Directorate for Mathematical and Physical Sciences

Government Performance and Results Act

FY 2001 Report

Introducing the "*Directorate for Mathematical and Physical Sciences Government Performance and Results Act (GPRA) Performance Report for FY 2001"*

It is with considerable pleasure that the Directorate for Mathematical and Physical Sciences (MPS) of the National Science Foundation presents its FY 2001 GPRA Performance Report.

In this Report we offer a small sample of examples of support for research and education fulfilling the Outcome Goals of the National Science Foundation. The broad portfolio of research and educational activities supported by the Directorate has resulted in a number of remarkable discoveries that have attracted the attention of the press and the public. These discoveries are only, of course, small pieces of a puzzle ultimately leading to development of a fuller, more accurate understanding of the world and universe we inhabit.

Progress in the mathematical and physical sciences is, of course, linked to other disciplines, and there are many examples of work jointly supported with other NSF Directorates of other agencies. In addition, the development of technology and progress in all fields of research are closely related, We wish to emphasize, however, that in all the research highlighted here, the education of future citizens and future scientists is becoming an integral component. The Directorate supports thousands of graduate students and postdoctoral students in the physical sciences. These individuals will form a major portion of the leadership of the physical sciences community in the coming decades.

We are committed to making the results of the research we support available and understandable to the general public. We are also attempting to increase the involvement of our community with teachers and with students in grades K-12. It is essential that our community become involved in improving the mathematical and science skills of all Americans. The report gives a number of examples of this type of activity.

I'm sure you'll agree this Report illustrates that MPS is not only alive and well, but that the research it is supporting is dramatic and forward-looking. I encourage you to contact us should you require further information on any aspect of the material contained within the Report.

Robert A. Eisenstein
Assistant Director for
Mathematical and Physical Sciences

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Directorate for Mathematical and Physical Sciences
GPRA Performance Report FY 2001

The Directorate for Mathematical and Physical Sciences (MPS) supports a strong and diverse portfolio of research and education in mathematics, astronomy, physics, chemistry, and materials research. The purpose of this work is both to deepen our understanding of the physical universe and to use that understanding in service to society both as a means of intellectual enrichment and as a wellspring to future economic development. The mathematical and physical sciences, supported across all Federal agencies, serve as the training ground for at least half of all doctoral scientists now employed in U.S. industry.

The Directorate places a high priority on multidisciplinary work and on partnerships. Within MPS the Office of Multidisciplinary Activities serves as a catalyst in emerging areas of research and education at disciplinary boundaries.

International partnerships are critical in the work MPS supports, especially in astronomy, physics, and materials research, all of which require large facilities in order to carry out state-of-the-art research. A critical objective of MPS is world leadership in the sciences MPS supports, and, over the years, numerous MPS-supported researchers have received the Nobel Prize or other awards of high international standing.

Postdoctoral training, Research Experiences for Undergraduate (REU) sites, graduate student traineeships, national facilities and centers, partnerships with the Directorate for Education and Human Resources (EHR), and workshops and conferences are means through which the Directorate for Mathematical and Physical Sciences helps develop the nation's next generation of scientists and engineers.

All Programs and Divisions within the MPS Directorate have provided background information for this report. Other sources include project reports, FY 2001 COV reports, budget justifications, press releases and related media materials, divisional annual reports, and formal external evaluations.

The Division of Chemistry

The mission of the Division of Chemistry (CHE) is to promote the health of academic chemistry and to enable research and education in chemistry at the highest possible professional, technical, and creative levels.

The Division of Chemistry provides about one-quarter of Federal research funds for academic chemistry. The National Institutes of Health provide about one-third of the Federal funds for academic chemistry, narrowly targeted to projects that directly benefit biomedical research. The chemical and allied processes industries (including pharmaceuticals) have sales of over $400 billion and invest about $18 billion per year in research. This industry segment employs about 94,300 scientists and engineers. In addition, other industries such as semiconductor, transportation, and agriculture, support and depend on chemistry research. These industry investments in research are usually short-term and targeted to a narrow purpose. Thus, the Division is the only significant source of funds to build the knowledge base and educate the future workforce on which this large, diverse, and economically important enterprise depends.

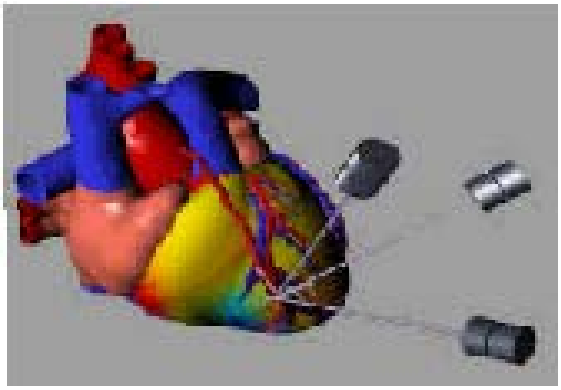
The Division places a high priority on support for high risk-high potential research, for adequate funding of academic investigators at the beginning of their careers, for support and encouragement of chemists who are members of underrepresented groups, and for projects integrating research and education. The Division is extensively involved in interdisciplinary and crosscutting NSF-wide programs.

The total FY 2001 Current Plan funding is $153.46 million.

The Division of Mathematical Sciences

The Division of Mathematical Sciences (DMS) supports over 65 percent of Federal academic investments in the mathematical sciences.

Today's advances in science and engineering, driven in part by increasingly sophisticated and readily available computing environments, lift the mathematical sciences to the forefront of science and engineering, reshaping modern science and engineering discovery through quantitative predictions, modeling, visualization, computational algorithms, and optimization methods. Science and engineering are becoming more mathematical and statistical, not only in the physical, engineering and informational sciences, but also the biological, geophysical, environmental, social, behavioral, and economic sciences. While the mathematical sciences are pervasive in science, technology and health, mathematics and statistics is often an invisible partner, encapsulated, for example, in algorithms, models, and software packages. Today the mathematical sciences play a fundamental role in the security of communications; in robust computation and



Experimenting with real human hearts isn't possible. Experimenting with accurate mathematical models is.

critical applications such as weather prediction and disaster modeling; and, in stochastic modeling in atmosphere and earth science.

In view of this, the National Science Foundation (NSF) and the Directorate for Mathematical and Physical Sciences (MPS) in FY 2001 are positioning the Division of Mathematical Sciences for a important role in an agency-wide priority area in the mathematical sciences with the first year of a 5-year investment strategy beginning in FY 2003. To jumpstart this investment, the Division is targeted with an additional $20M increase in FY 2002. At this date the precise budget for this priority area has not yet been determined by Congress and approved by the President, but this future multi-year investment will empower the mathematical sciences on three frontiers: (a) advancing fundamental mathematical sciences, (b) advancing the mathematical sciences in interdisciplinary science and engineering, and (c) advancing the nation's mathematical skills and literacy.

The total FY 2001 Current Plan funding for DMS is $121.48 million.

The Division of Physics

The Division of Physics (PHY) has major stewardship responsibility for the university sector of the physics community. The field of physics provides the basis for the fundamental understanding of the physical universe, from the basic building blocks of matter to the evolution and structure of the universe. Physics also contributes conceptual underpinnings and technologies to many other fields. Moreover, physics contributes strongly to the training of the technological workforce. Broad contributions from the field of physics include lasers, medical imaging and therapy technologies, global positioning technology, nuclear power, communications and networking technology, defense technology, and many technologies used by industry. The PHY mission is to support forefront research and education across physics' broad intellectual sweep, including emerging interdisciplinary areas of opportunity. PHY provides support for individual investigator awards (IIAs), for groups, large and small, for centers, and for user facilities within the sub-disciplines of physics.

Multidisciplinary activities are seen, increasingly, as rich in scientific opportunities. Astrophysics is an area where an increased PHY investment will have particularly strong

scientific payoff. Biophysics is another. The interface between physics and computer science is also an area showing great promise. Along with nurturing such emerging scientific opportunities, PHY plans a commensurate response to broaden the role physics plays in postdoctoral, graduate, and undergraduate education in these new research areas.

The total FY 2001 Current Plan funding for PHY is $187.53 million.

The Division of Astronomical Sciences

NSF is the lead Federal agency for the support of ground-based astronomy. Within the Division of Astronomical Sciences (AST) a broad base of observational, theoretical, and laboratory research is aimed at understanding the states of matter and physical processes in the solar system, our Milky Way galaxy, and the universe. Coordination takes place between NSF and NASA, and the two agencies often engage in significant partnerships or joint undertakings. AST also supports advanced technologies and instrumentation, university radio observatories, and a variety of special programs. The Division's National Centers (National Optical Astronomy Observatory - NOAO, National Solar Observatory - NSO, National Radio Astronomy Observatory - NRAO, and National Astronomy and Ionospheric Center - NAIC), maintain state-of-the-art instrumentation and observing capabilities accessible to the community on the basis of scientific merit. AST also provides the U.S. share of funding for the operation of the Gemini Observatories, an international partnership involving seven other nations for two 8-meter optical/infrared telescopes. In FY 2001 advanced design work continued on the Atacama Large Millimeter Array (ALMA), a telescope that will operate at millimeter wavelengths that involves a partnership with the European community.

The total FY 2001 Current Plan funding for AST is $148.64 million.

The Division of Materials Research

The Division of Materials Research (DMR) is the unit of the Federal government with primary responsibility for the overall health of materials research and education in the nation's colleges and universities. Materials research integrates a wide range of activities spanning both science and engineering. These extend from investigations of phenomena in condensed matter physics and solid-state chemistry to research on functional materials including metals, ceramics, polymers, biomaterials, and electronic, photonic and magnetic materials. Materials research addresses the synthesis, processing, characterization, and properties of materials together with the prediction and control of materials behavior, encompassing the discovery and understanding of materials and condensed matter phenomena and the basis for their translation into technological application. Its practitioners include physicists, chemists, materials scientists, and engineers, and it benefits from the participation of researchers from an even wider range of disciplines such as biochemistry, biology, earth sciences, mathematics, computer science, and medicine. The technological and societal significance of the field is immense: "Everything is made out of something." DMR supports education, fundamental research and facilities that are critically important to the future advancement of industries and technologies ranging from electronics and communications to information technology, transportation and aerospace, energy, environmental protection, manufacturing, medicine and health care, packaging, and civil infrastructure.

The total FY 2001 Current Plan funding for DMR is $209.75 million.

The Office of Multidisciplinary Activities

The Office of Multidisciplinary Activities (OMA) facilitates MPS support of particularly novel, challenging, or complex multidisciplinary research projects whose realization might otherwise be hampered by existing institutional or procedural barriers. Its purpose is to foster the

realization of imaginative ideas emanating from the scientific and engineering community that currently do not fit naturally into established MPS programs. OMA supports meritorious projects proposed by the scientific and engineering community and submitted to one of the regular programs of the MPS divisions. The proposal is evaluated by merit review and judged by the MPS Division as appropriate for OMA consideration. Since the intellectual scope of the OMA includes all of MPS, it does not function as a conventional program office and does not accept unsolicited proposals directly. It promotes joint ventures across existing organizational boundaries within NSF and with research universities, private industry, and other Federal, state, and local government agencies.

The total FY 2001 Current Plan funding for OMA is $29.91 million.

Funding Priorities

Within the three NSF Outcome Goals of People, Ideas, and Tools, the MPS Current Plan for FY 2001 provided $87.07 million for People, $546.52 million for Ideas, and $210.83 million for Tools. About one-third of the entire MPS budget is spent on graduate education and postdoctoral training, primarily in the "Ideas" part of the budget. MPS places a high priority on support for high-risk, high-potential research, for adequate funding of academic investigators at the beginning of their careers, for support and encouragement of scientists who are members of underrepresented groups, and for projects integrating research and education. The Directorate is extensively involved in interdisciplinary and crosscutting Foundation-wide programs. Through education and curriculum renewal, postdoctoral training, REU sites, graduate student traineeships, national institutes, partnerships with the Education and Human Resources (EHR) Directorate, and workshops and conferences, the MPS Directorate is working to develop the nation's next generation of science and engineering personnel.

The Relationship of Resources to Outcomes

In establishing budgets for future years, the MPS Directorate undertakes annual management and program reviews of each of its Divisions. At that time discussions are held as to new initiatives proposed by the Divisions, the scientific results obtained by the investigators currently being supported, and priorities within each Division. In addition, MPS discusses its priorities and initiatives with the Directorate's Advisory Committee and occasionally solicits opinions from external bodies (such as the National Academy of Sciences). The Directorate places a high priority on multidisciplinary initiatives, and as mentioned earlier, the Office of Multidisciplinary Activities assists in such efforts. MPS also pays close attention to managing ongoing projects and to timing the phase-out of ongoing activities in order to support new initiatives.

Organizational Highlights

Division of Chemistry

The 1998 Division of Chemistry's Committee of Visitors (COV) recommended that the Division develop means for consistently evaluating large multi-investigator proposals. In order to improve the evaluation process for center and group proposals, in accordance with this recommendation, the Division established the Collaborative Research in Chemistry competition. The first of these competitions took place in FY 2001.

Division of Physics

In FY 2000 the Physics Division issued a solicitation for a new program within the Division – Physics Frontiers Centers (PFCs), with the first competition and funding in FY 2001. The purpose of the PFC program is to enable major advances at the new intellectual frontiers of physics by providing needed resources not usually available to individual investigators or small groups. PFCs make it possible to address major challenges that require,

for example, combinations of talents, skills, and/or disciplines; specialized infrastructure; large collaborations; and centers/institutes that catalyze rapid advances on the most promising research topics. Characteristics of PFCs include: (1) the potential for a profound advance in physics, broadly defined; (2) a major impact on another field or benefit to society; (3) a synergy or value-added rationale that justifies a center-like approach; and (4) creative, substantive activities aimed at enhancing education, diversity, and public outreach. Annual funding for a PFC ranges from $500 thousand to $4 million. The second PFC competition will be run this year. In FY 2001, the Division received 48 preproposals, which in turn led to 14 full proposals and 4 awards. The second competition will be held in FY 2002.

Division of Astronomical Sciences

The Division continues to act on realizing several organizational changes in response to recommendations from the 1999 Divisional Committee of Visitors (COV) and from other program reviews and community recommendations that took place in FY2000, such as the Portfolio Allocation and Review (PAR) Committee. FY 2001 saw a restructuring of the Division's grants programs for individual investigators. This restructuring unified the 5 major research programs with a common deadline and an umbrella administrative structure, called the Astronomy and Astrophysics Research Grants. This change permitted a more flexible organization of panels for the review of proposals, with the creation of several new panel topics that spanned the traditional program boundaries and facilitated the co-review of proposals with other divisions, particularly with the Physics Division.

FY 2001 also saw the first year of the NSF Astronomy and Astrophysics Postdoctoral Fellowship program, partly in response to the recommendations from the COV and PAR. This program is designed to provide an opportunity for highly qualified young investigators within 3 years of obtaining their PhD to carry out an integrated program of independent research and education at the institution or national facility of their choice. The program is intended to recognize young investigators of significant potential, and provide them with experience in research and education that will establish them in positions of distinction and leadership in the community. Ten fellowships were awarded in FY2001 from a pool of 51 applicants.

