPS
Joseph Dehmer, Director Division of Physics
Luis Echegoyen, Director, Division of Chemistry
Eileen Friel, Executive Officer, Division of Astronomical Sciences (present via phone)
Lance Haworth, Acting Division Director, Division of Materials Research
Janice Hicks, Executive Officer, Division of Chemistry
Deborah Lockhart, Executive Officer, Division of Mathematical Sciences
Peter March, Director, Division of Mathematical Sciences
Judith Sunley, Executive Officer, MPS
G. Wayne van Citters, Jr., Director, Division of Astronomical Sciences (present via phone)

Visitors
Arden Bement Jr., Director, NSF
Kathie Olsen, Deputy Director, NSF

Appendix II

Report of the MPSAC Subcommittee on the American Competitiveness Initiative
May 3, 2007

I. Background

The Augustine report,[1] "Rising Above the Gathering Storm" included the following overarching recommendation:

> *Sustain and strengthen the nation's traditional commitment to long-term basic research that has the potential to be transformational to maintain the flow of ideas that fuel the economy, provide security, and enhance the quality of life.*

The report further recommended an increase of 10% per year for 7 years in the nation's investment in long-term basic research in physical sciences, engineering, mathematics, and information sciences. MPS, in conjunction with its collaborative partners in ENG, CISE, OCI and ERE, is ideally situated to have a dramatic impact on achieving the goals of ACI as well as the Innovation Agenda already circulating in Congress. Both short-term and long-term planning is required to provide guidance to the directorate regarding areas for future investment. There is a strong sense that economic competitiveness comes from fundamentally new innovations, not from incremental improvement of existing technology. ***Truly transformational outcomes will result only from increased and sustained investment in basic physical sciences, mathematics and related fields.***

The subcommittee was charged with reviewing past investments as well as recommending future areas of interest. The committee met by teleconference on 3/1/07, 3/14/07, 3/29/07 and 4/24/07 to review the FY 2008 budget request and to suggest areas for increased visibility.

II. Review of the FY 2008 budget request vis-à-vis ACI

A large fraction of the FY 2008 budget request could be aligned with ACI, particularly in the areas of ***Science Beyond Moore's Law***, which was a major feature in several divisions' requests. These and others are further articulated below:

- In AST, funding that enhances cyberscience and cyberinfrastructure including the development of tools to manipulate and analyze large and heterogeneous data sets represents a major alignment with ACI. AST facilities, such as the Atacama Large Millimeter Array that is currently under construction, exemplify the unique, technologically advanced, large-scale "tools of science" that ACI calls out as essential to maintaining US leadership in the global economy.
- In CHE, nearly all areas of the portfolio can be viewed as aligned with ACI: nanoscience, complexity and the molecular basis of life processes facilitate the discovery of new materials as well as new molecular processes that support both nanotechnology and the pharmaceutical industry; science beyond Moore's law is aimed at discovery of single-molecule electronic devices and self-assembling schemes to facilitate the electronics industry; sustainability issues address the growing needs of the US chemical, energy and agricultural industries to utilize natural resources in an environmentally sound fashion; cyber-enabled discovery is aimed at computational modeling of molecular processes that have ramifications in

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[1] *Rising Above The Gathering Storm: Energizing and Employing America for a Brighter Economic Future,* Natl. Acad. Press, 2007.

remote sensing or characterization of reactive species.

• In DMR, all areas of experimental and theoretical research have a bearing on ACI including condensed matter physics, solid-state chemistry and polymers, biomaterials, structural and high temperature metals and ceramics, nano-scale material systems, electronic, magnetic and photonic materials. New materials are critical to the ACI issues of energy, sustainability and feedstock for manufacturing. Basic advances in our understanding at the atomistic level of fundamental reactions and interactions and how they control properties will open new avenues for designing and synthesizing novel complex materials with unique and adaptive properties.

• In DMS, the area of science beyond Moore's law is clearly aligned with ACI, and DMS can provide fundamental advances in algorithm design, scalability, and quantification of errors and uncertainty. Through fundamental research, DMS strengthens the core of many disciplines that apply mathematics and statistics, and like AST, contributes to the analysis and understanding of large data sets.

