UNITED STATES GOVERNMENT

M E M O R A N D U M

DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

Date: October 25, 2005
From: Assistant Director, MPS
Subject: **MPS Response to Recommendations of the MPS Theory Workshop**
To: MPS Advisory Committee (MPSAC) Members

I want to thank the organizers of the MPS Theory Workshop, its participants, and especially the Chair of the workshop, Dr. Thomas Appelquist of Yale University, for this report. I believe the workshop represented the first time participants from all of the MPS disciplines convened to discuss the support of theory within the MPS sciences.

Since acceptance of the report by the MPSAC at its Spring 2005 meeting, MPS has been discussing and developing a response to the report's recommendations.

Our response to the report follows. The response consists of the report's preamble to each recommendation, the recommendation, and the MPS response. The same format is used in the response of each of the MPS divisions to division-specific recommendations.

I look forward to discussing our response to the report at the November meeting.

Sincerely,

Michael S. Turner
Assistant Director

A. The Science and its Support:

----A1----

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

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

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

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

MPS Response A1: We concur. The support of unsolicited proposals from the science community will remain a very high priority for all of the Divisions within the MPS Directorate.

----A2----

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

MPS Response A2: MPS sponsors theoretical research in the physical sciences and mathematics through its five divisions and the Office of Multidisciplinary Activities. The MPS divisions will continue to be responsive and flexible to new opportunities in theoretical science including those that cut across traditional boundaries.

----A3----

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

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

MPS Response A3: The balance between center support, group support and the support of individual investigators in theoretical science is one that is dynamic and changing. The MPS Divisional Committees of Visitors (COVs) are and will be asked to assess the current balance of center, group and individual investigator support across the division and make recommendations.

----A4----

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

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

MPS Response A4: MPS agrees that an award should be supported at a level and duration consonant with the proposed research. The norm for the duration of awards in awards supporting theory is 3 years. Awards with

durations longer than this are considered on a case-by-case basis. The size of theory awards in the MPS Divisions has been increasing over the last few years. The divisions look carefully at the tradeoff between award size, duration and success rate.

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

Recommendation A5. MPS should ensure that adequate mechanisms are in place for the review and support of proposals for theoretical research at the boundaries of the established disciplines, as well as theoretical research that combines several disciplines. The success rate for such proposals should be the same as for disciplinary proposals of comparable quality. The Office of Multidisciplinary Affairs (OMA) should play a more active role at the individual and small-group levels.

MPS Response A5: The success rate of theoretical proposals in interdisciplinary fields is dependent on the quality of the proposals that are received and on available budgets. Program Directors actively consult with their counterparts in other Divisions and Directorates on interdisciplinary proposals, and they will be encouraged to continue to do so. The Office of Multidisciplinary Activities' role is to actively encourage and assist in the support of multidisciplinary proposals.

----A6----

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

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

MPS Response A6: MPS will, as appropriate, consider inclusion of theoretical science in MPS initiatives, solicitations, and the support of new facility projects.

----A7----

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

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

MPS Response A7: We concur. MPS is an active participant in the development of an Office of Cyber Infrastructure within NSF. There is an MPS working group that meets on a weekly basis providing input into various aspects of cyberinfrastructure. The Divisions of Chemistry (page 16) and the Division of Materials Research note that they are strongly committed to providing adequate levels of support.

----A8----

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

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

MPS Response A8: Funds that were available through MPS under the Information Technology Research priority area are now part of Divisional budgets, and we will continue to seek funds to augment this area.

----A9----

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

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

MPS Response A9: We agree. This is an emerging area that is attracting increasing numbers of research scientists in the MPS disciplines, we are strongly supportive of this area, and we will coordinate efforts in this area among the MPS Divisions and with other Directorates.

----A10----

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

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

MPS Response A10: MPS is well aware of the problem of over-committed staff, and it is not limited to theory. Likewise, it is important to have a balance between permanent and visiting scientists at NSF. Committee of Visitors have brought this to our attention, and we will work towards a balance of permanent staff and visiting scientists. In addition, it is important that the community work with NSF in suggesting the names of individuals who might consider coming to NSF.