Independent Assessments of MPS Divisions

Committees of Visitors

Division of Mathematical Sciences

The activities of the Division of Mathematical Sciences for FY 1998, 1999, and 2000 were thoroughly reviewed by an external Committee of Visitors (COV) in February 2001. The COV stated that the Division is "doing an excellent job of achieving its strategic goals" and rated the Division as "Successful" for all indicators related to the strategic performance goal of PEOPLE, "Successful" for *all* indicators related to the strategic performance goal of IDEAS, and "Successful" for *all* indicators related to the strategic performance goal of TOOLS.

The COV report on the Division of Mathematics is attached to this Directorate report. A summary of its conclusions and recommendations follows:

In addition to finding that the Division was successful in achieving the NSF Outcome Goals for the three years under review, the COV had the following comments:

- It felt that the use of Screening Panels was a very effective process for reviewing proposals and encouraged program officers to expand its use.
- With respect to the Broader Impact Criterion, the COV felt that responsibility for appropriate consideration of this criterion lies with the program officer.
- The COV supported the creation of more institutes, having different characters, foci and modes of operation.
- The COV encouraged increasing and systematizing shared funding of

interdisciplinary programs, involving the Division and a funding agency from another discipline.
- The COV felt that the mentoring program for new program officers should be expanded.
- The GOALI and the IGMS programs were suffering from lack of quality applicants.
- Research Experiences for Undergraduates (REU) sites and supplements should be expanded.
- The COV felt that the Division should increase its presence on the NSF web site and encourage the creation and maintenance of accessible web sites by other parts of the mathematical sciences enterprise.
- The COV was concerned with shortages of human resources and, in particular, the number of American students pursuing graduate-level mathematical sciences.
- The problem of increasing participation in the mathematical sciences and statistics by underrepresented minorities and women continues to be unsolved.

The response of the Division and the Directorate can be found in the attached COV report.

Division of Chemistry

The activities of the Division of Chemistry for FY 1998, 1999, and 2000 were thoroughly reviewed by an external COV in February of 2001. The COV stated that the Division is "doing an excellent job of achieving its strategic goals" and rated the Division as "Successful" for *all* indicators related to the strategic performance goal of PEOPLE, "Successful" for *all* indicators related to the strategic performance goal of IDEAS, and "Successful" for *all* indicators related to the strategic performance goal of TOOLS.

The COV report on the Division of Chemistry is attached to this Directorate report. A summary of its conclusions and recommendations follows:

In addition to finding that the Division was successful in achieving the NSF Outcome Goals for the three years under review, the COV had the following comments:

- The COV noted that Division is operating well. It applauded the efforts the Division has made to integrate research and education and commented that the Divisional workload is staggering.
- The COV felt that clear guidelines need to be developed for proposal submission in areas where strong connections are to be made between research and education.
- The COV stated that it was time to have another close look at the instrumentation program, and wanted to make sure "that Centers are more than groupings of PIs who get together only when site visits take place."
- The COV stated "the chemistry academic community, the NSF and the Division of Chemistry have not developed ways of increasing the representation of women and minorities [in tenure track positions]."
- The COV stated "There was strong sentiment in favor of reviving the competitive NSF postdoctoral fellowship program in order to broaden the training of young people."
- Support for graduate students was a major concern.
- The COV noted that increasing the number of funded proposals while maintaining the value of the award can only be done by increasing the Division's budget for core research.

The response of the Division and the Directorate can be found in the attached COV report.

Other Independent Assessments

Division of Astronomical Sciences

The Bush administration's 28 February 2001 FY 2002 budget summary document called for NSF and NASA to establish a Blue Ribbon Panel to "assess the organizational effectiveness of Federal support of astronomical sciences and, specifically, the pros and cons of transferring NSF's astronomy responsibilities to NASA." The panel could also consider and develop alternative options. NASA and NSF asked the National Academies, through the National Research

Council, to conduct the study, and the NRC formed the Committee on Organization and Management of Research in Astronomy and Astrophysics (COMRAA) and charged them to produce their report by 1 September 2001. The Committee recommended that NSF's astronomy and astrophysics responsibilities not be transferred to NASA, and that the Federal government should develop a single integrated strategy for astronomy and astrophysics research that includes supporting facilities both on the ground and in space. They further recommended the formation of an interagency planning board for astronomy and astrophysics that would receive input from the community through a joint advisory committee of outside experts. The report also contained specific recommendations for both NSF and NASA that address ways to improve the present overall management structure and strengthen NSF's ability to support ground-based astronomy and astrophysics. The report can be found at http://www.nas.edu/ with the prepublication copy available at http://books.nap.edu/html/integrated_program/comraa.pdf

Division of Chemistry

The American Chemical Society, the Council for Chemical Research, and other similar organizations publish periodic assessments of the current state and future prospects for chemical research. In addition, CHE along with the Chemical Transport Systems Division (CTS/ENG), currently support the National Academy of Sciences study of chemistry and chemical engineering research called "*Challenges for the Chemical Sciences in the 21st Century.*"[1] This survey of the current status of chemical sciences will evaluate trends and identify key opportunities and challenges.

The Division sponsored workshops in inorganic chemistry, materials chemistry, organic synthesis, and physical organic chemistry. These workshops served to inform the Division on emerging areas of importance to the community.

[1] CTS-9908440

Division of Physics

Until this year, the Physics Division had only one standing advisory committee, the Nuclear Science Advisory Committee (NSAC). The NSAC Reports to both the NSF and the Department of Energy, and management of the committee rotates between the two agencies on a 2-year basis. This year, the High Energy Physics Advisory Panel (HEPAP), formerly an advisory committee to the DOE alone, became a joint NSF-DOE advisor committee and now formally provides advice and reports to both agencies.

Division of Materials Research

The Division of Materials Research (DMR) supports topical workshops in all areas of materials research in part to obtain independent community assessment and guidance on future directions and topics of special interest. As well as providing guidance for NSF, workshops and ongoing programs build intellectual infrastructure in the research community.

Several symposia and workshops focused on the emerging area of nanoscale science and engineering. For example, a joint NSF-European Community workshop on nanotechnology (Toulouse, October 2000) provided guidance on potential areas of cooperation between US and European researchers in this rapidly growing field.

DMR also supports workshops and conferences in specific broad sub-fields of materials research and education to provide assessments of progress and guidance for future direction in specific programmatic areas. Current areas of emphasis in solid-state chemistry are described in the recent *Proceedings of the Workshop on the Present Status and Future Developments of Solid State Chemistry and Materials.*[2] [3] A second national solid-state chemistry workshop will be held in October 2001 at the University of California at Davis. The goals of this *2001 Workshop on Future Directions in Solid State Chemistry* are to articulate the solid-state

[2] *Journal of Solid State Chemistry,* **149**, 3-8, (2000)
[3] http://www.nsf.gov/mps/dmr/ssc.pdf

chemistry community's sense of opportunities and directions to be taken in the future.

Implementation of Merit Review Criteria

The two Committees of Visitors that met during the year examined the use of the merit review criteria both by reviewers and by program officers during the years FY 1998 – FY 2000. The Committee of Visitors for the Division of Mathematical Sciences examined approximately 300 jackets, while the Committee of Visitors for the Division of Chemistry examined approximately 180 jackets. Their findings are quoted below.

Division of Mathematical Sciences

a. Performance Goal: Implementation of Merit Review Criteria by Reviewers: NSF performance in implementation of the merit review criteria is successful when reviewers address the elements of both generic review criteria. Did reviewers adequately address the elements of both generic review criteria?

Committee Rating: Successful/Unsuccessful

"The reviewers always addressed adequately the intellectual merit criterion in their reviews. For disciplinary proposals, on the broader impact criterion, most reviewers' comments, if present at all, are limited to impacts on science and technology and training of graduate students and postdocs. These comments are more common in Computational Math. The broader impacts criterion was not usually addressed by reviewers unless issues relevant to that criterion (e.g. the presence of minority students) were raised by the proposer. In Applied Mathematics and in the various cooperative and interdisciplinary programs we looked at, impact on other sciences and applications was a major factor; impact on students was still rarely addressed by reviewers.

Reviewers rarely comment on diversity, infrastructure and dissemination. We suspect that most reviewers focus on the scientific aspects of a disciplinary proposal and tend not to read the reviewing instructions. Also, these criteria are relatively new and most reviewers may not be familiar with them. For infrastructure proposals (Institutes, VIGRE), both criteria seem to be used properly."

b. Performance Goal: Implementation of Merit Review Criteria by Program Officers: NSF performance in implementation of the merit review criteria is successful when program officers address the elements of both generic review criteria. Did program officers adequately address the elements of both generic review criteria?

Committee Rating: Successful/Unsuccessful

"Program officers always addressed adequately the intellectual merit criterion in their decisions. Program officers were inconsistent in addressing the broader impacts criterion in their decisions. The documentation was inconsistent in showing that the broader impact was considered (again, individual grants). We know from personal experience on panels that these issues have been discussed without being documented in the jacket, but cannot verify that this always happens from the jackets alone. If program officers regularly address these issues in their feedback on both successful and unsuccessful proposals, it would help generate new ideas in the mathematical community.

The responsibility for appropriate consideration of the second review criterion - the broader impacts criterion - lies with the program officer. The program officer should draw this to the attention of the reviewers, particularly in cases where this is a major factor in the decision. The program officer should ensure that this is documented in the jacket."

Division of Chemistry

"The infamous second review criterion of the NSF merit review criteria apparently has caused problems for reviewers and PIs. The Program Officers of the Division have saved the day by taking Criterion 2 into consideration as best they can in reaching decisions on awards. But, in our opinion, steps need to be taken to educate reviewers and PIs on the matter. We leave it to the Division and to the NSF as a whole to come

up with a suitable plan. Let it be clear that we understand the goal of Criterion 2 and we fully support it. We are optimistic that reviewers and PIs will provide the information that is asked for once they understand the goal."

"NSF review criteria are employed in reaching decisions on awards. The need to educate reviewers and PIs in the matter of Criterion 2 has been noted above. The COV found that the Program Officers have done an outstanding job in applying both intellectual merit and broader impact criteria in the evaluation of proposals."

More detailed discussions of the use of these criteria by the various programs within the Division of Chemistry are given in the attached COV report.

Cross-cutting and Coordination Activities

Interagency Activities

Division of Astronomical Sciences

The joint activity with the Air Force Office of Scientific Research (AFOSR) to make available to the US astronomical community observing time at the Advanced Electro-Optical System (AEOS) telescope on Maui, Hawaii was continued in FY 2001 for a second year of funding. The objective of the program is to provide funds to the astronomical community to support astronomers to use the 3.76-meter advanced technology telescope for scientific research.

A number of other projects in the area of particle and nuclear astrophysics continue in conjunction with the Department of Energy and the Physics Division within NSF. These projects include the Cryogenic Dark Matter Search Experiment (CDMS II), the Borexino Project, and the Auger Project. The last two of these also involve international collaborations and are administered in the Physics Division.

AST is making a concerted effort to work more closely with NASA, particularly their Office of Space Science. Both NSF and NASA are considering an initiative recommended in the recently published Decadal survey, the 'National Virtual Observatory (NVO).' There have been a number of meetings between NSF and NASA staff to explore mechanisms for working together in the realization of the NVO. This activity will continue into FY 2002, with a report expected in January 2002.

Division of Mathematical Sciences

The Division and the National Institute for General Medical Sciences at the National Institutes of Health (NIH) began a partnership in a new initiative in mathematical biology.[4] Revolutionary opportunities have emerged for mathematically driven advances in medical-related biological research. These opportunities are recognized by the National Institutes of Health and by the NSF.

The Division, along with the Computer-Communications Research in the CISE Directorate, began a partnership with the Defense Sciences Office of DARPA on research in "Computational and Algorithmic Representations of Geometric Objects (CARGO)".[5] Computational geometry has proven to be a rich area of mathematical and computational research with numerous applications in computer graphics, robotics, and computer-aided design (CAD). Research in this area is expected to have significant impact on engineering design, modeling of physical systems, and computational and geometric cartography.

Division of Chemistry

The Division supports the development and operation of a synchrotron beamline at the Advanced Photon Source jointly with the Division of Materials Research and the Office of Basic Energy Sciences at DOE.[6]
CHE also currently supports two awards in the NSF/Environmental Protection Agency (EPA) Partnership for Environmental Research (*Technology for a Sustainable Environment*). In

[4] NSF 01-128
[5] NSF 01-111
[6] CHE- 0087817

one of the projects K. Barry Sharpless of the Scripps Research Institute[7] is developing methodology for carrying out important classes of chemical reactions in water to construct useful molecules. The work has the potential to impact the pharmaceutical industry by developing highly reliable, aqueous-phase reactions for the preparation of complex structures of biological importance. William Goddard of the California Institute of Technology[8] takes advantage of recent advances in computation chemistry to calculate thermodynamic quantities that can be used to simulate chemical processes and to use the knowledge obtained to optimize commercial reaction processes to minimize effects on the environment.

The Committee on the Advancement of Women Chemists (COACh) consists of individuals who are concerned about the slow progress that is being made in reaching gender equity in professions in the Chemical Sciences. The Division of Chemistry, the Division of Chemical and Transport Systems and the NIH National Institute of General Medical Sciences jointly fund COACh.[9] COACh has been formed to (1) identify and examine the barriers that are inhibiting the careers of women in the chemical sciences; (2) work to educate the community on gender equity issues in the chemical sciences; (3) effect change in institutions and organizations that have hampered the progress of women chemists; (4) actively promote women in pursuit of their career goals; and (5) train women in professional skills that will empower them to achieve their full career potential. The initial focus of the efforts of COACh is on advancing the careers of women chemists and chemical engineers in academia.

The Division currently supports four Environmental Molecular Science Institutes (EMSI). The Chemical Sciences Division of the Office of Basic Energy Sciences, Department of Energy, the Division of Chemical and Transport Systems, and the MPS Office of Multidisciplinary Activities also provide support. Seven Collaborative Research Activities in Environmental Molecular Science (CRAEMS) awards, made to smaller research groups of three to five investigators, are also supported by the Division.

Division of Physics

Activities with the Department of Energy (DOE) include co-funding of a number of large detector projects by grantees of each agency. The U.S. Large Hadronic Collider (LHC) ATLAS and CMS detector projects, the Auger ultra-high energy cosmic ray detector, the G0 spectrometer for use in parity violation experiments at the DOE Jefferson Laboratory, and the CDMS II dark matter detector are examples. In addition, the two agencies jointly support some grants in plasma physics.

NSF and DOE also share a common advisory committee on issues of scientific priority within nuclear science – the Nuclear Science Advisory Committee (NSAC). NSAC is charged to develop a national long-range plan for nuclear science and advise when specific issues arise.

An advisory panel advising both agencies in the field of elementary particle physics–the High Energy Physics Advisory Panel (HEPAP) was created this year.

A third committee that advises the two agencies on large, national-scale astrophysics detector projects is the Scientific Assessment Group for Experimental Non-Accelerator Physics (SAGENAP).

Observers from NASA are invited to SAGENAP meeting, since there are many instances of common interest in the science programs of the three agencies. There are a number of detector projects that are now in the planning stage where opportunities exist for close cooperation in satellite-based physics or astrophysics research.