• In PHY, the ability to generate predetermined quantum states in atoms and molecules provides the underpinnings for a quantum-level technology that offers a revolutionary approach to the tools of computation and communication. Analytical and computational techniques needed for extraction of information from large data sets generated in experiments in elementary particle physics lead to new approaches for massive signal processing. Distribution of the data to the worldwide physics community fosters approaches such as grid computing. The advances in biological physics are aligned to the ACI's goals of developing the healthcare industry. Advances in accelerator technology also impact healthcare.

All of the divisions contribute in a major way to the training of a diverse and highly skilled technical workforce. The vast majority of the MPS budget is used to train students and provide advanced instrumentation for use by these students who will go on to be the nation's next generation of innovators. *This is of paramount importance to the ACI and should continue to be emphasized.*

III. Areas for continued/increased visibility in the FY 2009 budget

A December 2006 NSF workshop entitled "Sustaining America's Competitive Edge" outlined seven priority areas of special opportunity in science and engineering:

- Plant Science: from biofuels to nutrition
- Complex Structural Materials Systems: high performance materials for construction
- Electronic and Optical Materials and Systems: theory and design of new materials for communications and information technology
- Energy and Materials: photovoltaics, hydrogen generation, transport and storage, advanced nuclear technologies, advanced coal technologies, batteries, etc.
- Nanotechnology--Science and Applications: molecular assemblies
- Development of New Pharmaceuticals: from synthetic chemistry to biophysics
- Imaging Science and Technology: medical diagnostics, *in situ* techniques for dynamic studies of reactions and interactions, and remote sensing

All of the above areas can be enhanced by basic research activities in the MPS domain. Furthermore, they represent the largest sectors of our technology-based economy—energy, electronics, and pharmaceuticals—and so the long-term effects of fundamental research and innovation will be dramatic.

In the coming year, ***Sustainable Energy*** is thought to be an over-arching concern whose solutions can be addressed through investment in basic research. Meeting future demands for energy without overtaxing the environment is an enormous challenge that cannot be addressed by any single technology, or by any single funding agency. Interim solutions may rely on more efficient use of coal, ethanol and biofeedstocks, but long-term solutions that do not generate CO_2 must be sought now. Nine long-term challenges that are outlined in a recent *Science* perspective by Whitesides and Crabtree[2] are:

- The oxygen electrode problem: fuel cells and the production of H_2
- Catalysis by design: processes in the production and storage of energy
- Transport of charge and excitation: making cost-effective solar cells
- Chemistry of CO_2: large-scale physical and chemical properties of CO_2 in the environment
- Improving on photosynthesis: uptake and processing of CO_2 and other light-mediated fixation reactions
- Complex systems: understanding multi-component systems with non-linear interactions; emergent behavior
- Efficiency of energy use: new strategies for reducing wasted energy
- Chemistry of small molecules: H_2O, H_2, O_2, CO_2, CO, NO_x, O_3, NH_3, SO_2, CH_4, CH_3OH, HCl
- New ideas: growing the Earth's biomass, stimulating photosynthesis in the oceans, new nuclear power cycles, room-temperature superconductivity, biological production of H_2, new concepts in batteries, etc.

NSF and DOE must act synergistically as they do in other areas, and, for example, as NSF and NASA do in the field of astronomy. NSF should focus on long-term fundamental research from which transformational science will emerge providing entirely new strategies to attack sustainable energy problems. Partnerships between NSF and DOE might occur at the divisional level among specific programs that derive added benefit from such a joint approach.

The committee had the following recommendations for additional emphasis in 2009 beyond those just described.

- Increased emphasis of cyber-enabled research for handling and extracting knowledge from large and heterogeneous data sets, for assimilating observational and experimental data into computational models, for creating virtual environments that allow humans to interact with data and models, and for underlying advances in imaging and signal processing, including multi-modal and real-time aspects. While CISE contributes to the implementation of these aspects of cyberinfrastructure, MPS is a major driver and algorithmic enabler.
- Development of new algorithms and computational methods to model multiscale, non-equilibrium systems, and to understand interacting complex systems and emergent phenomena.
- Discovery of new molecular materials and science "Beyond the Molecule" to help understand complex phenomena. Additional support for the discovery of new reactions and new assemblies would impact health sciences and the pharmaceutical industry as well as materials science and technology. "Responsible chemistry" aimed at minimizing the impact on the global environment is a key aspect of this research.
- Photochemistry and photophysics aimed at understanding photodynamic processes and designing advanced photonic materials. These areas specifically impact energy and electronics.
- The biological interface with mathematical and physical sciences including chemistry

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[2] Whitesides, G. M.; Crabtree, G. W. *Science* **2007**, *315*, 796.

and physics of the brain, synthetic and computational mimicry of biological processes, biomolecular machines, and the human impact on the environment.

