

Minutes
MPS Advisory Committee Meeting
April 1-2, 2010
National Science Foundation

Thursday, April 1, 2010
Morning Session

Welcome, Introductions, and Agenda Overview

Dr. Iain Johnstone, Chair of the Mathematical and Physical Sciences Advisory Committee (MPSAC) opened the meeting at 9:15 a.m. He noted that this meeting was being conducted as a teleconference with members present at NSF or linked via phone. Working groups formed in 2009 would report throughout the day on topics including Climate, Energy, Computation, Life Sciences, Broadening Participation, and Science and Engineering Beyond Moore's Law/Quantum Information Systems (SEBML/QIS). Dr. H. Edward Seidel, the MPS Assistant Director, would review the FY 2009 - FY 2011 budgets. The meeting would conclude Friday, April 2 after a discussion with Tom Kalil from the Office of Science and Technology Policy (OSTP).

Remarks by MPS Assistant Director

Seidel began his presentation with a discussion of the FY 2009-2011 budgets. While the President has stated that discretionary funding within the Federal budget will be frozen for the next three years, NSF was still working on the assumption is that its budget would be doubling over the next few years. A case needs to be made for basic science with priority areas of climate and energy reflected in the budget. With respect to the FY 2009 Recovery Act funds (ARRA), \$490M had been provided to MPS, with \$402M for research and education grants. Close to 400 new principal investigators were supported and 85 CAREER awards, 70 energy-related awards, and 25 climate-related awards award were made. A total of \$88M was provided for facilities and instrumentation.

He noted that the Division of Chemistry (CHE) and the Division of Mathematical Sciences (DMS) Committee of Visitors (COV) meetings had been rescheduled from February 2010 to late May and June 2010 because of the severe winter storms that had taken place in the Washington area in February.

With respect to the FY 2010 budget, NSF had received \$6.87 billion and cyberinfrastructure, SEBML/QIS, climate, and energy research had all received support. As for the FY 2011 budget, \$7.4 billion had been requested and priorities are to support innovations in core programs, advance a strong scientific and technical workforce, and invest in research addressing national priorities. The budget request contained funds that would enable tripling the number of graduate research fellowships.

Seidel then turned to personnel matters. The NSF Director, Dr. Arden Bement, Jr. would be stepping down June 1, 2010. Dr. James Jim Ulvestad had become the Director of the Division of Astronomical Sciences (AST), and the CHE, DMS and Division of Materials Research (DMR) interviews for new Division Directors had been completed. The positions of Deputy Division Directors in AST and DMR were open.

Planning for FY 2012 had begun and at this meeting first steps would be discussions of divisional priorities and cross cutting initiatives, and, as had been mentioned by Johnstone, there would be a presentation and discussion with Tom Kalil of OSTP. There would also be a series of MPS internal discussions with its divisions, an MPS retreat to be held in May, and strategic plan discussions later in the year. At the NSF Assistant Director (AD) level planned NSF-wide activities included an FY 2012 budget retreat and discussions with OSTP.

Seidel described the proposed NSF Science, Engineering and Education for Sustainability (SEES) initiative that will result in a planned agenda for coordination and expansion of its portfolio of research and education associated with climate, energy, and sustainability. The research stemming from the systems-based approach implemented through the SEES portfolio will lay the foundation for decision capabilities and technologies aimed at mitigating against and adapting to environmental change that threatens sustainability. MPS is critical in this activity in providing basic research support and this is likely to be a major multi-year effort. Discussion on SEES included how one would evaluate the success of SEES in the future, how SEES would be effectively reviewed in a trans-disciplinary manner in order to support the best science, and, with respect to the intended

data management plan requirement, will NSF provide guidance to principal investigators on establishing infrastructure such as workshops and other ways to get them prepared and thinking in those terms?

MPSAC Climate Working Group Report

Dr. Barbara Finlayson-Pitts described what the activities of the group. She noted that there was limited representation of MPS areas in climate and there was a need for MPS to partner closely with other Directorates in the areas of climate prediction using earth system models, biodiversity, water, ocean acidification, and climate change education. She gave an overview of the Intergovernmental Panel on Climate Change (IPCC) report and where the working group felt MPS could make contributions. While there is currently a great emphasis on carbon dioxide (CO₂), it was only part of the story -- there is a need to look at lower atmosphere complex chemistry; aerosols (particles) are where major work needs to be done. Aerosols drastically affect climate and she described the areas in which research on aerosols is needed. In addition, multi-scale climate change analysis is needed at the temporal and spatial levels and we need improved understanding of climate at a more local level. Finlayson noted that models always have uncertainties, and there is the problem of how model uncertainty can be quantified in a meaningful way. Model hierarchies include economic models that incorporate sustainability, societal models (social disruptions and conflicts), epidemiological models, and models of extreme event mitigations

With respect to biodiversity what is needed is the valuation of biological diversity with new algorithms to deal with high uncertainties, statistical tools for detecting anomalies, and an integration of the various scales associated with these studies. New tools are needed for the study of water, not only to predict shortages, but also to predict water quality. Can it be assessed and modeled?

Finlayson-Pitts then turned to the working group recommendations for future efforts in this area for MPS. The group proposes a series of targeted workshops as a way to generate directions for MPS efforts in climate change. She noted that a workshop on current issues in the environmental chemical sciences was held by CHE June 8-9, 2009 with a few selected participants; the workshop discussed the importance of understanding the atmosphere at the molecular level. What had been done to date did not cover all MPS areas and there was great importance in partnering with other directorates. Areas of emphasis include climate prediction, biodiversity, water, and ocean acidification. In particular, there is an urgent need for basic research on the effects of aerosols and particulates on climate, with input from physics and mathematics essential.

MPSAC Energy Working Group Report

Dr. Theresa Maldonado described the activities of the working group. The question that had to be answered was how we fit mathematics and fundamental science into issues associated with energy, as sustainable energy is a complex and urgent problem. Another issue is the role of NSF as compared to the Department of Energy (DoE).