[7] CHE-9985553
[8] CHE-9985574
[9] CHE-0078913

Division of Materials Research

The NSF Nanoscale Science and Engineering Priority Area involves all NSF directorates and forms part of the multi-agency National Nanotechnology Initiative announced in FY 2000. MPS and the Engineering Directorate (ENG) are the two lead NSF directorates and DMR plays a key role in the overall MPS and NSF effort in this rapidly emerging area of science and technology. DMR-supported efforts in nanoscale science and engineering include every program in the Division and range from individual investigator awards and focused research groups to multidisciplinary centers. DMR accounted for a significant fraction of the total NSF investment in nanoscale science and engineering in FY 2001 ($58 million out of approximately $150 million. DMR invested $11.08 million in new awards under the NSF Nanoscale Science and Engineering competition in FY 2001, including support for 7 Exploratory Research awards, 25 Interdisciplinary Research Teams, and 5 Centers. DMR core programs independently made another 82 awards in nanoscale science and engineering amounting to over $26 million independently.

The National Institutes of Health provides funding for equipment and personnel at the DMR-supported Cornell High Energy Synchrotron Source (CHESS) through 'MacCHESS.' As a user facility, CHESS provides state-of-the-art synchrotron radiation facilities for research in physics, chemistry, biology, materials sciences and environmental sciences. MacCHESS supports special facilities at CHESS for protein crystallography and related studies.

The Center for High Resolution Neutron Scattering (CHRNS) is a joint NSF/ National Institute for Standards and Technology (NIST) national user facility supported by the Division within the Center for Neutron Research (NCNR) at NIST. CHRNS develops and operates state-of-the-art neutron scattering instrumentation, with broad application in materials research.

Several Federal agencies, including the Department of Energy, the Environmental Protection Agency and the Department of Defense provided co-funding for various DMR-supported activities in FY 2001. For example, the US Air Force Materials Laboratory at Wright Patterson Air Force Base provided substantial co-funding for instrumentation and equipment for a DMR-supported Focused Research Group at the Ohio State University addressing the design of metallic alloy systems. The award is also supported by NSF's Division of Civil and Mechanical Systems and by the State of Ohio.

The Department of Energy (DOE) supports the construction of high-field pulsed magnets at the National High Magnetic Field Laboratory (NHMFL). The NHMFL is operated for NSF by a consortium of institutions comprising Florida State University (FSU), the University of Florida (UF), and DOE's Los Alamos National Laboratory (LANL). The pulsed magnet facilities of the Laboratory are located at LANL.

The Spallation Neutron Source (SNS) is now under construction at Oak Ridge National Laboratory. Following discussions with DOE management and SNS management at Oak Ridge, NSF has deferred plans to support the development of a second (long wavelength) target station for the SNS. NSF and DOE staff are now exploring NSF's future role in providing a full suite of instruments for the high-power target station currently under construction. NSF's participation will help the US regain worldwide pre-eminence in research and education in neutron science with applications to materials science, condensed matter science, chemistry, earth science, biology and engineering.

Intra-agency Activities

The Divisions within MPS participate in the following NSF-wide activities:

- Minority Career Advancement Awards (MCAA).
- Faculty Early Career Development (CAREER) Program.
- Grant Opportunities for Academic Liaison with Industry (GOALI).

- Major Research Instrumentation (MRI).
- Professional Opportunities for Women in Research and Education (ADVANCE).
- Research Experiences for Undergraduates (REU).
- Research at Undergraduate Institutions/ Research Opportunity Awards (RUI/ROA).
- Small Grants for Exploratory Research (SGER).
- Minority Research Initiative.
- Environmentally Benign Chemical Synthesis and Processing.
- Science and Technology Centers.
- EPSCoR.
- Technology for a Sustainable Environment.
- Nanoscience and Engineering.
- Biocomplexity in the Environment.
- Information Technology Research.

Two cooperative agreements in the Model Institutions for Excellence program are also handled by MPS. The agreements are with the Universidad Metropolitana[10] and Xavier University of Louisiana[11] and have just been renewed for years six to eight. The maximum duration of the projects is eleven years.

Division of Astronomical Sciences

The Division participated in a number of NSF-wide programs in FY 2001, most significantly, the Information Technology Research (ITR) program. A total of $4.6 million in AST was available for the funding of proposals submitted to the ITR solicitation. The total requested amount in proposals that passed through the pre-proposal phase exceeded the funds available by more than a factor of 10.

Office of Multidisciplinary Activities

The MPS Office of Multidisciplinary Activities is sponsoring an increasing number of educational and outreach grants programs that bring together all the divisions of MPS in the preparation of program announcements and the review and administration of proposals submitted in response to these new opportunities. Two OMA-coordinated programs began in FY 2001- the MPS Distinguished International Research Fellowship (MPS-DRF) program, and the Internships in Public Science Education Program (IPSE). Of the 10 proposals to MPS-DRF that were finally considered for funding, 7 of them were in Astronomy, and 6 of these were funded. Three of the IPSE awards receiving funding had a strong astronomy component.

Most activities with other divisions occur on a more informal basis, and lead to significant co-funding of individual projects or investigators. Many of these occur in the area of astrophysics, in which AST, the Physics Division, and the Office of Polar Programs have a number of ongoing activities. Several of these are mentioned in the inter-agency activities described above. Examples of other co-funded projects that produced significant results in FY2001 are the Boomerang Project[12] and the Deep Extragalactic Evolutionary Probe (DEEP). AST also participates in significant co-funding activities with the Division of Atmospheric Sciences (ATM) in the Geosciences Directorate, the International Division (INT) and increasingly with the Division of Mathematical Sciences (DMS).

Division of Materials Research

DMR is a major participant in an increasingly wide range of intra-agency activities. The NSF-wide 'nano' and 'ITR' competitions in particular expanded rapidly from FY 2000 to FY 2001.

Overall, DMR supported about 760 REU students at REU Sites, MRSECs and National Facilities in FY 2001 and several hundred more REU students through individual-investigator awards).

About 120 pre-college teachers participated in Research Experiences for Teachers (RET) activities at REU Sites, Centers and Facilities supported by DMR in FY 2001. These RET awards were funded primarily by the MPS Office of Multidisciplinary Activities.

[10] DMS-9988401
[11] DMS-9911120
[12] AST-9813920 and OPP-9729121

DMR played a significant role in the NSF-wide Information Technology Research Priority Area in FY 2001. DMR supported (in whole or in part) 5 five-year "medium" ITR awards and 5 three-year "small" ITR awards.

DMR efforts to support human resource development and foster diversity in the materials field also continue to grow. Among many examples, supplementary support to DMR grantee Douglas Osheroff[13] provided funds for travel and local expenses for 54 African-American students to attend the Annual National Conference of Black Physics Students held at Stanford University this year. DMR supported a total of 61 Site awards for Research Experiences for Undergraduates in FY 2001, and 120 pre-college teachers participated in Research Experiences for Teachers at many of these REU Sites in FY 2001.

DMR programs co-review and co-fund a wide variety of activities with other NSF programs and administrative units. Examples include the Materials Computation Center at the University of Illinois (with CHE, DMS, PHY and ACIR); the Turbulence Center at Oregon State University (with PHY); the National Nanofabrication Users' Network (with Engineering); and scores of individual-investigator awards and Focused Research Groups (with CHE, PHY, DMS, ENG, BIO and others). Several DMR-supported Center activities are co-funded by other NSF units including Engineering and EHR (Education and Human Resources), and DMR supports two Collaboratives for the Integration of Research and Education (CIRE) awards through the Materials Research and Engineering Centers program. DMR programs supported 13 EPSCoR awards and 42 CAREER awards in FY 2001.

DMR is a key player in NSF efforts to stimulate and foster increased international cooperation in materials research and education (see paragraph under International Activities). The partnership in materials sciences between NSF and the European Commission provides an excellent example. Within NSF, DMR's partners in this endeavor include the MPS Chemistry Division, the Engineering Directorate, and the International Programs Division of SBE.

Division of Chemistry

Members of the Division serve on NSF-wide working groups in Nanoscience and Engineering, Biocomplexity in the Environment and Science and Technology Centers. Proposals were co-reviewed and co-funded, with among others, the Divisions of Materials Research, Physics, Molecular and Cellular Biology, Chemical and Transport Systems, and International Programs. The Division supported 19 new awards in FY2001 in the Experimental Program to Stimulate Competitive Research (EPSCoR) program.

Division of Physics

The Physics Division has very close ties with the NSF Astronomy Division in the area of astrophysics. The two Divisions have co-funded several large detector projects—the Borexino solar neutrino detector, the Auger high-energy cosmic ray detector, and the CDMS II dark matter detector. A number of other large projects are under consideration. This close cooperation has led to improved and consistent coverage of this increasingly exciting science.

Physics is finding increasing common ground with the other Divisions within MPS and with other NSF Directorates. Examples include mathematical physics (with DMS) and molecular physics and coherent quantum control (with CHE). Similar interfaces with biology, *i.e.* biophysics, and with computer science are emerging. Many biophysics proposals are now co-reviewed by the Physics Division and other divisions within the Biological Sciences Directorate (BIO). A very exciting interface with the Office of Polar Programs has emerged– the Antarctic Muon and Neutrino Detector Array (AMANDA) and IceCube detector projects. These projects exploit the south polar cap ice as a unique, large area detector for high-energy

[13] DMR-0107408

neutrinos and for the conduct of neutrino astronomy and neutrino physics observations.

Division of Mathematics

The Division of Mathematical Sciences and the Directorate for Geosciences support a Climate Simulation Laboratory at NCAR. The award supports a number of postdoctoral statistical scientists in the study of global climate modeling.

The Division, together with the Directorate for Education and Human Resources, is providing partial support for the International Mathematical Olympiad. This event is an international mathematics competition between high school teams representing countries from around the world and was held in Washington, DC this summer. It was the first time the US has hosted this competition in over 20 years.

The Division, together with the Directorate of Education and Human Resources, continues to invest in the Vertically Integrated Grants for Research and Education in the Mathematical Sciences (VIGRE) activity. VIGRE provides for undergraduate and graduate education, postdoctoral and professional training, and curriculum reform in the nation's Ph.D. granting mathematics departments. The Division, together with the Computing and Engineering Directorates, hosted a workshop on robotics to explore the scientific challenges and opportunities in 21st century robotics.

MPS's Office of Multidisciplinary Activities and the Division invested in several of the Division's programs including the new Focused Research Groups and the Divisional program (IGMS) for researchers to spend time in other science and engineering departments and in industry.

International Activities

With respect to cooperative international research and education activities, MPS is currently funding:

- Partnerships between individual scientists.
- Conferences and workshops.
- In PHY, an REU Site at CERN, including some K-12 teachers.
- In CHE, an REU Site at the University of Florida, involving exchanges of French and US students between CNRS laboratories and the University of Florida.
- In AST, an REU Site at the Cerro Tololo Interamerican Observatory in Chile (CTIO).
- Visitors to centers and institutes.
- Use of large-scale facilities.
- Construction of large-scale facilities.

These activities are concentrated in Europe, South America, and Japan. Significant opportunities in other Asian countries, Eastern Europe, Russia, South America, and Africa need to be explored and exploited. More extensive use of information technologies is being explored to facilitate international collaboration. The Division of International Programs plays an important supporting role in coordinating and monitoring international activities.

With respect to encouraging international exposure for US students and young faculty, MPS has just implemented the Distinguished International Postdoctoral Fellowship Program. Four were awarded this year.

Division of Astronomical Sciences

NSF serves as the executive agency for the Gemini Observatories, an international project with seven partner nations (the U.S., the United Kingdom, Canada, Australia, Chile, Brazil and Argentina). The Gemini Observatories consist of two 8-meter telescopes, one located in the southern hemisphere, in Chile, and one located in the northern hemisphere, in Hawaii. NSF provides 50% of the funding, providing merit-based access for the US national community to both telescopes.

AST provides funding for the Gemini Fellowships program. This program brings postdoctoral scholars from the Gemini partner countries of Argentina, Brazil, and Chile to U.S. institutions on research fellowships. AURA, Inc.

also has a program, in cooperation with Fondacion Andes, to provide opportunities for Chilean graduate students to pursue doctoral degrees in the U.S. Both of these programs serve to strengthen both the astronomical communities of our partner countries and the U.S. scientific community.

NSF/AST is also involved in the Atacama Large Millimeter Array (ALMA) project, to place a new radio facility in the Atacama desert of northern Chile. Originally conceived as The Millimeter Array (MMA), ALMA design and development has become a partnership between the NSF's NRAO and a European consortium consisting of the European Southern Observatory and funding organizations from France, Germany, the Netherlands, Spain, Sweden, and the United Kingdom. ALMA construction is envisioned as an equal U.S.-European partnership, with the likelihood of Japan as a third equal partner. ALMA is intended to study the origins of galaxies, stars, and planets by observing the gas from which these objects form.

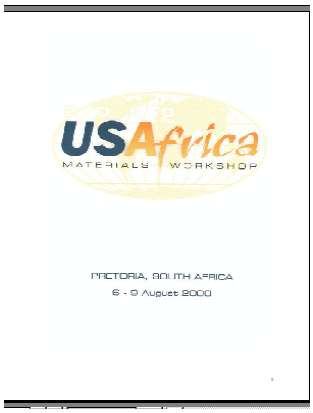
Division of Physics

NSF is the lead agency in the U.S. for ground-based gravitational physics. NSF is actively supporting cooperation between U.S. researchers in other countries that are constructing gravitational wave detectors to form a worldwide network linking such detectors: LIGO (U.S.), VIRGO (Italy), GEO (Germany, Scotland), TAMA (Japan), and AIGO (Australia). In addition, NSF is actively involved in cooperative support (with GEO and VIRGO) for research and development towards next generation detectors to enhance the capabilities of these facilities.

In high energy physics, NSF and DOE are both responsible for the health of the field. In the U.S. NSF has responsibility for an important part of the university community, while DOE, which also has a responsibility for the university program, has sole responsibility for the large U.S. national laboratory accelerators. NSF and DOE have joint responsibility for the U.S. part of the U.S-CERN LHC construction project. However, for the purpose of negotiation, DOE is the lead agency. In terms of international collaborations, NSF plays a lesser role in funding large detectors than DOE, but, nonetheless, an important role in support of individual investigators. The total US contribution will be $531 million, including $450 million from the DOE.

Another example is the Pierre Auger cosmic ray detector project. This is a multinational effort in which PHY and AST and DOE are contributing equally to the construction costs. The U.S. costs will be $15 million, about 15% of the total. NSF and DOE share the responsibilities for oversight of the US part, with neither agency designated as lead. NSF-supported researchers are leading this project.

Division of Materials Research



Over the past six years DMR has co-sponsored a series of workshops in different regions of the world with the goals of identifying specific areas and future directions for cooperation between US and foreign investigators in materials research and education, and to begin the development of a Materials World Net for international communication in the field of materials. Several of the workshops are now bearing fruit. An NSF Dear Colleague Letter issued FY 2000 and updated in FY 2001 describes opportunities for cooperative activities in materials research between US and European researchers to be supported by NSF and the European Community (EC). DMR plays a leading role in this partnership that involves three NSF Directorates together with the EC Growth Programme. Five NSF awards were made this year and more than 30 additional proposals are under review in the current phase of the competition. Comparable arrangements for international cooperation are

now being actively explored by NSF and its counterpart agencies in Canada, Mexico, and South America, and also by NSF and national funding agencies in Europe to complement the NSF-EC interaction. A workshop held in South Africa last year to address opportunities for US-African cooperation in materials research and education has already stimulated the development of regional materials networks in Africa.