B. Education and Training

The health of theoretical science relies critically on the education and training of young scientists. From the advanced undergraduate level on,

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

----B1----

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

Recommendation B1. MPS should encourage the Division of Undergraduate Education in the Education and Human Resources Directorate to expand workshops on professional development and teaching for faculty.

MPS Response B1: The coordination between MPS and EHR is being strengthened with the establishment of three working groups between the two Directorates. We will consult with EHR on these workshops and work with them on possible implementation of such workshops.

----B2----

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

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

MPS Response B2: MPS follows a flexible interpretation of the educational effort, and follows the spirit of the CAREER solicitation, which states "Successful PIs will propose creative, integrative, and effective research and education plans." Additionally, MPS wishes to note the solicitation statement that "Proposed education activities may be in a broad range of areas and may be directed to any level: K-12 students, undergraduates, graduate students, and/or the general public, but should be related to the proposed research". These are the types of efforts that are communicated to

prospective PIs, not only in the solicitation, but during conversations and presentations that arise before the submission deadline. They are also the efforts that are described to the reviewers and the panel. The Workshop recommendation emphasis on "K-12 opportunities" unnecessarily focuses attention on only one possible educational effort. General examples of possible educational activities are, in fact, presented in the solicitation, and efforts proposed by successful awardees are available in the published abstracts. Since NSF recognizes that there exists "no single formula for developing an integrated research and education plan", and "because there may be different expectations within different disciplinary fields and/or different organizations, a wide range of projects may be appropriate for the CAREER program", best practices (and expectations of the host institutions) for the proposed program should, by necessity, be conveyed in the proposal by the PI.

----B3----

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

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

MPS Response B3: MPS is strongly supportive of such summer schools and the Divisions are already supporting a number of such activities. MPS will encourage PIs to submit proposals for this type of activity and we will encourage them to explore the possibility of support by other agencies for this type of activity. We will partner with other agencies should they be interested in this activity.

----B4----

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

impact on the education of theorists and in suggesting possible actions by universities and by MPS.

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

MPS Response B4: This would be a major undertaking for the Directorate and a number of issues must be addressed prior to beginning gathering such information. How would "theory students" be identified? In addition, one would have to determine just what type of data should be gathered, and whether it would be available within the data provided with a proposal submission or in the annual and/or final reports on grants. We consider this to be a question applicable to both graduate students and postdocs and will consult with the Division of Science Resource Statistics (SRS) on gathering such data[1].

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[1] The Division of Science Resources Statistics (SRS) fulfills the legislative mandate of the National Science Foundation Act to . . .

> *provide a central clearinghouse for the collection, interpretation, and analysis of data on scientific and engineering resources, and to provide a source of information for policy formulation by other agencies of the Federal Government. . .*

To carry out this mandate, SRS designs, supports, and directs about 14 periodic surveys as well as a variety of other data collections and research projects. These surveys yield the materials for SRS staff to compile, analyze, and disseminate quantitative information about domestic and international resources devoted to science, engineering, and technology. Each year SRS produces about 30 publications, which can be roughly divided into the following categories:

- Detailed Statistical Tables reports containing an extensive collection of tabulated data from each of SRS's surveys;
- InfoBriefs highlighting results from recent surveys and analyses;
- Periodic "overview" reports, such as Science and Engineering Indicators or National Patterns of R&D Resources;
- Periodic reports on focused topics such as Women, Minorities, and Persons With Disabilities in Science and Engineering and International Science and Technology Data Update; and
- Special reports, such as Undergraduate Origins of Recent Science and Engineering Doctorate Recipients and International Resources for Science and Technology.

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

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

MPS Response B5: Support for such activities have taken place at times, primarily through centers and facilities. MPS will explore possibilities with the joint MPS/EHR working groups.