NSF staff and MPSAC members participated in multiple weekly teleconferences, and the working group received an updated charge in January 2010. The goal is to produce a high-level needs assessment for the MPS community, to produce a plan for possible paths forward, and to produce an estimate of resources needed over the next 5 years in this area. There is a need for a National Nanotechnology Initiative-like effort around energy and she made reference to the National Science Board (NSB) August 2009 energy report *Building a Sustainable Energy Future: U.S. Actions for an Effective Energy Economy Transformation* as well as the National Academy of Sciences (NAS) December 2009 report, *America's Energy Future: Technology and Transformation*. Sustained investments in NSF programs are needed for a generation.

With respect to topics for advanced energy technologies, there is a question of how to introduce nanotechnology into the oil and gas industry since renewable energy will be a small part of the energy portfolio for a long time. New materials and nanostructured materials are needed. Do we need a new distribution system instead of the status quo (e.g. gas pumps at stations)?

A focused energy workshop was held on March 15, 2010 to discuss the design of new materials, computational efforts, and systems integration. General observations that resulted from that workshop were that there are significant technical challenges at disciplinary interfaces and NSF needs to foster and cultivate new ideas and ways of thinking among groups of investigators. With respect to the design of new materials, one has to

understand the scalability of materials and incorporate multi-scale modeling into energy-related problems. Major computational efforts are required in energy studies, including the creation, mining, visualization, and maintenance of massive datasets. With respect to systems integration we need an integrated approach to efficient energy conversion, storage, delivery, real-time measurements, social impact, and cost.

MPSAC Broadening Participation (BP) Working Group

Dr. Sharon Neal noted that MPS is seeing some gains in the participation of women and racial/ethnic minorities. Some groups are starting to include sexual orientation and persons with disabilities.

The working group recommends that MPS frame its broadening participation programs around the topic of innovation -- the argument being that diversity is good for innovation. Diversity of thought and geographic differences are all advantages that the US holds. In addition, MPS should review the language in its solicitations and literature and utilize the innovation argument rather than the demographic changes argument.

MPS should apply the scientific method to design and implement BP. Efforts are now focused on how to do a good extra-curricular or remediation program to retain under-represented groups. But more sophisticated work could be done using the social science of research network formation. MPS should generate guidelines for BP programs and for assessment. MPS should explore a joint program with the Social and Behavioral Sciences Directorate (SBE). They are interested in the science of BP while MPS has the subjects, the students, *etc.* Also, MPS should promote BP program sustainability.

MPS should do a survey and find out what is happening at minority serving institutions (MSI). At national meetings, program directors can explain how to succeed with BP and to advertise new programs. One could form a corps of individuals who can serve as mentors for Minority Serving Institution's (MSI) writing large grants. MPS should make specific Research Experiences for Undergraduates (REU) awards for community college students to strengthen the pipeline, and, as is now required for all postdocs supported by NSF awards, consider having mentoring plans for graduate students and undergraduates. This would encourage principal investigators (PI) to educate themselves about mentoring.

Dr. Joseph deSimone commented that there are pockets of success with respect to broadening participation, but systemic improvements are needed. It would be good to tie into competitiveness. Dr. Myron Goodman, the Assistant Director for SBE said that SBE is willing to partner with MPS and conduct a workshop on these issues.

MPSAC Life Sciences Working Group

Dr. Maryanne Horn of DMS reported on the working group activities. She noted that she is also the co-chair of the MPS and Directorate for Biological Sciences (BIO) working group in this area.

Her presentation began with a quote from the 2010 National Research Council report *Research at the Intersection of the Physical and Life Sciences*: "Are efforts to understand biomolecules, the smallest of biological constructions, a facet of chemistry or biology? Are attempts to understand the environmental effects of greenhouse gases a concern of physical science or of biology? It is becoming increasingly irrelevant whether a particular research topic fits neatly into one discipline or another; in fact, many of the most interesting scientific questions and pressing societal issues will require the collective expertise from multiple fields." The report had gone on to identify 5 grand challenges in this area: Synthesizing Lifelike Systems; Understanding the Brain; Predicting Individual Organisms' Characteristics from their DNA Sequence; Interactions of the Earth, its Climate and the Biosphere; and Understanding Biological Diversity. Furthermore, the National Academy of Sciences had noted, in its 2008 report *The Role of Theory in Advancing 21st-Century Biology: Catalyzing Transformative Research* that "Theory is already an inextricable thread running throughout the practice of biology; but ... explicitly giving theory equal status with other components of biological research could help catalyze transformative research that will lead to creative, dynamic, and innovative advances in our understanding of life."

With respect to training challenges, faculty transitions, and interdisciplinary education, collaborative work requires researchers to understand the language of the other discipline. Transitioning from disciplinary research to interdisciplinary collaborations typically requires a significant time commitment for faculty, and interdisciplinary training at the student and postdoctoral levels requires support and commitment from all disciplines involved.

The MPS-BIO working group had identified three of these areas last year as well as needed training aspects such as MPS-BIO interface fellowships and midcareer planned activities. The Physical/Life Sciences Interface track (RCN-PLS) was developed between MPS and BIO to address research focused on a specific problem at the interface of the biological and mathematical or physical sciences that would be significantly advanced through a synergistic approach, requiring the expertise of both biologists and mathematical or physical scientists. Such proposals are expected to involve a balance of researchers from two or more disciplines, at least one in the biological sciences and one in the mathematical or physical sciences. Grants will provide \$100K/year for 5 years for travel and coordination.

Dr. Dennis Matthews commented that it is no longer a question of whether MPS should do something in this area but a question of what to do. MPS should hold a set of workshops with the National Institutes of Health (NIH).

MPSAC Science and Engineering Beyond Moore's Law (SEBML) Working Group

Dr. Luis Orozco reported on the working group activities. He began by noting that the first quantum revolution involved transistors. Now is the time to advance the second quantum revolution for communications and computation capability beyond the physical and conceptual limitations of current technologies. The technical center of the program should be MPS but the Engineering (ENG) and Computing and Information Science and Engineering (CISE) and the Office of Cyber Infrastructure (OCI) are natural partners.

There are six areas of research: New materials, devices, and processes; new computer architectures; new algorithms; new software; energy efficient computing; and new paradigms (quantum information). The first five represent the ending of first revolution and the last one – the beginning of the second revolution. New paradigms include quantum information. Quantum information is the use of entanglement and superposition. Quantum computers will be as different from our laptop as our laptop is from an abacus.