Division of Mathematics

The Division of Mathematical Sciences (together with the Division of Physics and the Division of International Programs) continued their support for postdoctoral fellows at the international institute IHES in Paris, France. This institute supports postdoctoral study in mathematical physics and geometry. As mentioned earlier, the United States will hosted the International Mathematics Olympiad this year in Washington, DC.

A new U.S.-Canada partnership to establish a mathematics research station in Banff, Alberta was announced this year.[14] The NSF is providing $1.27 million to support U.S. participation in the project. The Banff facility will provide a world-class venue to form collaborations, advance research and share information on developments in mathematics research throughout North America. NSF's participation reflects its pledge to increase federal investment in the fundamental mathematical sciences, which underlie all science and engineering discovery.

Division of Chemistry

The Division continues to develop contacts with chemistry funding agencies in Europe and the Pacific Rim. The Division organized an informal planning meeting of agency representatives from Pacific Rim countries at the December 2000 Pacifichem meeting in Hawaii. Representatives from China, Taiwan, Canada, Korea and Japan attended this meeting. The purpose was to identify areas and means for improving international collaborations among Pacific Rim countries.

High-Risk Investment Areas

The Division of Physics and the Division of Astronomical Sciences have undertaken a major effort[15] (in collaboration with the Department of Energy) to detect dark matter experimentally. Dark matter is believed to make up more than 90% of the mass in the universe. Only its gravitational field effects reveal its presence. It cannot be observed at any wavelength in the electromagnetic spectrum. Over the last ten years, at the Center for Particle Astrophysics, detectors have been developed to detect the extremely rare interactions of dark matter with ordinary matter.

The Laser Interferometer Gravitational-Wave Observatory (LIGO) has the goal of observing gravitational radiation, a phenomenon predicated by Einstein's General Theory of Relativity. While there is very strong indirect evidence that this radiation exists (the binary pulsar) gravitational waves have never been directly detected.

In FY 2001 the Division of Materials Research played a key role in the NSF Nanoscale Science and Engineering Priority Area focused on six high-risk/high-reward research areas. The six focus areas are:

- Biosystems at the Nanoscale.
- Nanoscale Structures, Novel Phenomena, and Quantum Control.
- Device and System Architecture.
- Nanoscale Processes in the Environment.
- Multi-scale, Multi-phenomena Modeling and Simulation at the Nanoscale.
- Societal Impact of Scientific and Technological Advances on the Nanoscale.

The largest number of NSF proposals was received in the *Nanoscale Structures, Novel Phenomena and Quantum Control* focus area in

[14] DMS-0124838

[15] AST-9978911

the FY 2001 competition, and DMR's role was correspondingly focused quite strongly – though not exclusively - on this aspect of the competition.

In FY 1991 DMR began support for the National High Magnetic Field Laboratory, operated by a consortium involving Florida State University, the University of Florida and Los Alamos National Laboratory. The project was perceived at the time as one with high risk and high potential for payoff in fundamental research. In the ensuing ten years, the NHMFL has developed from a design blueprint to reach fruition as the world's premier laboratory for the exploration of matter under high-field conditions, attracting the very best scientists and engineers as participants and users. In January 2001 NSF support for the NHMFL was renewed for a further 5-year period on the basis of a comprehensive review conducted during the previous year.

Areas of Special Emphasis in MPS in FY 2001

Division of Mathematical Sciences

During FY 2001, the Division of Mathematical Sciences invested approximately $4.2 million for research in mathematical biology. Larger divisional investments: included $8.1 million support for the national mathematical sciences institutes: The Mathematical Sciences Research Institute/Berkeley (MSRI); The Institute for Mathematics and Its Applications/Minnesota (IMA); and, The Institute for Pure and Applied Mathematics/UCLA (IPAM).

The Division continued its major effort to enable education and training reform in departments of the mathematical sciences through an investment of $10.0 million in its VIGRE activity. These awards are to departments in the mathematical sciences to carry out innovative educational programs in which research and education are integrated and in which undergraduates, graduate students, postdoctoral fellows, and faculty are mutually supportive.

A total of $9.2 million was invested in Focused Research Groups (FRG) activity. The new FRG activity allows groups of researchers to respond to recognized scientific needs of pressing importance, to take advantage of current scientific opportunities, or to prepare the ground for anticipated significant scientific developments in the mathematical sciences.

Division of Chemistry

In order enable groups of researchers to respond to recognized scientific needs, to take advantage of current scientific opportunities, or to prepare the groundwork for anticipated significant scientific developments in chemistry, broadly defined, the Division held its first competition in FY 2001 in the Collaborative Research in Chemistry program. This activity supports collaborative research involving three or more investigators, each of whom has a well-established research group.

Division of Materials Research

Special 'Nanotech' issue of Scientific American, September 2001

NSF priority areas in which the Division of Materials Research is involved are Nanoscale Science and Engineering ($58.82 million from DMR in FY 2001), Information Technology Research ($7.28 million), and Biocomplexity in the Environment ($1.07 million). DMR is a key player in the 'nano' area and has a significant role in Information Technology Research.

Interdisciplinary research and university-industry cooperation are supported through Focused Research Groups (FRGs), centers and GOALI awards. A broad spectrum of activities in education and human resource development, thematic workshops, and international activities in materials research and education are also

supported. The Division now supports about 50 active FRG awards (including new awards under the Nanoscale Science and Engineering competition in FY 2000).

Division of Physics

A new program, Physics Frontiers Centers (PFC), was begun in FY 2001 providing support for a physics-based centers program spanning the parts of physics under Physics purview, and extending to emerging new areas as well. The PFCs program supports university-based centers and large groups in cases where this mode of research is required to make transformational advances in the most promising research areas. The purpose of the PFC program is to enable major advances at the intellectual frontiers of physics by providing needed resources not usually available to individual investigators or small groups.

Areas of particular emphasis within the Physics Division include nuclear and particle astrophysics, quantum information science, biophysics, and mathematical physics. These emphases developed from a pattern of increasing proposal pressure over the past several years. For example, we are now seeing extremely exciting new developments in the area of applying single atom manipulation techniques to probing biological systems at the molecular level.

Division of Astronomical Sciences

Much of the research supported by the Division contributes substantially to the creation of scientific databases and tools to use them. Observational projects, in particular the many extensive surveys now underway, routinely create extensive databases that are made available over the web to the astronomical community, and to the public. Projects include the Optical Gravitational Lensing Experiment (OGLE) project, which is known for its massive database and 'early alert' system, the Galactic Ring Survey (GRS), a project to map the ^{13}CO emission from a large portion of the plane of the inner Milky Way, the Southern Galactic Plane Survey, a survey of the 21-cm line and continuum emission in the inner Milky Way, the galaxy surveys to support cosmological studies, and extrasolar planet searches.

I. OUTCOME GOAL: PEOPLE

FY 2001 Annual Performance Goal

NSF is judged successful when

In the aggregate, results reported in the period demonstrate significant achievement in one or more of the following indicators:

- Improved mathematics, science, and technology skills for U.S. students at the K-12 level and for citizens of all ages, so that they can be competitive in a technological society.
- A science and technology and instructional workforce that reflects America's diversity.
- Globally engaged science and engineering professionals who are among the best in the world.
- A public that is provided access to the benefits of science and engineering research and education.

FY 2001 Areas of Emphasis across NSF

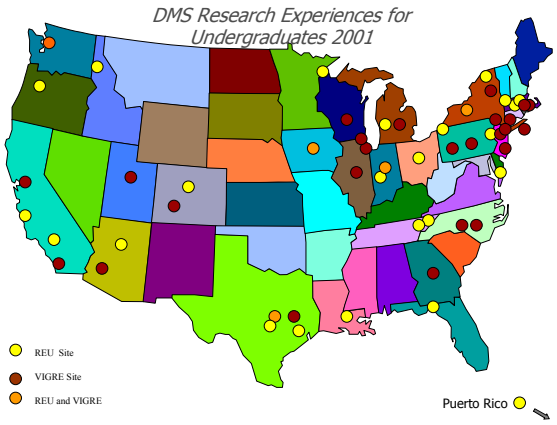
- K-12 systemic activities
- Enhancing Instructional Workforce
  - Center for Learning and Teaching
  - Graduate Teaching Fellows in K-12 Education
- Broadening Participation
  - Tribal Colleges
  - Partnerships for Innovation
- Addressing near-term workforce needs
  - Advanced Technological Education

Introduction

Mathematics

The fundamental mathematical sciences – embracing mathematics and statistics – are not only essential for the progress of research across the disciplines; they are also critical to training a mathematically literate workforce for the future. Technology-based industries help fuel the growth of the U.S. economy, which relies, in turn, on large numbers of college graduates, well versed in mathematics, science and engineering. Even firms not at the forefront of technology rely increasingly on computer control systems, electronic data management, business forecasting models, and modern economic theory. For the United States to remain competitive among other nations with strong traditions in mathematical education, we must attract more young Americans to mathematical careers. Our country must also provide all citizens with the mathematical training to succeed in the workforce, and to make effective decisions concerning their lives.

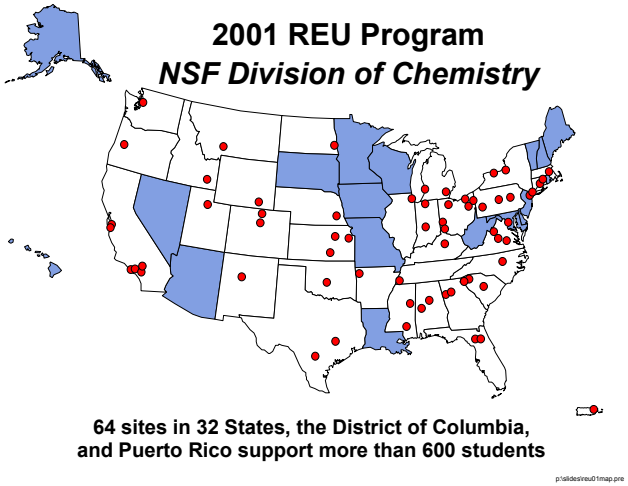
As the role of mathematics has expanded in science and society, the resources devoted to three key areas – fundamental mathematical research, interdisciplinary collaboration between mathematics and other disciplines, and mathematics education – have not kept pace, thus limiting the nation's scientific, technical, and commercial enterprises. To address this challenge, the NSF proposes a Mathematical Sciences Investment Priority Area as a national imperative.



In FY 2001, the Division of Mathematical Sciences (DMS) supported 1293 investigators on approximately 700 awards from among approximately 1800 proposals. The Division supports the training of a globally-oriented workforce of scientists through a variety of mechanisms including formal postdoctoral fellowship programs, postdoctoral activities at VIGRE sites, postdoctoral training at the Division's national institutes, and postdoctoral support on research grants. In FY 2001, DMS supported 317 postdoctoral fellows and 1387 graduate students. DMS supported 243 undergraduates on research awards and an additional 296 undergraduates at 29 Research Experiences for Undergraduates (REU) sites. The Division's most significant investment in developing the U.S. scientific workforce is through its VIGRE program. Currently thirty-one projects are being funded. The average award provides three years of full-time support for twelve graduate trainees, three years of half-time teaching for five postdoctoral fellows, and research experiences for twenty undergraduate students. Awards are for five years, contingent upon an assessment during the third year, and average $600,000 per year.

Chemistry

The Division of Chemistry (CHE) has one of the largest investments in REU sites in the National Science Foundation. Through this program undergraduate students are introduced to meaningful scientific research and in most cases are motivated to go on to studies for an advanced degree in the sciences. The Division supports 64 sites in 32 states at which more than 600 students are supported each summer. Half the participants are female, and 23% are from underrepresented ethnic or racial groups.



Astronomy

The Division of Astronomical Sciences (AST) supports the goals of training and enabling a diverse, globally oriented workforce of scientists and engineers through a variety of activities coordinated through the astronomy National Facilities and carried out by individual investigators or groups of investigators. Over 100 undergraduate students and over 250 graduate students are supported on individual research grants in AST, and an additional 125 undergraduates are engaged in research activities at REU sites across the country. AST also supports telescope operations and scientific research at privately owned

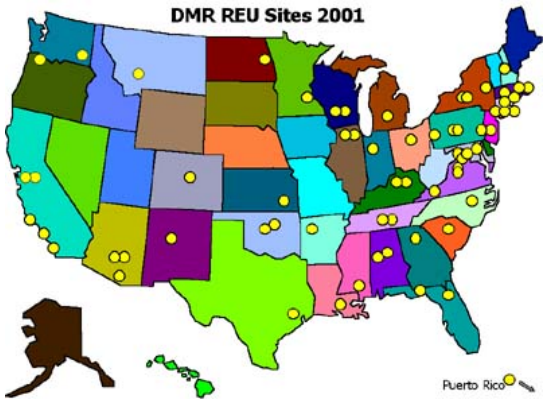
university-based radio observatories, which play a major role in training the future generations of radio astronomers. AST also supports over 100 postdocs on awards to individual investigators, and has established a prestigious postdoctoral fellowship that not only recognizes and supports the training of the next generation of scientists, but supports them in their efforts to combine their interests and activities in education and outreach with their research programs.

Physics

The Division of Physics (PHY) supported 55 REU sites in 2001, providing undergraduate research opportunities for roughly 700 students. Eight of the physics REU sites also include Research Experiences for Teachers (RET) programs to bring high school teachers into the research experience. A hallmark of the REU program is its diversity, not only in terms of the participating students, but also in the geographic locations, participating institutions, and available research areas. REU sites are located across the country, and two of the programs also allow students to participate in international research collaborations at CERN in Switzerland. At all REU sites participating students choose research projects from a full spectrum of both traditional and interdisciplinary physics topics. One newly funded site led by L. Magnani of the University of Georgia[1] provides opportunities in exciting interdisciplinary areas blending physics with fields including biology, computer science, and genomics.

Each PHY-supported facility also has outreach programs. Growth in outreach is entering a new phase, and PHY plans to extend it by supporting further facility-based informal educational activities. An example is building upon the educational opportunities that LIGO offers. PHY is also supporting K-12 teacher enhancement activities in which research experiences (e.g. the REU program) will extend to current and future science teachers.

Materials Research



The Division of Materials Research (DMR) supported the research efforts of well over 1000 undergraduates in FY 2001, including 760 at REU Sites, Materials Research Science and Engineering Centers (MRSECs) and National Facilities, and several hundred more through individual-investigator awards. About 350 students participated in summer research experiences at 36 locations established through the annual NSF-wide REU site competition. Two sites are co-funded with the Division of Physics, one with Chemical and Transport Systems (Directorate for Engineering), and two with the NSF-EPSCoR program. Four are affiliated with MRSECs. In addition, 23 MRSECs supported by DMR in FY01 incorporated REU Sites as an integral part of the MRSEC efforts; about 380 students participated. DMR user facilities including the National High Magnetic Field Laboratory and the Synchrotron Radiation Center also supported REU Sites involving 30 students.[2]

About 120 pre-college teachers participated in Research Experiences for Teachers (RET) activities at REU Sites, Centers and Facilities supported by DMR in FY 2001. These RET awards were funded primarily by the MPS Office of Multidisciplinary Activities.