C. Broadening Participation

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

----C1----

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

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

MPS Response C1: This is an NSF-wide issue and we will bring this recommendation to the attention of NSF senior management.

----C2----

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

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

MPS Response C2: Broadening participation in research and engineering is an area NSF strongly supports. In particular, we encourage REU sites to make strong programs in broadening participation, and will continue to do so. We will encourage theorists to participate in the REU sites at their institution and we will also encourage, through divisional newsletters, theory groups to submit to the REU program.

----C3----

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

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

MPS Response C3: Support for graduate students and postdocs is part of the normal request within proposals, and is considered on the basis of each proposal received. Supplements are considered on an individual basis, subject to budget constraints. In all instances, principal investigators are encouraged to draw from a diverse pool of candidates. In instances where specific students are identified, diversity and potential impact on broadening participation are among the decision factors.

----C4----

Recommendation C4. MPS should regularly examine the diversity of speakers and organizing committees at meetings that it supports involving theoretical scientists. It should do the same for the advisory panels for the facilities and centers that it supports. MPS

should identify, promulgate and reward best practices. It should take into account recent practice in making funding decisions for all meetings and workshops.

MPS Response C4: We are in full agreement with this recommendation. We will ensure that all of the MPS divisions are aware of this and we will expect MPS divisions to follow this to the extent that is practical in any particular situation.

D. Outreach

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

----D1----

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

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

– Publicizing and taking credit for MPS-supported theoretical research. This can be done through NSF publications themselves and by working with the private-sector media. NSF can learn from the best practices of other agencies.

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

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

MPS Response D1: We agree with this recommendation, and are working with OLPA to publicize and take credit for MPS-supported research. We will encourage MPS-supported principal investigators, through our divisional newsletters, to include a link to the NSF home page. We will also look at other means of encouraging PIs in theory to submit nuggets to us. We will encourage the submission of proposals for workshops that are designed to implement the recommendation concerning journalism, and we will work with NSF's Office of Legislative Affairs (OLPA) about informing journalists on MPS-supported work.

----D2----

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

MPS Response D2: We will encourage principal investigators to include such activities within proposals and coordinate such activities with the Education and Human Resources Directorate.

IV. Division-Specific Observations and Recommendations

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

A. Astronomy (AST)

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

AST Response: We appreciate the Theory Workshop endorsement of the organizational structure of the unrestricted individual investigator grants program in AST. We believe PIs with proposals in all techniques and astronomical topics, including those covering multiple techniques (observations, theory, laboratory) and topics, are best served with the no-boundary structure of the program. Furthermore, this structure maintains the flexibility to respond to shifting interests and newly burgeoning areas of research. AST will continue to follow the practices described in this recommendation. In particular, it is AST practice that review panels are made up of experts in the same range of activities as the proposals before the panel.

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

AST Response: The AST Astronomy & Astrophysics Postdoctoral Fellowship (AAPF) program was designed to provide a comprehensive professional development experience for the Fellows. The AAPF fellowships are awarded to the individual to recognize and develop professional independence and to foster flexibility and portability. They include an educational component that is intended to integrate the fellow into the educational activities of the host institution and to provide fellows with experiences that will prepare them for the next stage of their careers.

The AST AAPF approach is intended to expose applicants to the proposal writing and review process, to increase diversity among the award recipients by removing perceptions of reputation and influence, and to judge AAPF proposals in a manner similar to that used with regular AST research proposals. Proposals to the AAPF program are reviewed according to the intellectual merit and broader impacts of the proposed research and education projects. Additional review criteria are used in the evaluation process to consider the qualifications of the applicant, the suitability of the proposed host institution, and the prospective benefits to the applicant, host institution and scientific discipline. The majority of AAPF review panelists consistently report that letters of recommendation would not be beneficial to the program or the review process. AST considers both the diversity (49% women, 11% non-Asian minorities) and caliber of AAPF awardees as demonstrative of a robust review process.