There is a need for NSF to maintain, enhance and lead this area. Current interest will require a vision of the possibilities, and a sustained investment on this area. There is significant potential for interagency partnering and NSF should take the lead in this. The investment could easily be \$100M/year, roughly double the current level (~\$50 M).

(NOTE: The presentations of the MPSAC Matter by Design Working Group and the MPSAC Cyber Working Group were delayed due to the end of the day due to the lateness of the schedule. The presentations are being inserted here for integration with the other working group reports.

MPSAC Matter by Design Working Group

Dr. Andrew Lovinger of DMR presented the working group report. He began by providing a definition of "Matter by Design." It is the ability to design and create any type of matter for any desired combination of properties, ideally through first principles. It departs from the traditional Edisonian (trial-and-error) techniques and starts with an integrated theoretical, modeling, and experimental approach and extends beyond "materials": It may be a quantum object, a molecule, an assembly, a hierarchical system, conceivably even an organism. It is frequently inspired by nature and its complexity typically requires extensive cyber-tools. Matter by Design involves very close interactions among many disciplines and major necessary components are: theory / modeling; synthesis / assembly; structure / characterization; processing / properties; instrumentation / facilities. It is important to note that innovative processing is often a critical requirement.

He then discussed why this area was important now. "Matter by Design" has long been an unattainable "Holy Grail," but there have been recent powerful breakthroughs in theory and modeling, in new synthetic and self-

assembly techniques, in our ability to emulate and be inspired by nature, in our understanding and control of the physical world down to the quantum realm, in our processing capabilities all the way down to the nanoscale, and in new, advanced instrumental and cyber tools

Opportunities in this area include complex matter; hierarchical matter such as self-replicating matter, bio-mimetic and bio-inspired matter that could result in materials for bio-therapeutics and biomedicine; bio-alien matter; metamaterials; and self-healing matter.

Other opportunities in this area include new electronic, photonic nanostructures; single-molecule electronic devices, molecular biochemical machines, new design concepts and materials for alternative energy sources, for environmental sustainability, and for security, and new underlying biological, chemical, physical, mathematical, theoretical, computational, processing and instrumental concepts.

An NSF/MPS initiative in this area would integrate new theoretical concepts and modeling, would extend broadly across MPS and could involve ENG, BIO, CISE, and OCI. It would promote highly interdisciplinary education and will require a center or large group mode of funding, and, because of the breadth of this area, require an initiative focused down to one or two sub-topics.

MPSAC Computational Science Working Group

Dr. Sharon Glotzer presented the preliminary report of this group. The group held meetings with the MPS Cyber group, held one-one discussions, and considered recommendations from recent reports and community input. Questions that were addressed by the group included what should MPS should be doing in Computational Science, and what critical activities in Computational Science are important to the community but not adequately (or at all) addressed/supported by MPS or elsewhere at NSF. The group deferred questions on how should MPS undertake new programs in Computational Science, how should/can MPS activities leverage CF21, and what aspects of Computational Science should MPS take the lead on, versus Partnering with OCI?

The group has the following recommendations:

1) MPS and NSF should embrace Computational Science (and Engineering) as a “discipline” in its own right - it has its own identity that should be recognized as such. The group notes that supporting theory, modeling, and simulation activities is not synonymous with supporting computational science and the activities that must be supported, and which are not being supported now, are already recognized by the community and by NSF as important – but they fall between the cracks, because no one owns them. Examples include new software, new and “staple” community codes, open source codes, codes for new or nonconventional architectures, algorithms, models, data, cyber tools for collaboration, sharing, re-use, and education, training and workforce development

Consequences of this lack of “identity” at NSF and a concomitant lack of a visible, permanent commitment to Computational Science are that the critical infrastructure supporting US Computational Science is eroding or missing, universities are wary of creating permanent programs and faculty lines in an area where there is no clear line of funding, and there are too few students trained in computational science. As a result, computational science cannot realize its full abilities as an equal partner to experiment/observation and theory/modeling, and science suffers.

2) Longevity: MPS must commit to long-term support of the computational science community, and put in place programs that are permanent, provide substantive, long-term, pan-generational funding, support endeavors for which scientific impact may be many years off, and this should be done in partnership with other directorates and OCI where it makes sense. MPS should think strategically of how to do this.

She discussed implementation of this recommendation and commented that this should be a bottoms-up approach with a program directors managed effort, and not a top-down activity

3) With respect to software, MPS should support software development, dissemination, maintenance and stewardship. This would be difficult to do within the existing program structure but it is a key to scientific

discovery in all MPS divisions. She emphasized that software is the single most important tool in computational science; without it, one can do nothing. It must be supported for the critical infrastructure that it is.

4) MPS should encourage interdisciplinary interactions between domain scientists and mathematicians on the topic of uncertainty quantification, verification and validation, risk assessment, decision making.

5) MPS should support workforce development to expand literacy and broaden participation in computational science at the undergraduate, graduate, and postdoctoral levels.

6) MPS should support unconventional and high-risk activities in computational science, and be nimble to evolve while maintaining a long-term, pan-generational commitment, to achieve transformative change

In conclusion, Glotzer stated that the MPS AC Computational Science working group would happy to continue working with MPS to advise on both strategic issues AND tactical implementation

Lunch Adjournment Followed by Divisional Breakout Sessions

MPSAC members had lunch with the MPS Divisions in the divisional breakout sessions. Topics discussed during these sessions included long-range planning issues and FY 2012 budget ideas.

Thursday, April 1, 2010

Afternoon Session

Reports from Divisional Breakout Groups

The MPSAC reconvened in plenary session at 4:15 PM.

Division of Astronomical Sciences (AST)

Dr. John Peoples presented the AST breakout session report. AST is unique in MPS in the way it carries out its science in that it invests 56% of its budget in facilities. AST is the only steward of ground-based astronomy in the radio spectrum. In the optical spectrum, astronomy also has privately supported facilities. The perennial challenge for AST is balancing principal investigator support and facilities support.