[1] PHY-0097457
[2] http://www.nsf.gov/mps/divisions/dmr/research/c_reusites.htm

PERFORMANCE INDICATORS FOR PEOPLE

A. Summary Comments by the Committee of Visitors for the Division of Mathematical Sciences on the Performance of the Division for this Outcome Goal during FY 1998 – FY 2000:

a) Improved mathematics, science and technology understanding and skills for US students at the K-12 level;
b) Improved mathematics, science and technology understanding and skills for citizens of all ages, so that they can be competitive in a technological society;
c) A science and technology and instructional workforce that draws on the strengths of America's diversity;
d) A science and technology and instructional workforce that has global career perspectives and opportunities;
e) Globally engaged science and engineering professionals who are the best in the world; and
f) A public that is provided access to the processes and benefits of science and engineering.

Rating: **Successful in all categories**

"Within the constraints imposed by its tightly limited resources, the DMS has succeeded in having a positive impact on the mathematically trained workforce. By supporting researchers who in turn train postdocs and students, DMS is helping to create a community of mathematical scientists who in turn enrich mathematical education throughout the community. The well documented and worrying decreases in mathematical human capital at all levels clearly would have been more severe without these very creative efforts.

a. This is an important area in which more needs to be done. The NSF has funded conferences for high school teachers and a number of lectures at the high school and junior high school level (reported in the DMS Annual Report for FY 2000).

b. NSF programs we have reviewed contribute to a healthy mathematical atmosphere at undergraduate institutions (RUI, REU) and also to dissemination of mathematical ideas among scientists from other fields. Support of the Mathematical Sciences Institutes also contributes to public understanding of science and of mathematics in particular. Many expository lectures are placed on the World Wide Web for wide dissemination. MSRI has been especially innovative, with such programs as "Journalist in Residence", internships, "conversations with teachers," and the Bay Area Math Olympiad.

c. The POWRE program (to be replaced by ADVANCE) contributed to the professional development of women mathematicians. The success rate for applications of minorities in the individual grants is higher for minorities than in the general population (but the numbers are very small). Despite attempts to ameliorate the problem, our dominant impression is that the participation of minorities in research mathematics remains extremely small. The most relevant programs here are those that address the most junior people. However, the proportion of NSF applications from women remains much lower than the proportion of PhDs going to women. In contrast to the situation of minorities, the success rate for applications by women seemed if anything lower than the average.

d. The NSF program keeps US science at a global level. One of the ways it does this is to support US scientists traveling abroad to conferences and collaborations. Another very important mode is the support of many mathematicians in the United States who are not US citizens/permanent residents. This is an extremely important and forward-looking activity, which is essential for keeping US science at a global

standard. The programs IGMS[3] and GOALI[4] attempt to keep academic scientists connected with vital industrial mathematics and with sciences in which applications of mathematics are made. These two programs seem to have a hard time getting first-rate applications, and may need bolstering.

e. The NSF engages with other countries through its division of International Programs and in many activities within the DMS itself to keep US mathematicians well aware of global trends.

f. There are many isolated examples of public outreach programs that are providing access to the public of the benefits of mathematics research. For example, MSRI runs a Journalist-in-Residence program; hosts public programs such as "Mathematics in Arcadia; an interview with Tom Stoppard" (available on videotape); hosts many lectures (produced at MSRI and elsewhere, for example the Dartmouth CHANCE Lectures) for the public on its web site in the form of streaming video. Another good example is the film (now in production) being produced by Dan Rockmore (DMS-0086157). The panel felt that it would be good for the NSF to cultivate such things more systematically. A bureau providing press releases (as done by the physicists, by NASA, e.g. the Hubble telescope) could be very valuable (Curt Supplee, then at the Washington Post, now at NSF, has outlined what would be required for this at a conference on Math in the Media at MSRI in fall 1998; his lecture is available in streaming video on the MSRI web site). (NOTE: the references to MSRI are not intended to be exclusive; they merely represent the knowledge present on this panel.)"

B. Comments by the Committee of Visitors for the Division of Chemistry on the Performance of the Division for this Outcome Goal during FY 1998 – FY 2000:

"The Division is *successful* in its support of a diverse, internationally competitive and globally engaged workforce of scientists, engineers, and well-prepared citizens.

The Division supported 1400 graduate students and 514 postdoctoral students in FY2000. Diversity remains a problem for the academic chemistry profession. Approximately 33% of all chemistry Ph.D. degrees are granted to women. Only 12.5% of the senior faculty in science and engineering are women. In FY2000, 14% of the Division's principal investigators and co-principal investigators were women. This percentage has not changed substantially since FY1996. A similar situation obtains for minority researchers. While 11% of the U.S. population in 2000 were Hispanic and 12% African-American, only 2.2% of the PhDs in chemistry were awarded to Hispanics and 1.7% to African-Americans. In FY2000, 4.1% of the Division's principal or co-principal investigators were underrepresented minorities. The Division has done a good job of supporting women and underrepresented minorities in proportion to their representation in tenured or tenure-track academic positions. The chemistry academic community, the NSF and the Division of Chemistry have not developed ways of increasing the representation of women and minorities in these positions.

Two activities that the Division supports may in the long run help to improve this situation. The Division is an active participant in the Research Experience for Undergraduates (REU) program. In FY 2000 it supported 550 undergraduates at 56 sites in 33 states. Typically half of the undergraduate participants are female and over 21% are from underrepresented groups. The other activity is the Research Sites for Educators in Chemistry (RSEC) program. In this program, faculty at undergraduate institutions, including community colleges, are brought together with faculty from research universities to develop joint research programs and to bring the "culture" of research back to the undergraduate institutions. Many of these undergraduate institutions have large minority populations. Three awards were made in

[3] Interdisciplinary Grants in the Mathematical Sciences (IGMS)
[4] Grant Opportunities for Academic Liaison with Industry (GOALI)

FY1999 and a second round of competition will take place in FY2001. This activity has great potential but must be closely monitored to make sure that it accomplishes what it is designed to do.

In 1999, Isiah Warner of Louisiana State University (CHE-9942514) received the Presidential Award for Excellence in Science, Mathematics and Engineering Mentoring and was recognized by the American Association for the Advancement of Science with the Mentor Award for Lifetime Achievement as a "great teacher, mentor, and friend who affected the climate of a chemistry department and significantly increased the number of minority and underrepresented students pursuing and completing doctoral degrees." The Division supports Warner in the development of a comprehensive program in environmental chemistry and education at LSU and Southern University. Daniel Akins, City College of New York (CHE-9872777, 9616128) was the recipient of the Presidential Award for Excellence in Science, Mathematics and Engineering Mentoring in 2000 for his activities that have led to City College being one of the nation's leaders in providing PhDs to minority students."

On the following pages the Directorate for Mathematical and Physical Sciences presents highlights of some of the Fiscal Year 2001 activities focused on teachers, students, the public, and those young people who are likely to become the next generation of scientists. Together they effectively address all of NSF's Outcome Goals for People – to improve mathematics, science, and technology skills for US students and citizens, to create a workforce that reflects America's diversity, to provide the public with access to the benefits of scientific research, and to ensure that scientists are globally oriented.

Examples of MPS Directorate Performance for FY 2001

Indicator 1. Improved mathematics, science, and technology skills for U.S. students at the K-12 level and for citizens of all ages, so that they can be competitive in a technological society.

MPS Primary Area of Emphasis: Enhancing Instructional Workforce

Mathematics

- **High School Outreach.** Within the CAREER awards program DMS has funded the proposals of Ludmil Katzarkov of the University of California at Irvine[5] and Fedor Bogomolov of New York University[6] that support a secondary school outreach program in which they jointly participate. This year the program supports the CAREER award to Brian Conrad of the University of Michigan at Ann Arbor[7] that features a high school outreach program. This project also involved supervising a student who was a semi-finalist and a winner of the top mathematics prize at the Intel International Science and Engineering Fair (ISEF).

Chemistry

- **Research Sites for Educators in Chemistry (RSEC).** This Division of Chemistry program is completing its second cycle of awards in FY 2001. Initial awards were made in FY 1999. The aim of this program is to bring together faculty at undergraduate institutions (two-year community colleges, baccalaureate colleges, and master universities) with faculty at research universities for the purpose of enhancing the research and educational opportunities in chemistry at all participating institutions. In FY 2001, awards were made to establish three new RSEC programs, resulting in a current total of five such programs.

- Thomas McCarthy of the Polymer Science and Engineering Department at the University of Massachusetts at Amherst[8] and colleagues at Amherst College, Holyoke College, and Smith College have joined to form the core of this institution's new RSEC. Planned research themes are (1) rational heterogenation of homogeneous catalyst, (2) molecular imprinting of polymeric materials, (3) surface modification to control wettability and biocompatibility, and (4) control of protein adsorption through chemistry and topography. One of the goals of this RSEC is to increase the number of undergraduate

[5] DMS-9875383
[6] DMS-0100837
[7] DMS-0093542
[8] CHE-0113643

chemistry majors at all of the participating institutions by injecting polymer and materials chemistry into existing courses at all levels and by developing a one-semester course in polymer chemistry complete with notes and instructor's guide.

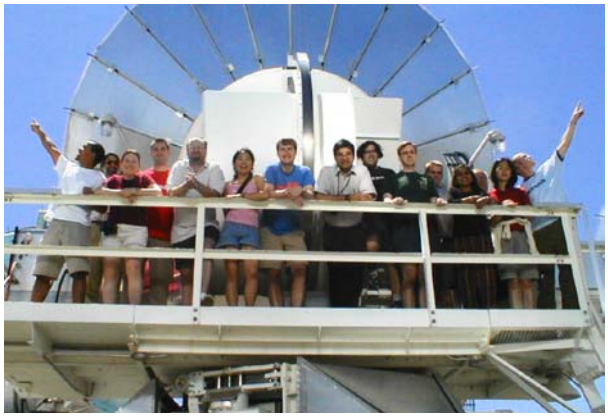
- Paul Rillema at Wichita State University (WSU)[9] of the third new RSEC will focus on approximately 30 two- and four-year institutions via the development of research collaborations. A second component of the WSU RSEC is a teacher training program for postdoctoral fellows who plan on being involved teaching and in research at two- or four-year institutions. A team of WSU faculty and the two- and four-year faculty participants will provide the training.

- The work of Michael Fitzgerald of Duke University[10] contains an exceptionally strong educational component through creation of a High School Science Teacher Outreach Program at Duke University. Fitzgerald is collaborating with the Office of Instructional Services at Duke and eight high school principals in the Durham public school system. The plan brings teachers to Duke University for a summer research experience and aims to provide them with the tools they need to enliven the high school science curriculum.

- Matthew Platz of Ohio State University[11] initiated a new course for local high school science teachers designed to update and enhance the participants' knowledge of chemical concepts and to improve the learning of chemistry in their classes. Twenty-two participants, including eleven women, were trained through laboratory and interactive lectures and problem-solving discussions.

Astronomy

- **Reaching out to Students and Teachers.** One example is the California Submillimeter Observatory (CSO) work with the University of Hawaii Hilo Upward Bound Program or the hosting of local Hawaiian associations and clubs. Another is the activity of the public outreach officer of the Owens Valley Radio Observatory (OVRO) in leading visits from local K-12 classes or his publication of astronomy articles for the local press.



Students at the June 2001 BIMA summer school pose on the platform of one of BIMA's 6.1m-diameter dishes.

The national astronomy centers are engaged in a wide variety of outreach and educational activities that reach a broad public. In FY 2001, the National Optical Astronomy Observatories (NOAO) began a new teacher education program that expands on the activities of their "Research Based Science Education" program with "Teacher Leaders in Research Based Science Education" (TLRBSE). This multi-year activity supported by NSF's Directorate for Education and Human Resources (EHR) is designed to train master teachers through workshops and other interactions at NOAO, who then train other teachers in their home schools and districts. The program provides encouragement and support to both experienced and novice science teachers in communities throughout the country.

[9] CHE-0113972
[10] CHE-0113972
[11] CHE-9909416

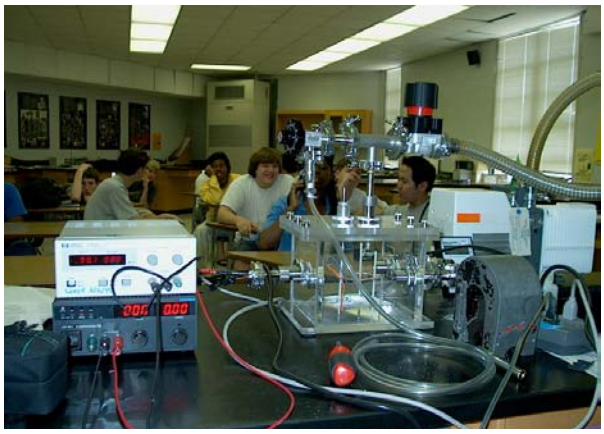
Physics

- **Physics Teacher Education Coalition (PhysTEC).** There is growing enthusiasm within the physics research community for making stronger connections with science education at the K-12 level. Through a joint effort led by F. Stein of the American Physical Society (APS)[12] the APS, the American Institute of Physics (AIP), and the American Association of Physics Teachers (AAPT), the Physics Teacher Education Coalition project (PhysTEC) was developed to address the national need for better-trained and educated physics and science teachers, and to strengthen the role of physics departments in teacher preparation. PHY, the Office of Multidisciplinary Activities, the Division of Materials Research within MPS, and the Education and Human Resources Directorate jointly fund the project. The influence of the professional associations will provide guidance for efforts at a set of selected Primary Program Institutions (PPI) to change the way courses for pre-service teachers are taught at the university level, and to build bridges between physics and education departments on these campuses.

LIGO Summer Undergraduate Research Fellowship (SURF) program

- **LIGO Research Experience for Teachers.** During the autumn of 2000, twenty-one teachers from Livingston Parish schools in Louisiana participated in the INTECH training program. INTECH is a program designed to help instruct teachers on the different ways of incorporating technology in the classroom and in their own educational methods. As part of the training, the teachers enjoyed a field trip to the LIGO Livingston Observatory. The purpose of the visit was to educate the teachers in LIGO's search for gravitational waves, to understand how gravity shapes the universe, and to learn a little about the science and technology that fuels LIGO's quest.

[12] PHY-0075528, PHY-0108787



Dusty Plasma Device Delights High School Students

- **Portable Dusty Plasma Device Delights Local High School Students.** Edward Thomas, Jr. of Auburn University[13] has developed a summer/academic year outreach program of high school students and teachers as part of his CAREER award. He has recently developed a small transparent (Plexiglas) vacuum system that is being used for some new dusty plasma experiments. The advantage of this chamber is that it is small and light enough to transport as a demonstration device. The pictures show the first time this new demonstration plasma device has been used in a high school classroom setting.

Materials Research

- At the National High Magnetic Field Laboratory's Center for Integrating Research and Learning,[14] signature programs, REUs, and RETs enable students to participate in authentic laboratory experiences. Forty-three teachers have been challenged to extend their understanding of how science is done in the real world and to create classroom materials for over 2,200 K-12 students.