- Quantum computing, molecular electronics, and science "beyond Moore's law" should continue to be a driver for the development of quantum-based technology, an approach that uses the quantum behavior of individual quantum states, e.g. of molecules or spins, as the basis for information storage and manipulation.
- New materials for applications in extreme environments characterized by high temperature, high pressure, stress, corrosion, oxidation, or intense irradiation. These span needs in the nuclear, coal, gas, and photovoltaic energy generating systems as well as hydrogen production facilities. The operational environments envisioned for advanced energy technologies place stringent demands on materials, and to meet the challenge, new strategies for designing, producing and assessing properties of materials systems are needed. This requires discovery of the fundamental atomistic processes, reactions and interactions operating in these environments and of how they dictate macroscopic properties.

IV. Development of a technical workforce skilled in physical sciences and mathematics.

Regarding the workforce, MPS should continue to provide leadership in expanding and diversifying the scientific workforce. Given national trends of diminished interest and lower achievement in science and math among school children, especially minorities, major initiatives should be launched to achieve a "Sputnik-like" call to action bringing the best young minds to science. For example, the I2U2 program that utilizes GRID technology to involve K12 students and teachers with physical science in large-scale projects goes beyond any one small experiment to create a national and international network.

With foreign enrollments declining at US institutions, the technical workforce should be increased domestically, particularly through outreach programs to underrepresented populations.[3] In addition, mechanisms to retain the best foreign students in the US would be desirable since many US-trained Asian students are now being courted back to their countries of origin due to rapidly rising investments in science and technology in China and India.[4] Current US immigration policies pose very substantial barriers for foreign students wishing to launch their scientific careers in the US.

The February 2001 Hart-Rudman report on National Security/21st Century listed as their second key recommendation for change, *"revitalizing America's strengths in science and education,"* including a doubling of the science budget by 2010. MPSAC responded in May 2002 by suggesting that NSF should expand its role as the steward of US science research capabilities, and toward that end, a number of cross-disciplinary workshops were organized evaluating the state of the art of various scientific frontiers. In addition, MPSAC suggested that the Directorate should take a leadership role in coordinating efforts with other funding agencies. Ongoing educational efforts such as REU, RET, IGERT and VIGRE programs were also highlighted in

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[3] *Land of Plenty: Sustaining America's Competitive Edge in Science, Engineering and Technology.* A Report of the Congressional Commission on the Advancement of Women and Minorities in Science, Engineering and Technology Development, September 2000. http://www.nsf.gov/pubs/2000/cawmset0409/cawmset_0409.pdf

[4] For information concerning the decline of the workforce in Chemistry, see the recent Casey report: *The Future of US Chemistry Research: Benchmarks and Challenges,* National Research Council, 2007. ISBN: 978-0-309-10533-0

that report.

MPS science areas are often showcased in the media and can be effective in recruiting the most brilliant and ambitious young minds into science and technology fields. Combining accessible narratives with captivating imagery from cosmic to nano-scales, researchers from MPS will continue to capture the imagination and convey the excitement of technology-enabled research at the frontiers of knowledge and innovation. These efforts should be enhanced to strengthen the pipeline of students entering scientific disciplines.

V. Past investments that can be articulated in terms of ACI

Reviewing the MPS web pages indicates that the Directorate has effectively been supporting ACI-related physical sciences and mathematics for a number of years. Many examples are highlighted at:

Astronomy: http://www.nsf.gov/news/index.jsp?prio_area=2
Chemistry and Materials: http://www.nsf.gov/news/index.jsp?prio_area=4
Mathematics: http://www.nsf.gov/news/index.jsp?prio_area=9
Physics: http://www.nsf.gov/news/index.jsp?prio_area=11

The subcommittee recognizes that the Division Directors are well poised to distill from their individual portfolios the past investments that best represent ACI-aligned outcomes, and it recommends that the Directorate continue to seek this valuable input from them. Publicity concerning MPS-funded science and mathematics educates the public, guides teachers and researchers, informs legislators, and improves the image of scientists, thereby attracting new students for the as yet unimagined science careers of the future.