The Division has a number of challenges. The United Kingdom (UK) is providing 25% of the support for Gemini, and they have announced that they are withdrawing from the Gemini Observatories. The university based 4-meter telescopes are old, but are innovative and have many users. A major issue for the Division is how it makes itself relevant today in the context of national priorities such as energy and climate. Another challenge is management of the radio frequency spectrum allocation.

Dr. Suzanne Hawley commented that national astronomical facilities are essential and suggested (1) that NSF ramp up funds for a program to support operations and management (O&M) for facilities, and (2) document how O&M is to be provided for any project ready for MREFC funding. Peoples added that facilities are needed to address the scientific questions of most importance to the AST community. Hawley commented that MPS and NSF should invest in infrastructure at the observatories, address the Gemini Observatories funding problem, work towards a down select for the Giant Segmented Mirrors Telescopes concept, and make progress on the support of the Large Synoptic Survey Telescope (LSST). Broadening participation is another issue, as is data management.

Division of Physics (PHY)

Dennis Matthews gave the summary of the PHY breakout session. The issue of the role of PHY in SEES was discussed. What kind of role is there in the specific research solicitations that have been released? More flexibility is needed to fund “out of the box” ideas. The climate is good for promoting basic research and its contributions to the innovation ecosystem. There are temporary budget issues concerning support for the Deep Underground Science and Engineering Laboratory (DUSEL) in FY 2011. PHY has a strategy for portfolio

balance that reserves 50% for PI support but DUSEL funding problems could jeopardize this. It would be inappropriate to use principal investigator support to solve such facility problems and MPS must look for other ways to deal with this issue. Support of mid-scale instrumentation must also be addressed.

Orozco stressed the importance of giving higher priority to core research in budget planning. Seidel commented that he has brought up the issue of the importance of basic research with OSTP, and MPS is working on the issue of support of midscale instrumentation.

Division of Chemistry (CHE)

Dr. Barbara Finlayson-Pitts gave the CHE report. She thanked Dr. Tito Abruna for his service on the committee, particularly with respect to leading the Division Director recruitment search committee. Thanks were due to Dr. Luis Echegoyen for his service as Director of CHE and his service to NSF. The realignment of CHE has gone well and added growth in activity and connection to modern issues. The breakout group felt that an *ad hoc* mail review with the program director in charge has distinguished NSF. Panels may not have the expertise, could be distorted by personality, and may not be good for broadening participation and interdisciplinary work. The group recommends staying with *ad hoc* reviews although this requires more staff. Ways to lessen the burden on program directors in view of increasing numbers of proposals would be a “three strikes” rule and limits to the number of proposals a principal investigator can submit. Some colleagues are now not responding to requests to review proposals. Perhaps CHE could consider copying the department chair when thanking a review, making an honor role of reviewers, or publishing a general list of all reviewers at the end of the year.

There are many exciting areas in chemistry, but there is already a problem with the number of awards versus the size of the awards. The funding level is too small, and some may not bother submitting to NSF. In commenting on the structure of this meeting of the MPSAC, she felt that AC members should be physically present at NSF for the meetings. The experiment on teleconference of the Office of Cyberinfrastructure AC meeting showed that it is only appropriate for shorter meetings on narrower topics.

Seidel thanked Finlayson-Pitts for the comments and said that MPS would reconsider whether to conduct teleconference AC meetings in the future.

Division of Materials Research (DMR)

Dr. Theresa Maldonado presented the DMR report: At the breakout session the first hour and a half were spent discussing the review process. The increasing number of proposals being received is of growing concern given the limited number of staff.

Matter by Design was discussed. ENG has the Emerging Frontiers in Research and Innovation (EFRI) program, which provides awards of \$500K for a period of 4 years on one or two topical areas. DMR is considering duplicating this idea in new areas. With respect to the MPS Solar Energy Initiative (SOLAR) program, the group discussed how to expand it further to include more participation across NSF. The question of how to measure success was discussed.

The international materials institutes were discussed. There are two in energy, and SOLAR has an opportunity to collaborate with Germany. The SEES could also become international. The idea of partnerships with the Education and Human Resources Directorate (HER) was discussed. Professional masters degrees could help the materials field and industry involvement would be desirable. This idea also has potential for support of instrumentation, in a “Bell Labs” mode for master-level professionals. The group also discussed support for new principal investigators, and how to make interdisciplinary opportunities more widely known. Another topic was funding for instrumentation below the MRI range, say, in the range of \$100K. This needs to be addressed.

The idea of “sustainable infrastructure science” was discussed. There is crumbling infrastructure and MPS should consider a collaboration with ENG and the Directorate for Geophysical Sciences (GEO).

Dr. Sharon Glotzer commented that increasing proposal pressure is also burdening the reviewer community. The system is broken on both sides. She asked how DOE handles things, and how NIH and DOE get out in front on timely issues, but still protect core support.

Division of Mathematical Sciences (DMS)

Dr. Fred Roberts presented the DMS report. The group first talked about ARRA and solicitations. ARRA funding proved that there are outstanding unfunded proposals. Solicitations involving climate and SEES are being prepared. The DMS workshop on sustainability will produce a new report on the science of sustainability its challenges. The group also heard from Dr. Lee Jameson of DMS on cyber activities. It appears that panels tend to be negative about support for software development.

Another topic was the increasing number of solicitations. This raised a real question on the recognition of mathematics as a fundamental science. Does the shift to solicitations reflect the natural priority of basic mathematics? Does it weaken the core disciplines? All divisions ask this question. The group wonders if MPS should make a strong statement about this. With respect to solicitations, there is a solicitation on networks. The activities are not as large as institutes. Is this a model for MPS, for NSF? One will have to observe the outcome of these solicitations.

The group discussed the future NRC report *Math Sciences 2025*. This report will focus on research disciplines and try to influence policy at the university level. Impact on other disciplines will be another emphasis.

Also discussed were the Vertical Integration of Graduate Research and Education (VIGRE) program evolution and workforce in general. VIGRE is mature after 10 years. DMS has concluded that it should be discontinued due lack of interest in the community in proposing for this program.