- "This research experience provided me with the additional insight as to how I want to inspire my students towards a science career. The research projects gave me new ways in which to incorporate basic knowledge and techniques into my lesson plans. I was most impressed by the spirit of collaboration and the excitement of research that was exhibited by everyone I came into contact with. It was the sharing of ideas and information that made the biggest impression on me. This is the feeling I want to bring back to my students, that science is interesting, challenging and exciting." – Dara Stone, Chestnut Accelerated Middle School, Springfield, Massachusetts, a University of Massachusetts at Amherst MRSEC/RET participant.

Tech on Wheels. The MRSEC at Stanford/UC-Davis/IBM Almaden Research Center[15] collaborates with the San Jose Tech Museum of Innovation to bring the museum exhibits to nearby schools. The Tech on Wheels Van Project is a joint effort aimed at promoting materials science education in local elementary and middle schools. The van is used to transport to the local schools education modules that connect The Tech exhibit themes with materials science concepts. The activities in the modules are consistent with the California State science content standards for each grade.

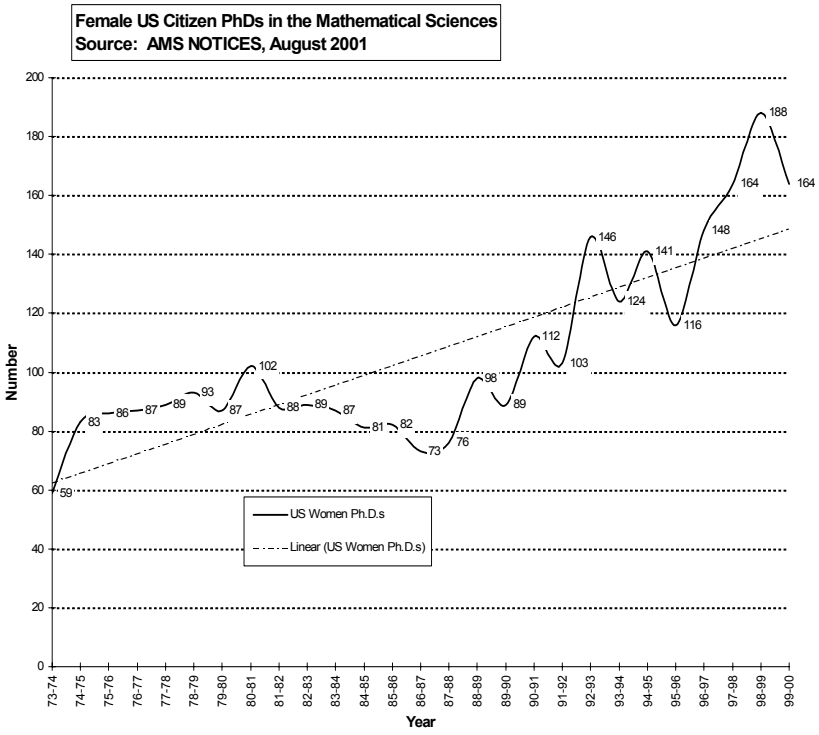
[13] PHY-0096254
[14] http://education.magnet.fsu.edu/
[15] DMR-9800354 and DMR-9400354 (http://www.stanford.edu/group/CPIMA/education/index.htm)

Examples of MPS Directorate Performance for FY 2001

Indicator 2. A science and technology and instructional workforce that reflects America's diversity

MPS Primary Area of Emphasis: Broadening Participation

Mathematics



- **Diversity.** Full participation of U.S. citizens, women, and members of minority groups continues to be a struggle in the mathematical sciences. However, as the above graph indicates, for the period 1973 – 2000, there is slow but steady progress (from ~60 to ~165) in the Ph.D. production of women in the mathematical sciences. An example of the results of efforts made by the Division to increase the participation of underrepresented groups is the Mathematical and Theoretical Biology Institute (MTBI) at Cornell University[16] directed by Carlos Castillo-Chavez. It continues to increase the number of underrepresented minorities attending graduate school in the mathematical sciences. Since its creation in 1996, 58% of the program's U.S. undergraduate students have enrolled in graduate or professional school programs.

- **Training of Undergraduates.** Maria-Carme Calderer of Pennsylvania State University[17] sponsored Zachary Battles in an REU project. Battles, who has been blind since infancy, graduated from Pennsylvania State University with three degrees and will be studying at Oxford University on a Rhodes Scholarship. He was featured earlier this year in an article in People Magazine.[18]

- **Conferences and Workshops.** Programs within the Division support special conferences on important computational topics and exploratory workshops on emerging research areas. The programs continues to strongly urge conference organizers to encourage and support the inclusion of members of

[16] DMS-9977919
[17] DMS-9704714, DMS-0042863
[18] *People*, **55**, No. 12, March 26, 2001, pp.81-82

under-represented groups as invited speakers, presenters of contributed papers, and, in general, as conference participants.

Chemistry

- **COACh.** The Committee on the Advancement of Women Chemists (COACh) consists of individuals who are concerned about the slow progress that is being made in reaching gender equity in professions in the Chemical Sciences. The Division of Chemistry, the Division of Chemical and Transport Systems, and the NIH National Institute of General Medical Sciences jointly fund COACh.[19] COACh has been formed to (1) identify and examine the barriers that are inhibiting the careers of women in the chemical sciences, (2) work to educate the community on gender equity issues in the chemical sciences, (3) effect change in institutions and organizations that have hampered the progress of women chemists, (4) actively promote women in pursuit of their career goals, and (5) train women in professional skills that will empower them to achieve their full career potential. The initial focus of the efforts of COACh is on advancing the careers of women chemists and chemical engineers in academia.

- **Mobile Chemistry Laboratory.** Gary Long and colleagues at Virginia Polytechnic Institute[20] have developed a Mobile Chemistry Laboratory (MCL) that in FY 2000 received initial startup support from the Division. A number of other private, public, and corporate funding sources also provide support. The current program expands the use of the MCL into more rural regions of southwestern Virginia and establishes two additional weeks of high school teacher workshops. In addition, a kit-based program will be developed for those high schools that have adequate laboratory space but limited budgets and equipment. Plans are to continue to develop the curriculum they initiated in 2000, and increase efforts to recruit high school teachers from underrepresented areas.

- **Research Sites for Educators in Chemistry (RSEC).** Jeffrey Roberts at the University of Minnesota[21] leads this institution's RSEC program, which is oriented around four interdisciplinary areas: chemical biology, computational chemistry, environmental chemistry, and materials chemistry. The RSEC leadership team plans to recruit a group of approximately 20 undergraduate chemistry departments as RSEC participants. Recruitment plans include partnering with the "Native American Undergraduate Fellows" program at the University of Minnesota to encourage the participation of regional minorities, and special efforts to include the participation of community college faculty.

[19] CHE-0078913
[20] CHE-0111501
[21] CHE-0113894

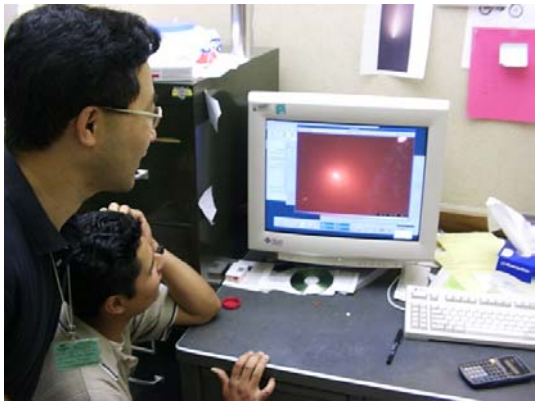
- **International REU Site.** An international REU site at the University of Florida is under the direction of Randolph Duran.[22] More than 20 faculty from French institutions are available to serve as REU mentors for U.S. students. Each summer ten students travel to France to participate in a 10-12 week program at several French institutions, including the Université Pierre et Marie Curie, the University of Montpellier, the Centre Nationale de la Recherche Scientifique (CNRS), and the University of Strasbourg. (Through French funding, a similar number of French students, recruited from the same institutions, will be doing summer research at the University of Florida.) Recruitment efforts will extend nationwide, targeting more then 80 institutions with noted minority enrollments. Student research topics center on materials chemistry. A mid-program science workshop affords students the opportunity to hear one or two lectures on a focused topic and to interact scientifically. The student participants see research performed in a different manner and within a different cultural context from the traditional U.S. model. Student participants conclude the program with a project summary presentation at the French institution where the research is being done. An enhanced evaluation of the program takes the form of a longitudinal study via interviews and surveys aimed at examining the impact the international experience has on students' career choices and cultural attitudes.

Astronomy

The REU sites supported in AST play a crucial role in providing a science and technology workforce that reflects America's diversity. For example, of the 125 undergraduates supported in FY2001, fully 50% of them were women, and 15% were from members of underrepresented minorities.

- **Research Experiences for Undergraduates.** Many REU students change their educational and career plans as a result of the positive experiences they have during their REU programs. As an example, two students, Melvin Thomas and Vincent Davis, participating in the REU program at the Kitt Peak National Observatory, were recently featured in the Arizona Daily Star, where they said that their project, hunting for asteroids, has had such a profound effect on them that they plan to enter astronomy as a result. "I've always been a lover of the stars, but this project alone has convinced me I want to go into astronomy," said Davis, a junior majoring in physics at Elizabeth City State University in North Carolina.

- **Asteroid is a Comet.** Three students working as a part of the California State University at Los Angeles[23]-led Consortium for Undergraduate Research Experience (CURE) found that a recently discovered asteroid is in fact a new comet. CURE focuses on bringing REU opportunities to minority students in the Los Angeles area.[24] The students made their discovery while working at the JPL Table Mountain Observatory tracking near-Earth asteroids. The precise determination of the



[22] CHE-0131446
[23] AST- 9820546
[24] http://AstroMm.calstatela.edu/cure/

comet's position shows that the yet unnamed comet orbits the Sun every 7.7 years on a very elongated orbit. The unusual orbit for the comet suggests that it was once a distant member of the solar system that was recently deflected by Jupiter to a closer and tighter orbit, and that it represents an opportunity to learn about the composition of the primordial solar nebula.

Physics

- The REU site specifically directed by Robert Thews at the University of Arizona[25] targets the local population attending community colleges. The site directed by Joseph Becker of San Jose State University[26] targets non-traditional students. All REU sites make special efforts to attract participants from groups traditionally underrepresented in physics.

- **LIGO Research.** At Southern University[27] (SU), a historically black university (HBCU) located in Baton Rouge, Stephen McGuire has developed a program that integrates research in advanced detector development for LIGO, a research program in gravitational physics for SU students, and an outreach program. The advanced detector research and development focuses on the study of impurities in optical systems of interest to LIGO. The group will also study to correlate gamma-ray bursts with gravity waves that LIGO expects to observe when its sensitivity is extended to detect events at cosmological distances. The relative proximity of SU to the LIGO site at Livingston, Louisiana Observatory greatly enhances the outreach program since SU students will have access to research projects at the site while they are enrolled in classes at SU.

- **Pion Lifetime and Quantum Chromodynamics.** A group at Hampton University[28] (HU), an HBCU located in Hampton, Virginia is a short distance from the Thomas Jefferson National Accelerator Facility (JLab). It is leading a very high priority experiment at JLab designed to test the Standard Model of elementary particles by making a precise measurement of the pion lifetime. They will also compare the pion lifetime with calculations based on the full theory of the strong interaction–Quantum Chromodynamics. The HU group received a Major Research Instrumentation[29] award in FY 2000 to fabricate the detector needed for this measurement. They have successfully implemented a longer-range construction project for central elements of the Large Hadronic Collider (LHC) ATLAS detector. The detector is designed to search for the Higgs particle – a particle believed to be closely linked to the mass spectrum of all elementary particles. The HU group also competed successfully for one of the new Physics Frontiers Centers.[30] This Center will help other HBCU faculty and students make contributions at the frontiers of particle and nuclear physics

Materials Research

- **Minority Research Planning Grants (MRPG)** enable new minority faculty to jump-start their research and obtain preliminary results they can build upon. Theodore Goodson just completed a very successful MRPG at Wayne State University[31] in which he studied the photodynamics of polymers. As a result, he published papers in *Phys. Rev. B, J. Phys. Chem.*, and *Chem. Phys. Lett.*, with additional papers in press in *J. Appl. Phys*. and *Macromolecules*. He trained one MS and two undergraduate students and had Detroit high-school students work in his laboratory.

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[25] PHY-9987664
[26] PHY-9988064
[27] PHY-0101177
[28] O. Baker, K. McFarlane, PHY-0072686
[29] A. Gasparian et al., PHY-0079840
[30] C. Keppel et al., PHY-0099540
[31] DMR-9908418

- **Collaboratives to Integrate Research and Education (CIRE).** The Division supports two Collaboratives to Integrate Research and Education, one between the University of Puerto Rico at Humacao[32] and the Materials Research Science and Engineering Center (MRSEC) at the University of Pennsylvania,[33] and the other between Florida A&M University[34] and the MRSEC at Carnegie Mellon University.[35] The Collaboratives are designed to improve minority education in materials-related areas by using both the human and practical resources of the MRSECs to establish joint research programs and sponsor summer exchange programs. A new Masters program in materials physics, the first graduate program at UPR-Humacao, has been developed through the collaboration with the University of Pennsylvania. The annual University of Pennsylvania-UPR CIRE meeting was held in Puerto Rico in October 2000.[36] The meeting featured Alan MacDiarmid who gave an inspirational talk to over 400 undergraduate and high school students in Humacao. This was the first meeting MacDiarmid attended after he was recognized with the 2001 Nobel Prize in Chemistry earlier that month.


EL ORIENTAL

Deportes

En suelo humacaeño Premio Nobel de Ciencia

Inauguran Terminal Sur de Humacao

Municipio de Yabucoa adquiere Teatro San Rafael

Pequeñanpor condiciones de escuela Rufino Vigo

[32] DMR-9872689
[33] DMR-0079909
[34] DMR-9982872
[35] DMR-0079996
[36] http://www.lrsm.upenn.edu/lrsm/outr.html#CIRE

Examples of MPS Directorate Performance for FY 2001

Indicator 3. Globally engaged science and engineering professionals who are among the best in the world.

MPS Primary Area of Emphasis: Broadening Participation

- **Nobel Prize.** The 2000 Nobel Prize in Chemistry[37] was awarded to Alan Heeger of the University of California at Santa Barbara,[38] Alan McDiarmid of the University of Pennsylvania,[39] and Hideki Shirakawa of the University of Tsukuba "*for the discovery and development of conductive polymers*." Alan Heeger has been a grantee in the Division of Materials Research for many years. His research has focused on the photophysics of conducting polymers. The Divisions of Materials Research and Chemistry supported both Heeger and McDiarmid through individual grants since the 1970s when their work on conductive polymers began. Research into electroactive polymers has brought forth plastic transistors, light-emitting diodes, lasers and other photonic devices, as well as applications such as "electronic paper." The work of chemists such as MacDiarmid and others laid the groundwork for the area that is now known as nanoscience, a strategic priority area for the NSF.