The AST AAPF program follows rules and policies that govern NSF fellowship programs in general. Under these rules non-US citizens are not eligible to receive fellowship awards. We believe that making the award to the individual and not to the institution is a strength of the fellowship program.

It is AST practice that review panels are made up of experts comprising the same range of activities as the submitted proposals under review. Thus, theorists are represented on AAPF review panels as appropriate. In every year that the AAPF program has been active, the percentage of theorists on AAPF review panels has exceeded the percentage of submitted theory proposals. Fellows engaged in theoretical work constitute roughly one third of current fellowship awards, an award ratio very similar to that in the regular research grants programs.

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

AST Response: Given the goals and the charge for the AST Senior Review and given suggestions from our advisory groups, the core grants program in AST will not be on the table for in-depth consideration by the 2005 Senior Review process. The Review committee will be free to express their view of the appropriate balance between facilities and grants, including the possibility of increased grant support over the current level.

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

AST Response: This recommendation will be passed on to the managing organizations of our National Astronomy Centers.

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

AST Response: Review panels in the AAG program will be informed that proposals structured as group grants are legitimate modes for AST support, if there are any proposals in the panel that meet this description. Any statement regarding legitimacy of group grants will apply to all such proposals regardless of technique (observation, theory, laboratory) and topic. Irrespective of the detailed organizational structure of the proposal, all proposals in the panels will be evaluated on the basis of the two NSF review criteria of intellectual merit and broader impacts.

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

AST Response: AST is supportive of this recommendation in spirit, but the restrictions on the MREFC funding account prohibit use of MREFC funds to support activities outside of facility construction. Recently submitted proposals for major research facilities include a theory challenge component. However, any support for theory challenges would have to be found in the already heavily pressured Division budget, and thus compete with other high

priority activities and recommendations from the community. AST will continue to weigh this recommendation with many others in this and other community reports and to work to implement it as we see opportunity to do so.

B. Chemistry (CHE)

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

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

CHE Response: As the principal steward of U.S. theoretical and computational chemistry, CHE has historically strongly supported this subdiscipline and is committed to continuing to ensure its development by providing adequate levels of support.

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

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

CHE Response: CHE certainly welcomes submission of collaborative, theory-intensive proposals to the CRC program. There is no restriction on

the nature of projects supported by the CRC program, nor by the other multi-investigator programs in CHE, viz., CBC, EMSI, and CRIF. Any of these programs could serve as vehicles for collaborative chemical research and education involving small groups of theorists, and CHE will work to make the community aware of this opportunity.

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

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

CHE Response: CHE is receptive to the concept of establishing institutes focused on theoretical chemistry whose activities would be complementary to the division's TCC single-investigator-based investments.

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

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

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

- **Base support for supplies, travel, and computation**

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

CHE Response: CHE/TCC fully endorses the spirit of this recommendation and its awards are typically at or close to the levels recommended above for individual PIs. This is particularly challenging in times of flat or declining budgets, as success rate is compromised when award size and duration are expanded. TCC has been pro-active in providing four-year awards, creativity extensions, and SGER awards, and in obtaining co-funding from other NSF divisions when appropriate. PIs are encouraged to request appropriate salary support consistent with their institution's guidelines, as well as adequate support for supplies, travel and computation.

In closing its response to these recommendations, CHE notes that there are extraordinary opportunities for the TCC PI community to provide leadership to the national chemistry community in three priority areas that CHE is coordinating: the molecular basis of life processes, sustainability, and cyber-enabled chemistry. The division anticipates investing substantially in leadership-caliber projects in these areas. CHE urges the TCC PI community to engage with the broader chemical sciences community to help shape these future directions in chemical research and education.

C. Materials Research (DMR)

Condensed Matter Physics is a vibrant and broad subfield of physics, one of its essential strengths being the close coupling of theory and experiment. Although it often has important consequences for technology, frontier theoretical condensed matter physics research, as in other areas of theoretical physics, is most often curiosity-driven, rather than application-driven.

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

DMR Response: DMR supports this recommendation.