VI. Mechanisms of enhancing the MPS investment for competitiveness and innovation.

MPS funding aligned with ACI can take many forms in terms of the types of grants awarded. In order to attract and retain some of the nation’s best scientists, awards to individual “ACI Fellows” would be effective. As the problems tackled become more complex and interdisciplinary, additional funding for centers and collaborative research projects will be necessary. Advanced instrumentation, facilities and cyberinfrastructure will be required to keep US science and mathematics researchers and educators competitive in their work. Importantly, these enhancements should not erode the individual investigator awards in core disciplines since these are the incubators of new knowledge and innovation.

MPS has a strong tradition of fostering innovative ideas in education that help diversify the workforce and expand the participation of underrepresented groups in science and engineering. New and continuing funding mechanisms should guide researchers toward best practices in broadening participation.

VII. Summary

Advances in economic competitiveness stem from fundamentally new innovations, not from incremental improvements in existing technology. Transformational outcomes must be seeded by increased and sustained investment in basic physical sciences and mathematics.

The subcommittee identified many components of the FY 2008 budget request that, in alignment with ACI, would promote the major sectors of our economy, including energy, health, and electronics. Briefly, these include science beyond Moore’s Law, cyberscience and the analysis of large data sets, the molecular basis of life processes, new synthetic methods and advanced materials with tailored or functional properties.

Areas for continued and increased visibility in the FY 2009 budget request include all of the above with additional emphasis on sustainable energy and the global environment, science “beyond the molecule”, cyber-enabled research, new algorithms and computational methods, quantum computing and molecular electronics (including advances beyond Moore’s Law), photochemistry and photophysics, advanced material systems and the biological interface with physical sciences and mathematics.

Critical to America’s competitiveness is the education of the next generation of innovators supported by an expanded technological workforce. MPS should continue to provide leadership in science and math education, teacher training and outreach activities, and the provision of tools that support the nation’s science education efforts. Captivating, recruiting, and retaining the nation’s best young minds in physical and mathematical sciences should be given very high priority.

The subcommittee recommends that division directors continue to bring forward their best examples of ACI-related outcomes from their portfolios in order to inform and stimulate a scientifically-minded public.

Mechanisms must be found to spur new collaborations, to recruit and retain the best scientists working in innovative areas, and to broaden participation in physical sciences and mathematics while fostering the core disciplines.

Subcommittee Members:

Dr. Cynthia J. Burrows (Chair)
Distinguished Professor of Chemistry
University of Utah

Dr. Susan Coppersmith
Professor & Chair of Physics
University of Wisconsin

Dr. Larry R. Dalton
George B. Kauffman Professor of Chemistry & Electrical Engineering
University of Washington

Dr. David E. Keyes
Fu Foundation Professor of Applied Mathematics
Columbia University

Dr. Jose N. Onuchic
Professor of Physics
University of California, San Diego

Dr. Eve Ostriker
Professor of Astronomy
University of Maryland

Dr. David W. Oxtoby
President & Professor of Chemistry
Pomona College

Dr. Ian M. Robertson
Donald B. Willett Professor of Engineering & Materials Science
University of Illinois at Urbana-Champaign

Advisory Members

Dr. Michael Witherell (Chair, MPSAC)
Vice Chancellor of Research & Professor of Physics
University of California, Santa Barbara

Dr. Morris Aizenman
Senior Science Associate
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Appendix III

MPSAC Cover Letter to MPS Assistant Director Tony F. Chan

June 21, 2007

Dr. Tony Chan
Assistant Director for Mathematical and Physical
Sciences National Science Foundation

Dear Tony,

I am enclosing two brief reports from the MPS Advisory Committee. The full committee discussed these documents at our teleconference on May 30, and we developed final versions based on changes suggested as part of that discussion.