Henry R. Glyde of the University of Delaware[40] received the *John Wheatley Award* for his "*enduring commitment and multifaceted contributions to the development of physics in Thailand, which include innovative creation of scientific links between North American research universities and Chulalongkorn University, inspiring collaboration with leading Thai physicists, and the marshaling of financial and intellectual resources to establish new regional research centers.*"

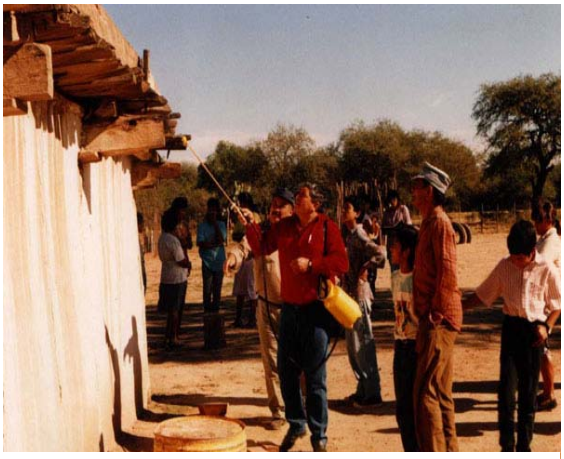
Terence Langdon of the University of Southern California[41] was awarded the *Henry Marion Howe Medal* for 2000 by ASM International, and in 2001 he was awarded a Senior Fellowship by the Japan Society for Promotion of Science for his collaborative research with colleagues at Kyushu University in Japan.

Mathematics

- **U.S. - Canada Partnership.** A new U.S.-Canada partnership to establish a mathematics research station in Banff, Alberta was announced this year.[42] The NSF is providing $1,270,000 to support U.S. participation in the project. The Banff facility will provide a world-class venue to form collaborations, advance research and share information on developments in mathematics research throughout North America. NSF's participation reflects its pledge to increase Federal investment in the fundamental mathematical sciences, which underlie all science and engineering discovery.

[37] http://www.nobel.se/chemistry/laureates/2000
[38] DMR-9730126, DMR-0099843
[39] CHE-7702207
[40] DMR-9972011
[41] DMR-0093011
[42] DMS-0124838

- **Mathematical Model of Chagas Disease.** Joel Cohen of Rockefeller University and Columbia University[43] and his colleague Ricardo Gürtler of the Universidad de Buenos Aires have identified improved control tactics for a vexing public health problem. American trypanosomiasis, or Chagas disease, caused by the protozoan parasite *Trypanosoma cruzi* and transmitted by blood-feeding triatomine bugs, is a chronic, frequently fatal infection that is common in Latin America. Neither adequate drugs nor a vaccine are available. A mathematical model, developed by these researchers, calibrated to detailed household data from three villages in northwest Argentina, shows that householders could greatly reduce the risk of human infection by excluding domestic animals, especially infected dogs, from bedrooms, removing potential refuges for bugs from walls and ceilings, and by using domestically applied insecticides. The mathematical model makes it possible to do computational experiments that could not be done ethically in a real household and shows how simple and inexpensive methods for disease prevention can be provided. This research was featured in an article in Nature.[44]



People being shown how to spray to reduce bugs.

- **International Mathematical Olympiad**. The United States hosted the 42nd International Mathematical Olympiad (IMO) this year.[45] The IMO was last held in the U.S. in 1981. This prestigious event brought approximately 500 of the most talented high school age mathematicians from more than 80 countries to the U.S. The Olympiad was held in Washington, DC, with opening ceremonies held on July 4, 2001 and closing ceremonies held on July 13, 2001. The American mathematics community used this opportunity to promote the importance of mathematics for all students and celebrated the accomplishments of our best and brightest students. During the competition students worked individually over a two-day period on six challenging problems and presented their solutions as essay-style proofs akin to those produced by research mathematicians. While the grading of the papers took place the IMO students were treated to American hospitality, visiting attractions in and around the capital and experiencing American life and culture.

Chemistry

The Division continues to develop contacts with chemistry funding agencies in Europe and the Pacific Rim. The Division organized an informal planning meeting of agency representatives from Pacific Rim countries at the December 2000 Pacifichem meeting in Hawaii. Representatives from China, Taiwan, Canada, Korea, and Japan attended this meeting. The purpose was to identify areas and means for improving international collaborations among Pacific Rim countries.

- **Some Comments from Division of Chemistry COV.** "The REU includes experiences for foreign students in the US and for US students in foreign countries. The NSF rigorous peer review process does an outstanding job of funding excellent, world-class researchers in TCC & EPC. Their global

[43] DEB-9981552 (Systemic and Population Biology award, co-funded by Applied Mathematics and Computational Mathematics)
[44] *Nature*, **293**, July 27, 2001, pp. 694-698
[45] DMS-9977906 and DMS-0097092

engagement is highly apparent in their representation in international publications, conferences, workshops, and scientific collaborations.

a. Area of inorganic organometallic and bioorganic supported by NSF is strong by international standards. Many PI's within the IBO program have traveled to international meetings and maintain close scientific relationships with colleagues throughout the world. Even stronger ties, involving collaboration, are maintained by others. Examples:
Brian Hoffman (0091364), Northwestern (collaboration with A.G.M Barret, Imperial College): The PI exploits a long and fruitful collaboration with Barret in England. Jointly they pursue the synthesis of porphyrazine-ligated metal complexes with potential applications to biomedical imaging, optical sensors, and chiral separations/catalysis.
James Ibers (0041354), Northwestern (collaboration with Vladimir Ferorov in Novosibirsk, Russia). The PI is collaborating with Ferorov in Russia on the synthesis of soluble metal selenides and tellurides. Ibers requested an International Supplement to cover travel expenses for exchange visits for scientists between the two labs.

b. ASC/AMP-supported PIs have won internationally recognized chemistry awards (8 in FY 2000 alone)."

- **Anharmonicity in Molecular Vibrations.** Janet Del Bene of Youngstown State University[46] and Dr. Meredith Jordan of the University of Sydney (Australia) are studying anharmonicity in molecular vibrations with a view to increasing our understanding of hydrogen bonding and the interpretation of infrared spectra in systems ranging from condensed water to complex biomolecules. This work is providing more powerful tools for examining hydrogen bonding in a variety of chemical and biological systems.

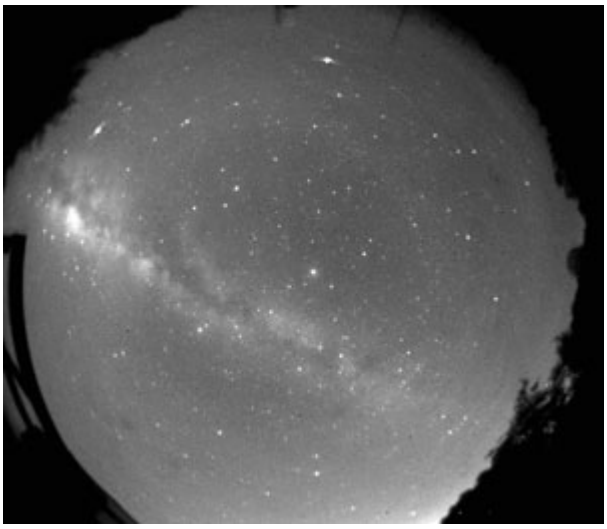
- **GOALI.** Through the GOALI mechanism one post-doctoral fellow in Nicholas Farrell's group at Virginia Commonwealth University,[47] Holger Rauter, spent a six-month period in the laboratories of Boehringer Mannheim Italia (BMIt) studying the industrial approach to compound synthesis and drug development. In a return visit, an employee of BMIt, Dr. DeCillis, spent three weeks in Farrell's laboratory at VCU studying molecular modeling.

- **Small Angle Neutron Scattering (SANS) Studies of Nanodroplet Aerosols.** Barbara Wyslouzil and her associates at Worcester Polytechnical Institute,[48] Rinehard Strey of the University of Cologne, Gerry Wilemski of the University of Missouri-Rolla, and John Barker of NIST Center for Neutron Research (NCNR) / Center for High Resolution Neutron Scattering (CHRNS) have recently made the first definitive scattering measurements on the nucleation and growth of binary fluid nanodroplets. By continuously forming droplets *in-situ* by expansion in a supersonic nozzle inserted in the SANS sample chamber, they have obtained data on the internal structure of binary fluid nanodroplets needed to test current theories in atmospheric physics. For example, their measurements on deuterated alcohol/water mixtures clearly show that the alcohol concentrates in the surface regions of the droplets before they reach 100 nm in size, a result that will help refine realistic models for chemical reactions in the atmosphere.

[46] CHE-9873815
[47] CHE-9615727
[48] CHE-9729274

Astronomy

- **Rooftop Cameras.** In a project led by CAREER awardee Robert Nemiroff of Michigan Technological University,[49] anyone with web access can view the night sky live through a wide-angle lens, thanks to rooftop cameras being installed at astronomical observatories in the United States and overseas. The cameras, dubbed CONCAMs, create a continuous record of the sky that allows astronomers, as well as students and teachers, to track changes over time. The first instrument, installed at NSF's Kitt Peak National Observatory in Arizona, has been recording the night sky since May 2000 and has documented several unanticipated events, including the spectacular March 31 2001 auroras, rarely seen so far south. Another CONCAM is operating at Mauna Kea in Hawaii, and others are planned for Mt. Wilson Observatory in California and for Utah, Israel and Argentina.[50] Scientific objectives of the CONCAM project include the tracking of bright stars and highly variable phenomena such as novae, supernovae, optical counterparts to gamma-ray bursts, while for observers they provide valuable information about weather and seeing conditions. CONCAM images are uploaded soon after being acquired to a publicly accessible web page and are considered public domain immediately upon recording.

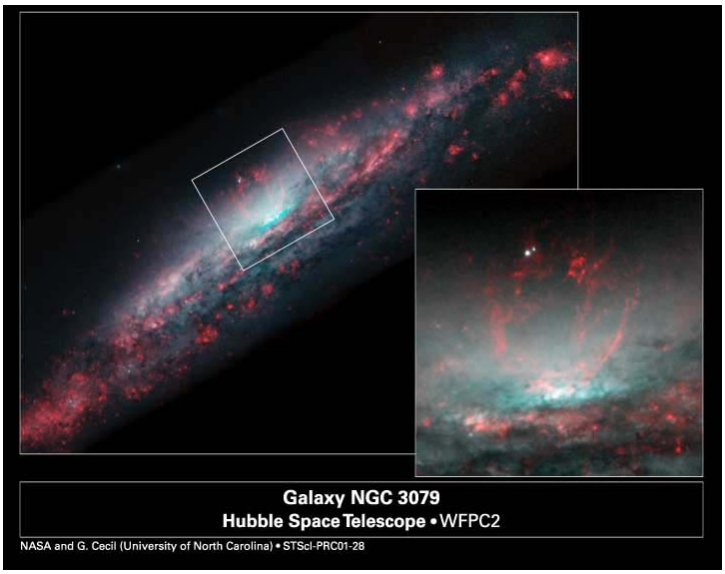


- **Pulsars.** Victoria Kaspi of the Massachusetts Institute of Technology,[51] using her CAREER award, has been involved in the Australian Parkes Multibeam Survey, the most successful radio pulsar search and discovery project ever undertaken, which has discovered nearly 650 new radio pulsars. While its primary goal is an understanding of the Galactic population of neutron stars, the discovery of individual objects has led to significant results in FY 2001. For example, her discovery, with collaborators, of two objects with the largest magnetic surface fields ever observed in radio pulsars has demonstrated that radio emission can be produced in such fields, and blurred the lines between conventional radio pulsars and the exotic hypothesized 'magnetars.' The result may have major implications for the population as a whole, as it opens up the range of parameters in which young neutron stars can exist. The discovery of a young radio pulsar in a relativistic binary orbit, most likely with a white dwarf star, is the first example in which the companion is unlikely to be another neutron star. This source is especially interesting because, after monitoring for several years, it will allow the precise determination of the mass of a young neutron star, as well as precise tests of general relativity.

- **Superwinds in Active Galaxies.** CAREER awardee Sylvain Veilleux of the University of Maryland[52] has made very good progress on his studies of superwinds in active galaxies and galactic fountains in normal galaxies. In the latter project, in collaboration with graduate student Scott Miller, he is working to determine the extent, origin, and source of the ionization of the material that is seen well out of the plane in normal spiral galaxies. By studying a sample of edge-on spirals they have learned that the mass and extent of the warm extra-planar material is correlated with the local star formation rate in the

[49] AST-9701716
[50] http://www.concam.net
[51] AST-9875897
[52] AST-9874973

disk, and photoionization by hot, massive OB stars appears to be the primary source of the ionization. It appears that an additional source previously thought necessary is required in only a few galaxies. His work on superwinds in active galaxies, in collaboration with Gerald Cecil of the University of North Carolina at Chapel Hill, Joss Bland-Hawthorne in Australia, and Alex Filippenko of the University of California at Berkeley, looks at the effects these powerful events have on the host galaxies and the surrounding environment. Ground-based Fabry-Perot data are combined with radio and X-ray data and Hubble Space Telescope images to track the energy flow through various gas phases. The data show spectacular ionized filaments on the outskirts of the host galaxies, sometimes extending well beyond the HI extent that normally defines the galaxy extent, as in this image of NGC 3079.



Sodium laser tests from Cerro Tololo Inter-American Observatory. These tests are part of a joint effort by Gemini, CTIO and ESO to characterize the seasonal variations in the atmospheric sodium layer in preparation for adaptive optics laser guidestar systems like Gemini's Altair and the planned Multi-Conjugate system currently being designed by Gemini.

- **Pulsars at Low Frequencies.** Joanna Rankin of the University of Vermont observes pulsars at very low frequencies.[53] Images map a pulsar's emission pattern produced several hundred kilometers above the 10-kilometer (radius) star's 300-meter magnetic polar cap. The low frequency observations, when compared with those of higher frequencies, reveal the trajectories of relativistic particles above the star. Rankin collaborates with several Russian radio astronomers in the work and the Division of International Programs also supports the award.

Laser Guide Stars. NSF serves as the executive agency for the Gemini Observatories, an international project with seven partner nations (the U.S., the United Kingdom, Canada, Australia, Chile, Brazil and Argentina). The Gemini Observatories consist of two 8-meter telescopes, one located in the southern hemisphere in Chile, and one located in the northern hemisphere in Hawaii. NSF provides 50% of the funding, enabling merit-based access for the U.S. national community to both telescopes. The project has also played a pivotal role in sodium laser tests sponsored by Gemini, the Cerro Tololo Inter-American Observatories, and the European Southern Observatory. Designed to characterize the annual variations in the sodium layer of the atmosphere, this work is critical to the development of sodium laser systems to be used

[53] AST-9986754 and AST-0098685

in Gemini's adaptive optics systems such as Altair (upgrade) and the Multi-Conjugate Adaptive Optics system currently under development.

- **Gemini Fellowships Program.** AST provides funding for the Gemini Fellowships program that brings postdoctoral scholars from the Gemini partner countries of Argentina, Brazil, and Chile to U.S. institutions on research fellowships. AURA, Inc. also has a program, in cooperation with Fondacion Andes, to provide opportunities for Chilean graduate students to pursue doctoral degrees in the U.S. Both of these programs serve to strengthen both the astronomical communities of our partner countries and the U.S. scientific community.

- **International Conference.** Other initiatives at the Gemini Observatory in FY 2001 have included a very successful scientific conference "*Astrophysical Ages and Time Scales*" that was held in Hilo, Hawaii and represented a partnership between Gemini and several other Mauna Kea observatories. The conference was considered a huge success by all involved and attracted over 160 astronomers from around the world who met for 5 days in late February 2001.