The Mathematical Science Institutes are unique because there are no sunset limits. They undergo changes in personnel and emphases. The announcement of the new winners is imminent, and another solicitation will be posted in a few months. An issue is the evaluation of these institutes.

With respect to the climate working group report, the breakout group discussed possible next steps.

Roberts, on behalf of the group, thanked Dr. Peter March, the DMS Division Director, for his sustained and significant contributions to the community.

Maldonado asked March to comment on the impact of VIGRE. He responded that while CHE is naturally hierarchal DMS is highly stratified. VIGRE was a large departmental project to link students/postdocs/faculty. The success of the effort is that people now believe that undergraduates can work at the frontiers. Maldonado then asked about broadening participation. March responded that broadening participation is a core value and VIGRE created new structures. Therefore, this is an opportunity for broadening participation.

Seidel noted that DMS could participate in many solicitations and DTRA is a good example. He was aware about the lack of support by reviewers for software but new solicitations may help. On sustainability it is necessary that MPS plan and there is time to influence future solicitations.

Presentations by the MPSAC Matter by Design Working Group and the Computational Science Working Group

(At this time, two presentations originally scheduled for the morning were presented: Matter by Design, by Dr. Andrew Lovinger, and Computational Science, by Dr. Sharon Glotzer. A report on their presentations can be found above.)

Adjournment

The meeting was adjourned at 5:45 P.M.

Friday, April 2, 2010
Morning Session

The MPSAC convened at 9:00 A.M.

Report from CEOSE

Dr. Theresa Maldonado, the MPSAC/CEOSE liaison to the CEOSE, presented a summary of the recommendations in a CEOSE committee report to Congress. This report has yet to be issued because there were discrepancies across 11 agencies and the CEOSE committee wished to make clarifications to its recommendations. A discussion about the recommendations followed. Maldonado noted that CEOSE is undertaking a comprehensive review of broader participation and CEOSE considers people as part of infrastructure. With respect to the advancement of women, a women of color mini-symposium was held with about 150 participants. The symposium found that considerable numbers of women left science and engineering during job/career transitions. There was a particularly high drop out rate in rural areas.

Maldonado discussed the 2011 budget request and noted that there had been much discussion at the CEOSE committee. The budget request states that three legacy programs involving broadening participation will be combined. Seidel commented that there had also been considerable discussion about this at the AD retreat and Maldonado added that this was an opportunity to reexamine the entire matter.

Report from the Environmental Research and Education (ERE) Advisory Committee

Dr. Fred Roberts, the MPSAC representative to the ERE Advisory Committee (EREAC), began his presentation with a brief review of the history of the EREAC. The EREAC was established in 2000. Up until 2010, its primary job has been interpreted to be “advocacy” for the topics with which it deals. It advocates interdisciplinary environmental research and to date has produced five publications that are available at its web site. The publications on “Complex Environmental Systems” have influenced development of NSF programs. Now, with substantial new initiatives at NSF on environmental research and education, the role of the EREAC is moving from advocacy to implementation. This new role will require rethinking of the tasks of the committee.

At its most recent meeting much of the discussion centered on the new NSF SEES Initiative. SEES integrates issues of environment, energy, and economics and is concerned with the two-way interaction of human activity with environmental processes. If one combines existing and new monies, the SEES budget is \$660M in FY2010 and is estimated to be \$765M in FY2011. He felt that there are clearly roles for MPS research, particularly in the role of creative mathematical, statistical, and computational methods for analysis and simulation. EREAC strongly endorsed the new SEES initiative.

Because there is considerable emphasis on the role of SBE and the many problems of decision making, human responses, land use patterns, *etc.* that are intimately related with environment, energy, and climate change, Roberts felt there are opportunities for MPS/SBE interconnections in this initiative. SEES illustrates how environmental research at NSF is now closely related to energy research, so EREAC has to rethink its expanded scope of responsibility. At the meeting, members of EREAC heard from ADs and Deputy ADs from BIO, MPS, OCI, GEO, SBE, CISE, ENG, and the Office of Polar Programs (OPP). All stressed the interdisciplinarity of the problems and their commitment to support the new initiatives. All of the NSF staff who spoke at the meeting were very committed to SEES and other programs at the interface among environment, energy, climate change, *etc.*, and one speaker felt it is the major scientific challenge of the century. However, there was much discussion of the definition of “sustainability” and no consensus on this was reached.

Roberts felt that it will be very difficult to evaluate the new environmental/energy/climate change initiatives since they are aimed at long-term processes, and a major challenge will be to develop appropriate ways to evaluate the success of programs like SEES in the short run. EREAC will be advising on metrics for measuring the success of the SEES initiative.

There was a great deal of discussion of the challenges of interdisciplinary education and discussion of the need to educate the public to be better decision makers in their personal lives and as voters. It was felt that this

education needs to start even in the K-5 level. The same concerns about evaluating interdisciplinary education programs were raised as were raised for interdisciplinary research programs, including evaluating proposals, faculty at universities, and NSF programs.

A substantial part of the EREAC meeting was devoted to the climate change programs at NSF and presentations were made on the five major FY2010 climate research programs: Dimensions of Biodiversity; Water Sustainability and Climate; Ocean Acidification; Decadal and Regional Climate; Prediction Using Earth System Models; and Climate Change Education . While MPS is only involved in the Earth System Models initiative, it was clear from the discussion that MPS disciplines are relevant to all five initiatives.

The meeting included a presentation from Jeff Nesbitt, Director of NSF Office of Legislative and Public Affairs. Nesbitt noted that since “climategate,” about 50% of the US public is now skeptical about climate change. When EREAC asked Dr. Bement about support for this initiative, he responded that the Congress was strongly supportive of the effort.

Roberts concluded his presentation of the new SEES program by stating that future tasks of the EREAC would be the development of metrics for success of the new program, the determination of program goals, and how NSF is to know if these goals have been achieved. It will also be concerned about climate change education of the public and of students.