The first report is “Research and Education Opportunities in the Mathematical and Physical Sciences.” Three sections of this report describe compelling research opportunities that bridge multiple divisions within MPS. The fourth section addresses some aspects of developing the scientific workforce that we think need more attention.

I would like to put this report in context, based on our discussion of May 30. Each of the five divisions within MPS has a well-developed program of research that advances the frontier of disciplinary science. Every year, we hear from Committees of Visitors and other experts about how compelling these scientific programs are and how much excellent science goes begging because of insufficient money to fund it all. The report we are submitting concentrates on some specific opportunities in compelling cross-disciplinary research that should also be given attention.

The NSF is now receiving annual increases that are somewhat beyond inflation, with a special emphasis that includes mathematical and physical sciences. We hope that over time these increases will make it possible to fund more of the compelling science that is receiving high priority within the divisional review process, and at the same time take advantage of opportunities such as those identified in our report. We are submitting this report of exciting interdivisional opportunities to complete the broad spectrum of research that we believe should be supported. We are not doing it to displace the strong programs coming forward from the divisions. We understand that the important management challenge is to get the right balance between strengthening the core programs and building the new capabilities.

I am also enclosing a document called "Comments on Outreach from the Mathematical and Physical Sciences Advisory Committee." The committee wanted to make a strong statement about the importance of outreach activity to NSF and the need for new approaches. It is somewhat different from our other reports in that it addresses programs that are not the sole responsibility of MPS.

I hope that these documents provide valuable input to you and all of the people within MPS that are developing the research and education directions for the future.

Sincerely,

Michael Witherell

Michael Witherell
Chair, MPS Advisory Committee

Appendix IV

Research and Education Opportunities in Mathematical and Physical Sciences

Learning from Biology

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

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

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

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

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

Beyond Moore’s Law

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

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

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

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

Understanding and Controlling Emergent Behavior in Complex Systems

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

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

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

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

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

Discovery from Massive Datasets

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

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

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

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

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

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

Developing the Scientific Workforce

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

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

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

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

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

Appendix V

Comments on Outreach from the Mathematical and Physical Sciences Advisory Committee

As the home for research in areas of compelling interest to the public, from the early history of the universe as recorded in the night sky to the chemistry and physics of global climate change to the molecular origins of life, the Mathematical and Physical Sciences Directorate at the National Science Foundation needs to take the lead in communicating that exciting science to the public. The goal is two-fold: first, to make the process of science more transparent and less mysterious, and second, to show the connections between pure science and mathematics and real-world applications. The benefits will be educating the public better to make political decisions in areas of science and technology, as well as raising the profile of science careers for Americans entering the workforce.

The range of new efforts toward public communication of science must extend from traditional placements of exciting discoveries in the print and broadcast media to the creation of compelling web sites that tell the story of science. This is needed to reduce the gap between what scientists do and the public perception and appreciation of science. The NSF is already supporting a wide variety of television shows that are designed to interest young viewers in math and science, such as "Fetch with Ruff Ruffman", "Cyberchase," and "Zoom." We applaud these efforts and encourage the agency to explore additional ideas, including:

(1) Bring in several scientists who are excellent communicators to a series of NSF-hosted day-long programs aimed at the public in cities around the country.

(2) Create a science quiz show to stimulate interest in the science that is taught in our schools.

(3) Join forces with entertainers and comedy shows to make a humorous traveling exhibit or broadcast program that shows how simple scientific concepts and methods are not only broadly accessible but useful to citizens.

In each case, connections to space, health, and energy could be used to attract interest, but the focus should be on the core areas of science and technology at the heart of NSF.

APPENDIX VI

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October 31, 2007
Dr. Tony F. Chan,
Assistant Director
Directorate for Mathematical and Physical Sciences
National Science Foundation
4201 Wilson Boulevard
Arlington, VA 22230

Dear Dr. Chan:

I have reviewed the final version of the minutes of the Directorate for Mathematical and Physical Sciences Advisory Committee meeting that was held on May 30, 2007 (attached), and am pleased to certify the accuracy of these minutes. Morris Aizenman has done an excellent job in recording the most significant parts of the discussion.
Sincerely,

Michael Witherell

Michael Witherell
Chair, Mathematical and Physical Sciences Advisory Committee