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

DMR Response: DMR has implemented this recommendation.

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

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

DMR Response: DMR will continue to collaborate and coordinate with relevant professional societies and governmental groups in order to communicate the excitement of materials research to both the scientific community and general public.

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

MPS-Wide Recommendation A8.

DMR Response: DMR supports this recommendation. Much of this research will be subsumed by Cyberinfrastructure.

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

MPS-Wide Recommendation A9.

DMR Response: DMR supports this recommendation. DMR has been a leader in supporting theory for biological physics and materials. DMR was primary organizer, with OMA, PHY and MCB, of the workshop on theory in biological physics and materials. DMR co-funds the PFC on Theoretical Biological Physics. DMR has recently established a group to coordinate its activities in biology within the division and with other divisions and directorates.

D. Mathematical Sciences (DMS)

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

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

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

DMS Response: This is a major issue for DMS and we are, in fact, continuing to monitor this balance and support the highest quality work.

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

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

DMS Response: DMS agrees that it is important to find ways to encourage and stimulate the many active, contributing mathematical scientists who are not supported by the necessarily limited number of individual research awards.

As stated in the report, DMS has addressed this issue in a number of ways. The mathematical sciences institutes function as national user facilities and represent a variety of core and interdisciplinary interests. The division's activity on Conferences, Workshops, and Special Meetings in the mathematical Sciences, provides participant support for conferences, workshops, and group international travel. Reviewing of these proposals stresses support for junior researchers and individuals who do not hold research grants.

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

MPS-Wide Recommendation B3.

DMS Response: DMS already supports a number of such activities and offers a specific competition for proposals of this kind. For example, several DMS-supported institutes run summer programs for graduate students in annually changing topics in the mathematical sciences. The DMS supported Park City-IAS Mathematics Institute has a component devoted to graduate students. DMS has also supported summer and winter "schools" for graduate students in a number of areas including number theory, analysis, and geosciences. Through its new "special meetings" activity cited above, DMS is actively seeking proposals for "summer schools" that will engage graduate students and new entrants to the field.

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

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

DMS Response: DMS agrees – in fact, it is currently working on an assessment of the effectiveness of the VIGRE program.

E. Physics (PHY)

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

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

PHY Response: The Physics Division normally asks its COV to address the issue of balance. The 2006 COV will be asked in particular to consider balance with respect to theoretical research. FYI: The first PFC started in response to the PFC solicitation began in FY02. Ongoing PFC-like (i.e. center synergy plus $ 1 M/year or higher funding level) activities have been moved into the PFC program.

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

MPS-Wide Recommendation A4.

PHY Response: The Physics Division recognizes that an award should be at a level of funding that will allow the research to proceed. In FY 05, theoretical sub-programs did receive incremental funding increases compared to other core programs. In times of budgetary stringency, increasing grant size must compete against the minimum cadre of grantees consistent with the health of the field. Increasing grant duration to typically 5 years vs the current typically 3 years reduces flexibility in times of budgetary stringency.

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

MPS-Wide Recommendation A5.

PHY Response: The Physics Division's Program Directors consult with PD's from other divisions and directorates to co-review interesting proposals at the boundaries. Some programs, such as Biological Physics, Plasma Physics, and Mathematical Physics, are inherently interdisciplinary and require co-review of most proposals. MPS (and NSF as a whole) should encourage Program Directors to be pro-active in interdisciplinary co-review and should recognize the efforts of Program Directors who engage in co-review and especially those who are leaders in this type of activity.

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

MPS-Wide Recommendation A6.

PHY Response: The Physics Division will include the status of relevant theory as a component of the review process for MREFC and mid-scale experimental proposals. Proposals that address gaps in the relevant theory will be accorded high priority on the basis of this potential broad impact.

C. Michael Turner Invitation Letter

Dear MPSAC Members and Theory Workshop Steering Group Members,

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

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

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

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

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

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

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

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

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

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

Sincerely yours,

Michael Turner
Assistant Director