In the question period that followed Roberts was asked what the MPSAC could do to advise NSF on the implementation of the initiative. Roberts responded that SEES is a massive initiative and MPS is clearly involved in it. There are opportunities for MPS/SBE collaboration in this activity. March commented that young people grasp the subject of sustainability and this may be a gateway to STEM. Roberts felt that environmental programs should be brought into the classroom. Dr. Zakya Kafafi, in noting public skepticism over climate change due to the “climategate” issue, asked if NSF is going to review data or validate it when skepticism exists. A new initiative might allow proposals to address the validity of data. Johnstone noted that there was an international committee formed and charged by the national science academies with reviewing the processes and procedures of the periodic climate change assessments of the IPCC. Hicks commented that the environment has become a polarization issue in political debates, and scientists need to pull out of this “tug of war.” Kafafi felt that SBE could play a major role in this. Aizenman stated that he was not as pessimistic about the future of the “green movement.” When word of the loss of ozone over the South Pole came out, the world responded. Now there is the “green movement” and he was optimistic about its future. It was noted that the ozone problem had not been an economic problem, but that the green movement was, to which Roberts responded that economics was part of the SEES initiative.

Seidel commented that he was very receptive to the MPSAC making suggestions on how MPS should be involved in ERE.

The Data Enabled Science Workshop

Dr. James Berger gave a presentation on the Data Enabled Science Workshop held March 29-30, 2010. The purpose of the workshop was to position MPS in Data Enabled Science (DES). The report of the workshop is in its draft stages. The workshop’s conclusion is that in order to realize the extraordinary potential for scientific advance inherent in the massive amounts of data being produced (a data flood) , two major hurdles need to be overcome: data management of massive data, and scientific inference from massive *or complex* data. Data management involves designing the data collection strategy; collecting the data, from either single or distributed sites; reprocessing the data (if necessary) to keep only the most essential data; storing the data, with appropriate meta-data to ensure usability; ensuring accessibility of the data by scientists, possibly through layered distribution of the data to multiple sites; providing platforms and software that enable efficient use of the data by scientists, as well as allowing for capture of the scientists’ post-processing of the data; and ensuring curation and preservation of the data.

With respect to challenges in scientific inference from massive or complex data the workshop felt that scalability is a primary concern and the example of the Sloan Digital Sky Survey (SDSS) was given; less than 10% of the SDSS imaging data have been accessed and analyzed by scientists. This has to be considered in the context of

the Large Synoptic Survey Telescope (LSST), which will acquire one SDSS equivalent amount of imaging data each and every night for 10 years.

MPS is well positioned with respect to mechanisms for transference of methodologies between disciplines because mathematics and statistics have traditionally been the major disciplines for effecting transfer.

The overall recommendations from the workshop were that while one could have DES initiatives, it would be best to have targeted additional support to the MPS divisions for data-enabled science. Funding of DES will require the same process care by NSF program officers as funding of interdisciplinary research (and computational science infrastructure). It would be necessary to instruct peer reviewers as to the unique evaluation metrics and have dedicated DES review panels at the divisional level and possibly the directorate level. MPS should develop tracking mechanisms to insure DES accountability.

With respect to the workforce, there should be CAREER awards in DES research areas. MPS should also consider fellowship programs (graduate and postdoctoral), provide REU supplements in DES, develop educational initiatives in DES, support workforce development in careers associated with data handling and understanding, and provide research support for scientists working in large data-producing projects during construction, commissioning, and early operations phases, enabling early science results from these facilities specifically from the people who know the facility and its data the best.

The workshop had the following recommendations with respect to data management: For facilities, data management is a major (often unfunded) component of operating costs; it should be a central part of the overall NSF strategy for funding facility operating costs. Project proposals which deal with massive data should include a data management plan consistent with the size, collaborative structure and funding of the project. This plan should address meta-data, access, long term funding, data storage, computational requirements, and standards. The workshop felt that data management with massive data requires significant innovation, and one must be prepared that initial efforts may fail. Vehicles for sharing of data management innovations across facilities and disciplines should be created, and NSF should continue to seek mechanisms to ensure that data arising from NSF projects become public.

Berger then described the recommendations on scientific inference with massive or complex data. Advances in fundamental mathematics and statistics are needed to provide the language, structure, and tools for many needed methodologies of data-enabled scientific inference. He provided several examples. Furthermore, algorithmic advances in handling massive and complex data are crucial, and visualization (visual analytics) and citizen science (human computation or data processing) will play key roles.

Progress in *new* areas of data-enabled science will require teams consisting of combinations of disciplinary scientists, data-scientists (including mathematicians, statisticians, and machine learners), and computational scientists. In this respect, the current mechanism of occasional joint initiatives between divisions is too transient for the future data-enabled science world.

The workshop also had specific sections and recommendations devoted to each of the MPS Disciplines. In particular, the mathematical sciences should become even more involved as a partner to other MPS (and external) sciences in meeting the data-enabled science challenge.

Following the presentation Roberts commented that information sharing is important and research is needed on the distributed nature of the data sources. Visual analytics are part of data. The nature of data and visual analytics is relevant to CISE and MPS. Dr. John Peoples said that while he agrees with conclusion of report he takes exception to the statement that the Sloan Digital Sky Survey (SDSS) data has not been fully utilized. There are analyses which use all data. A question was asked as to what is considered a massive data set. Berger replied that “massive” differs from “complex.” The definition of “massive” may be discipline dependent.

General Discussion on the MPSAC Working Group Reports

Seidel began the discussion by noting that all of the working group reports are extremely helpful. MPS must now determine how to take the reports to help refine programs and create new programs for 2012 and beyond.

Also, MPS has to determine the next step for the working groups. West commented that he was struck by the commonalities of the reports. All had common threads of being interdisciplinary and multidisciplinary and all involved sustainability and complexity. This is tied into basic research. However, basic research is perceived as an “add on” rather than an underlying theme. Basic research is the mission of NSF in comparison to other agencies. Sustainability should not only be energy and climate. Sustainability should deal with risk (*e.g.*, financial markets, urbanization). Much of what goes on in MPS can address complex adaptive systems and MPS should be involved.

A comment was made that the NSF budget request for FY 2011 is up by 8% while that of MPS is up 4% and the question was asked as to whether the working groups are doing the right thing in making the case for MPS. Seidel responded that MPS needs to find ways to articulate themes that resonate with OSTP. Roberts commented that the EREAC discussions expressed great concern about support for basic science and whether NSF becoming a mission agency. Dr. Eric Cornell commented that basic research *is* the NSF brand and MPS is most categorized by its support for basic research.

Meeting with Tom Kalil, OSTP Deputy Director for Policy

After introductions from the speaker and committee members Kalil made some introductory comments. He said that this was an exciting time to be in science and technology and that a number of very senior positions within the Administration were occupied by individuals with scientific training. He noted that the President is committed to the doubling of NSF budget. But there are obvious large financial issues and hurdles to be overcome. Walking in to budget discussions and being told “We need a 6% increase.” is not a good way of approaching this problem. There have to be concrete goals and objectives for the requests. One has to try to paint a picture of the future to the lay people that will be making the final decisions on budgets.

He then commented on three papers he had read on the intersection of science, engineering and policy. The three papers involved expansion of the nanoelectronics initiative, Quantum Information Science, and Matter by Design. With respect to the matter by design, OSTP was talking about new materials that would result in solar arrays that cost approximately \$1.00 per watt – installed. He also commented on the growing chasm between the rates at which we create data and the amount of time it takes to understand the data.

He then turned to broader science policy questions and addressed the question of what modes of funding are most productive. At present NSF supports individual investigators, centers, and facilities. He wondered whether one should fully fund small groups or researchers, or keep with the large centers. Is the support of high risk/high yield research being done correctly? Do faculty members have to “do the experiment” before they write the grant proposal?

Kalil concluded his comments by noting that President Obama considers science important and the research community needs to do more to get people thinking about how to bring the importance of science to the public. He then opened the floor to discussion.

Glotzer commented that computational science should really be considered as critical infrastructure. Dr. Dennis Matthews said that he would appreciate advice on which topics to pursue, and Kalil responded that he would like to be able to have all the disciplines produce materials similar to what he has seen from computer science. Neal commented that broadening participation was related to a country having a competitive advantage, and that this topic is normally brought up in the arena of ‘social justice’; the MPSAC proposes that this can also be framed as a tool to use diversity in search of innovative and creative solutions to problems.

Johnstone asked how one strikes a balance between major societal problems versus fundamental research. Cornell responded that “fundamental research” is a term that is tough to define. In general NSF funding increases come in response to societal needs, and this is OK. But it is time to realize that just asking for support for fundamental research is also OK. This does help bring in the best and brightest. When science is presented in this manner, it does help us fund ‘high risk/high yield’ science. You can also make a strong economic case for this, and the US needs to stay well ahead on the technology curve. “Surprise in science” creates jobs. The idea is that we can promote funding increases in a different way, not just as a response to a societal need.

The discussion then turned to centers. Matthews commented that at the center he directs they have tried to get the best scientific staff on board, but one size does not fit all. Dr. Luis Orozco stated that the center he co-directs (quantum information) has energized the people in this discipline. While he does not think the centers are the solution for everything, they do work. West agreed and commented on the Santa Fe institute and described the hybrid approach taken where some of the funding is Federal, but most is private. He added that this is the National Science Foundation, not the National Applied Science Foundation.

Glotzer added that one should not forget the single principal investigator grants. The best science has come from small groups that are well funded for a medium term. She mentioned DoD grants, where one receives \$1M a year for five years, and this works.

Peoples noted that the meeting had talked about support for individual grants, centers, but not about facilities. This is a dilemma and how do we deal with this? Seidel responded that facilities are critical to do the research, and support of their operations and management tend to eat away at the budget.

Echegoyen commented that in chemistry one gains a factor of 40 for each dollar invested in basic research.

This concluded the discussion and Johnstone offered the thanks of the MPSAC to the speaker for taking time from a very busy schedule to meet with the MPSAC.

MPSAC Working Group Comments

During the concluding session of the meeting, Johnstone asked for comments from the Chairs and members of the MPSAC working groups.

With respect to the climate working group and the energy working group, Roberts wondered whether the working groups should be expanded or combined. In favor of combining the groups was that the problems were so intertwined it would make sense to do so. On the other hand, each area has its own issues--energy in particular. For the moment, he felt that the groups should be kept separate, but more interaction between the groups was needed. Maldonado felt that one had to strengthen the priorities of the energy group and create a dialog between the groups, and Johnstone suggested that perhaps we could have the group leaders get together via phone.

With respect to the climate, Finlayson-Pitts felt that the case had to be made that MPS should be involved in each of the climate-related solicitation and it would make sense to pursue the climate change issues in a discipline-by-discipline approach.

With respect to energy, Maldonado felt that each Division within MPS needs to see how it can work with energy topics, and future workshops are critical.

In the area of broadening participation, Neal said that next steps depend on how MPS reacts to the broadening participation white paper. She noted that the working group had focused narrowly on items for the next funding cycle, and one now had to address the role of the working group in tackling the issue on a longer timescale. How can the group focus on longer timescales? Furthermore, there should be coordination between the group and the rest of NSF.

With respect to Life Sciences, Matthews felt that the group had to get focused on specific recommendations. In addition, there was the question of how each Division can work on the intersection of its activities with the BIO Directorate. He suggested that workshops should be held in the next year, and after that one should consider an interagency workshop involving NIH and DoD.

Orozco felt that the SEBML/QIS working group could try to help with the implementation of the Quantum Information Sciences Initiative. He also wanted the group to learn more about interagency activities in this area.

In computation, Glotzer said that they had to finalize and distribute the white paper within MPS, but she argued against another workshop. MPS needs to figure out how to implement its recommendations.

Seidel noted that the case for basic science had been well received, and that there would be follow up on facilities. The white papers the MPSAC had produced would be used at the Directorate level and would be circulated to other NSF Assistant Directors. Aizenman noted that there would be an MPSAC teleconference on Thursday, June 17th to consider the upcoming Committee of Visitor meetings of the Division of Chemistry and the Division of Mathematical Sciences. The next MPSAC meeting would take place at NSF on November 4th and 5th, 2010.

Johnstone and Seidel thanked members of the MPSAC and MPS staff for their participation in the meeting.

Adjournment

The meeting was adjourned at 2:00 PM.

APPENDIX I

ATTENDEES

MPSAC Members Present at NSF

Eric Cornell, JILA and the University of Colorado
Barbara J. Finlayson-Pitts, University of California, Irvine
Sharon C. Glotzer, University of Michigan
Iain M. Johnstone, Stanford University
Theresa A. Maldonado, Texas A&M University
Dennis L. Matthews, University of California, Davis
Sharon L. Neal, University of Delaware
Luis Orozco, University of Maryland
John Peoples, Jr. Fermilab
Fred S. Roberts, Rutgers University

MPSAC Members Present via Telecom

James Berger, Duke University
Daniela Bortoletto, Purdue University
Kevin Corlette, University of Chicago
Joseph DeSimone, University of North Carolina, Chapel Hill
Irene Fonseca, Carnegie Mellon University
Suzanne Hawley, University of Washington
David E. Keyes, Columbia University (present by phone)
Jerzy Leszczynski, Jackson State University
Ramesh Narayan, Harvard-Smithsonian Center for Astrophysics and Harvard University
Geoffrey West, Santa Fe Institute

MPSAC Members Absent

Hector D. Abruna, Cornell University
Taft Armandroff, W. M. Keck Observatory
Juan de Pablo, University of Wisconsin-Madison
James W. Mitchell, Howard University
Joel E. Tohline, Louisiana State University

MPS Staff

Morris Aizenman, Senior Science Associate, MPS
Carol Bessel, Division of Chemistry, MPS
Charles Bouldin, Program Director, Division of Materials Research
Denise Caldwell, Deputy Division Director, Division of Physics
Joseph Dehmer, Director, Division of Physics
Luis Echegoyen, Director, Division of Chemistry
Craig Foltz, Acting Director, Division of Astronomical Sciences
Janice Hicks, Executive Officer, Division of Chemistry
Mary Ann Horn, Program Director, Division of Mathematics
Lee Jameson, Program Director, Division of Mathematical Sciences, MPS
Zakya Kafafi, Director, Division of Materials Research
Deborah Lockhart, Executive Officer, Division of Mathematical Sciences
Peter March, Director, Division of Mathematical Sciences
Kathleen McCloud, Program Director, Division of Physics
Celeste Rohlifing, Head, Office of Integrative Activities
Edward Seidel, Acting Assistant Director, MPS
G. Wayne van Citters, Jr., Senior Advisor, Facilities, MPS

Visitors

Elizabeth Grossman, Lewis-Burke Associates

Tom Kalil, Office of Science and Technology Policy

Ani Mohan, American Chemical Society

James Murday, University of Southern California

Kate Von Holle, British Embassy

APPENDIX II

**BREAKOUT SESSION ROOMS
MPS Advisory Committee Meeting
Thursday Afternoon, April 1, 2010**

		DIVISIONAL ASSIGNMENTS FOR MPSAC MEMBERS						
		AST	PHY	CHE	DMR	DMS		
		Room	Room	Room	Room	Room		
		SII-535*	SII-545*	1020	1060	SII-585*		
Term Ends 09/30/10								
	JOHNSTONE					X		
	KEYES					X		
	MALDONADO				R			
A	ABRUNA							
	CORNELL		R					
	MATTHEWS		X					
A	TOHLINE	X						
Term Ends 09/30/11								
	BERGER					X		
	BORTOLETTO		X					
	FINLAYSON-PITTS			R				
	FONSECA					X		
	HAWLEY	X						
	NARAYAN	X						
	NEAL				X			
	PEOPLES	R						
	REICHMANIS					X		
A	WEST							
Term Ends 09/30/12								
A	ARMANDROFF							
	CORLETTE					X		
A	DE PABLO							
	DESIMONE			X				
	GLOTZER					X		
	LESZCZYNSKI			X				
A	MITCHELL					X		
	OROZCO		X					
	ROBERTS						R	
* - Breakout sessions will be held in Stafford II building								
A	Absent							
R	Breakout CHAIR, MPSAC member who will summarize Divisional meetings activities to MPSAC							

APPENDIX III

MPSAC Working Group Membership

Computation	Climate	Energy	SEBML	Life Sciences	Broadening Participation
Glotzer	Finlayson-Pitts	Maldonado	Orozco	Matthews	Neal
Keyes Tohline Fonseca Leszczynski	Johnstone Roberts Armandroff Reichmanis	Abruna Bartoletto Peoples West	Cornell Corlette DeSimone Mitchell	de Pablo Berger Narayan Mitchell	Hawley Matthews Leszczynski DeSimone
Lee Jameson (DMS) 703-292-4833 ljameson@nsf.gov	Zeev Rosenzweig (CHE) 703-292-7719 zrosenzw@nsf.gov	Carol Bessel (CHE) 703-292-4945 cbessel@nsf.gov	Charles Bouldin (DMR) 703-292-4920 cbouldin@nsf.gov	Mary Ann Horne (DMS) 703-292-4879 mhorn@nsf.gov	Kathleen McCloud (PHY) 703-292-8236 kmcccloud@nsf.gov

MPSAC Working Group Membership

Matter by Design	Basic Research	Data Enabled Science Workshop	Energy Workshop
De Pablo	Cornell	Berger	Maldonado
Glotzer Maldonado Reichmanis Leszczynski	Corlette DeSimone Hawleyf Reichmanis	Glotzer Keyes	Bartoletto Abruna
Andy Loveinger (DMR) 703-292-4933 alovinge@nsf.gov	Morris Aizenman (OAD) 703-292-8807 maizenman@nsf.gov	Lee Jameson (DMS) 703-292-4833 ljameson@nsf.gov	Carol Bessel (CHE) 703-292-4945 cbessel@nsf.gov

APPENDIX IV

September 14, 2010

Dr. H. Edward Seidel,
Acting Assistant Director
Directorate for Mathematical and Physical Sciences
National Science Foundation
4201 Wilson Boulevard
Arlington, VA 22230

Dear Ed:

I have reviewed the final version of the minutes of the Directorate for Mathematical and Physical Sciences Advisory Committee meeting that was held April 1- 2, 2010 (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,

Signed

Iain Johnstone
Chair, Mathematical and Physical Sciences Advisory Committee