- **Advanced Solar Technology Telescope.** The National Academy of Sciences Decade Review listed the highest priority ground-based facility among the "moderate" initiatives to be a large-aperture, advanced solar telescope, now called the Advanced Technology Solar Telescope (ATST). During FY 2001, the National Solar Observatory (NSO) led preparation of a proposal involving collaborators from 19 US institutions and 5 foreign nations for a five-year design and development phase of the ATST.[54] The Astronomy Division and the Division of Atmospheric Sciences jointly funded the proposal. Six site testing telescopes (Solar Differential Image Motion Monitors) were constructed at Sunspot, and deployment began for sites throughout the world, with the first going to Sacramento Peak, Big Bear, and La Palma. A two-year site survey will select the optimal location for the ATST.

- **Solar Adaptive Optics.** NSO also collaborated with the New Jersey Institute of Technology, the Air Force Research Laboratory, and the Kiepenheuer Institute (Germany) to initiate, in FY 2001, an effort partially funded within NSF's Major Research Instrumentation program for the next step in development of higher-order solar adaptive optics.[55] This will construct cameras for use on the Dunn Solar Telescope, the Big Bear Solar Telescope, and the planned GREGOR telescope on Tenerife, in the Canary Islands.

- **Atacama Large Millimeter Array (ALMA).** AST is also involved in the Atacama Large Millimeter Array (ALMA) project. This project plans to place a new radio facility in the Atacama desert of northern Chile. Originally conceived as The Millimeter Array (MMA), ALMA design and development has become a partnership between the NSF's National Radio Astronomy Observatory (NRAO) and a European consortium consisting of the European Southern Observatory (ESO) and funding organizations from France, Germany, the Netherlands, Spain, Sweden, and the United Kingdom. ALMA construction is envisioned as an equal U.S.-European partnership, with the likelihood of Japan as a third equal partner. ALMA is intended to study the origins of galaxies, stars, and planets by observing the gas from which these objects form.

Physics

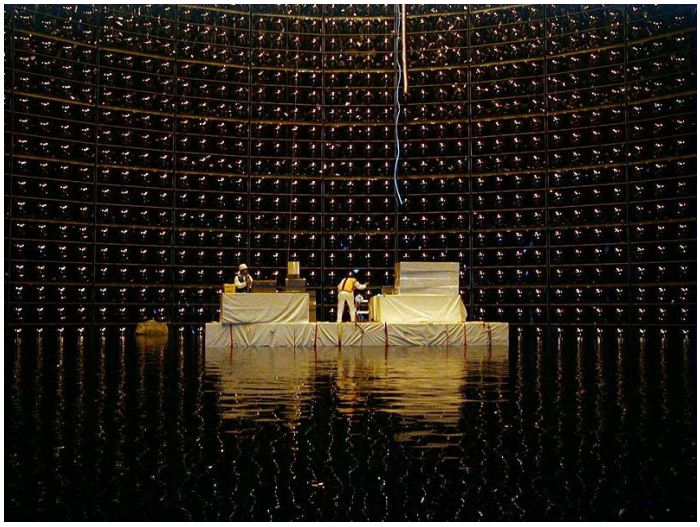
- **Gravitational Wave Detectors.** NSF is the lead agency in the U.S. for ground-based gravitational physics. NSF is actively supporting cooperation between U.S. researchers in other countries that are constructing gravitational wave detectors to form a worldwide network linking such detectors: LIGO

[54] http://www.sunspot.noao.edu/ATST/index.html
[55] http://www.sunspot.noao.edu/AOWEB/

(U.S.), VIRGO (Italy), GEO (Germany, Scotland), TAMA (Japan), and AIGO (Australia). In addition, NSF is actively involved in cooperative support (with GEO and VIRGO) for research and development towards next-generation detectors to enhance the capabilities of these facilities.

- **Large Hadron Collider.** NSF and the Department of Energy (DOE) have joint responsibility for the U.S. part of the U.S-CERN Large Hadron Collider (LHC) construction project. However, for the purpose of negotiation, DOE is the lead agency. In terms of international collaborations, NSF plays a lesser role in funding large detectors than DOE, but, nonetheless, an important role in support of individual investigators. The total US contribution will be $531 million, including $450 million from the DOE.

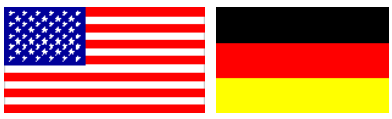
- **Pierre Auger Cosmic Ray Detector.** Another example is the Pierre Auger cosmic ray detector project designed to detect ultra-high-energy cosmic rays. This is a multinational effort in which NSF and DOE are contributing equally to the construction costs. The U.S. costs will be $15 million, about 15% of the total. NSF and DOE share the responsibilities for oversight of the US part, with neither agency designated as lead. NSF-supported researchers are leading this project.



- **Super-Kamiokande Neutrino Detector Observes Flavor Oscillations**: Super-Kamiokande is a 50-kiloton water-Cerenkov detector located at a depth of 1500 meters in the Kamioka-Mozumi mine of Japan. The detector was designed to explore neutrino properties by making high statistics measurements of neutrinos produced in the atmosphere by high-energy cosmic rays and neutrinos produced in the nuclear reactions of the sun. It is also the world's most sensitive detector for proton decay. Data obtained using this detector has included the first convincing evidence for neutrino oscillations and non-zero hence neutrino mass, using the atmospheric neutrino sample, and better then 3-sigma evidence for solar neutrino oscillations. A group led by G. Sullivan of the University of Maryland[56] is part of the Super-K collaboration and has successfully developed and deployed a new calibration source that has significantly reduced the main systematic error in the solar neutrino measurement. Undergraduates are involved in the project as well. There are currently two undergraduates in residence in Japan helping with the current upgrade to the detector.

Materials Research

- **International Interactions.** DMR continued to sponsor a broad spectrum of workshops in FY 2001. Many of these bring together scientists and engineers from different parts of the world and include a significant



[56] PHY-9816963

focus on questions of workforce and human development. One example is the bi-national U.S-Germany Workshop on Polymers[57] organized last year by Colleen Pugh and Wes Burghardt.[58] Speakers in this highly prestigious workshop are young researchers (usually at the Assistant Professor level) who can attend only once, so that each meeting is infused with the ideas of a new generation of scientists who usually go on to establish long-standing interactions.

- **International Conferences.** Various NSF funds are used to facilitate international collaborations through attendance at conferences overseas by US researchers or the attendance by foreign researchers at conferences held in the US. Examples of the former are the Aspen Conference Winter Workshop in Condensed Matter Physics where the topic was High Temperature Superconductivity,[59] the Gordon Research Conference on Condensed Matter Physics: Soft Condensed Matter,[60] and the Conference on Local and Nanoscale Structure in Complex Systems.[61] Opportunities to explore collaborations were provided by joint support to the Enrico Fermi ISP Summer School on High-Pressure Phenomena held in Varenna, Italy;[62] the Inter-American Workshop of the Use of Synchrotron Radiation for Research, a Symposium on Nanotechnologies held in Campina, Brazil;[63] and the 2001 International Conference on Strongly Correlated Electron Systems held in Ann Arbor, Michigan.[64]

- **U.S – Africa Cooperation.** Over the past six years DMR has co-sponsored a series of workshops in different regions of the world with the goals of identifying specific areas and future directions for cooperation between US and foreign investigators in materials research and education, and to begin the development of a Materials World Net for international communication in the field of materials. Several of the workshops are now bearing fruit. An NSF Dear Colleague Letter issued in FY 2000 and updated in FY 2001 describes opportunities for cooperative activities in materials research between European and US researchers to be supported by NSF and the European Community. DMR plays a leading role in this partnership, which involves three NSF Directorates together with the European Community Growth Programme. Five NSF awards were made this year and more than 30 additional proposals are under review in the current phase of the competition. NSF and its counterpart agencies in Canada, Mexico, and South America are now actively exploring comparable arrangements for international cooperation. NSF and national funding agencies in Europe are also exploring such arrangements. This would complement the NSF-European Community interaction. A workshop held in South Africa last year to address opportunities for US-African cooperation in materials research and education has already stimulated the development of regional materials networks in Africa.

- **Collaborations.** Examples of projects with co-support from NSF's International Division allow experiments to be conducted with unique facilities. Bogdan Dabrowski of Northern Illinois University[65] uses unique facilities in Switzerland to make muon spin rotation measurements. Himanshu Jain of Lehigh University[66] works with researchers in England.

[57] http://www.chem-org.nwu.edu/us-germany/usg-objectives.htm
[58] DMR-0080058
[59] DMR-0098816
[60] DMR-0113186
[61] DMR-0118222
[62] INT-0118576
[63] DMR-0094781
[64] DMR-0109063
[65] DMR-0105398
[66] DMR-9816402

- **Diversity and International Cooperation at the Frontier of Nanoscale Science and Engineering.** Mildred Dresselhaus' research group at the Massachusetts Institute of Technology[67] is engaged in nanostructural studies of carbon, bismuth and other materials. In addition to its outstanding research achievements, the group provides a fascinating example of the human side of materials research. Supported by the NSF grant are: Marcie R. Black, Electrical Engineering and Computer Science (EECS) graduate student; Sandra D. M. Brown, Physics graduate student (received Ph.D. June, 2000); Yu Ming Lin, EECS graduate student; Antonio G. Souza Filho, visiting Physics graduate student from Brazil (Brazilian Fellowship at MIT); Ado Jorio de Vasconcelos, Postdoc (Brazilian Fellowship with a supplement from NSF); Noriko Yoshizawa, Postdoc (Japanese Fellowship). Marcie Black and Dr. Yoshizawa are women and Dr. Brown is an Afro-American woman. Yu Ming Lin is an MIT graduate student in EECS from Taiwan. Dr. Vasconcelos is supported in part through an NSF-sponsored exchange program with Prof. Marcos A. Pimenta of the Federal University of Minas Gerais in Brazil. Antonio Souza Filho is a visiting graduate student from the Federal University of Ceara. Sandra Brown was partly supported by a fellowship from Lucent Technologies. NSF's Division of International Programs supports the group's interactions with Japan and Brazil.

- **NSF and the European Community.** The first two NSF-European Community projects with "new starts" on both sides of the ocean were jointly funded in FY 2001 (Carlos Levi, University of California at Santa Barbara[68] and Carter of the Massachusetts Institute of Technology[69]) by DMR, the Office of Multidisciplinary Activities and NSF's International Division. These projects involve four European countries in total (England, France, Germany and Sweden).

[67] DMR-0116042
[68] DMR-0099695
[69] DMR-0010062

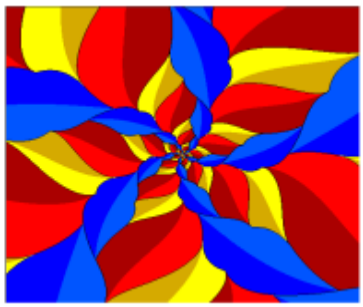
Examples of MPS Directorate Performance for FY 2001

Indicator 4. A public that is provided access to the benefits of science and engineering research and education

MPS Primary Area of Emphasis: Broadening Participation

Mathematics

- **Research Experiences for Undergraduates (REU).** In January 2000 the Department of Mathematics at the University of Maryland created the Experimental Geometry Lab, a research laboratory directed by William Goldman[70] and Richard Schwartz[71]. This laboratory supports research in geometric structures using experimental techniques. It houses more traditional mathematical materials such as models as well as computers, and maintains a web page[72] from which games, software and demos may be downloaded. It has been a vehicle for outreach to the general public as well as an invitation to prospective mathematics students. One game illustrates Galois theory by reflecting the sides of a regular pentagon and is available on the Wide World Web. Goldman and Schwartz, working closely with the University of Maryland's Undergraduate Research Assistant Program, have directed several undergraduate research experiences. Next year they plan to integrate experimental projects into the undergraduate course "Differential Geometry of Curves and Surfaces."



Construction of a hyperbolic 3-manifold bounding a complex hyperbolic 4-manifold.

Chemistry

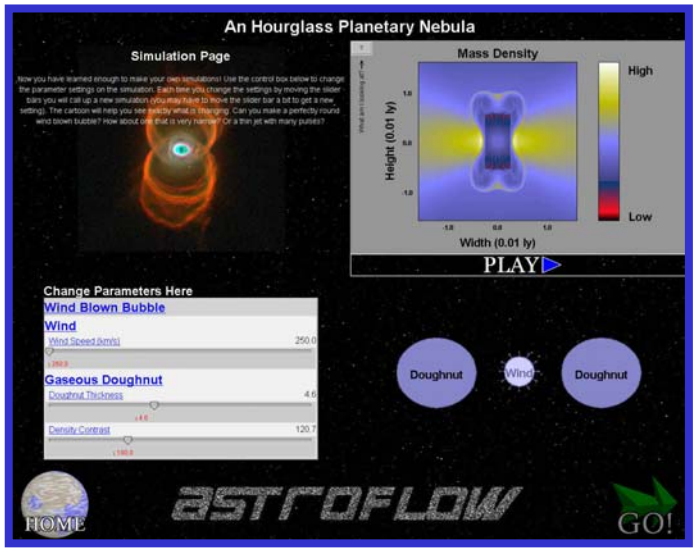
- **Identifying Molecules Remotely.** Michael Jackson of the University of Wisconsin at La Crosse[73] is studying high-resolution absorption spectroscopy. This molecular spectroscopy provides a way of both detecting and identifying molecules remotely and of determining their fundamental internal properties. Two of his undergraduate research students, Heidi Hocket and Michael Lauters, were selected in a national competition to participate in a poster session on Capitol Hill sponsored by the Council on Undergraduate Research. The event featured scientific and engineering research

[70] DMS-0103889
[71] DMS-0072607
[72] http://www.umd.edu/~res/egl
[73] CHE-0078812

conducted by undergraduates from across the country. The Hocket-Lauters poster was entitled "*Discovery and Investigation of Optically Pumped Laser emissions from Methanol Isotopes in the far-Infrared.*" They carried out some of their work at the National Institute of Standards and Technology in Boulder, Colorado in collaboration with Dr. Ken Evenson and Dr. Mike Allen. The figure illustrates Michael Lauters (left), Heidi Hocket, and Rep. Mark Udall (D-CO) discussing the Hocket-Lauters poster in the Rayburn Building on March 29, 2001.

Astronomy

- **Astroflow.** The activities of faculty members who are active in bringing their research results to the public are well illustrated by the work of Adam Frank, a CAREER awardee at the University of Rochester.[74] He and his research group make the results of their research directly available to the public through a variety of venues including programs at local grade, middle and high schools. A program called Astroflow is a suite of software tools allowing users to interactively control, visualize, and explore realistic simulations of cosmic events: exploding stars; comets diving into planetary atmospheres; jets of hypersonic gas driving through interstellar clouds and more. Astroflow gives students and non-scientists the opportunity to learn by experimentation and exploration. Currently Astroflow is installed in a specially designed kiosk at the Strasenburgh Planetarium in Rochester NY. The technology behind Astroflow has been successfully commercialized.



- **Catching the Wave.** The National Radio Astronomy Observatory project *Catching the Wave* was funded by the Education and Human Resources Directorate's Informal Science Education Division to develop interactive exhibits and new programs for visitors and schools in West Virginia. Exhibits are being field tested in the summer of 2001 for installation in the new Science Education Center being constructed in 2002.

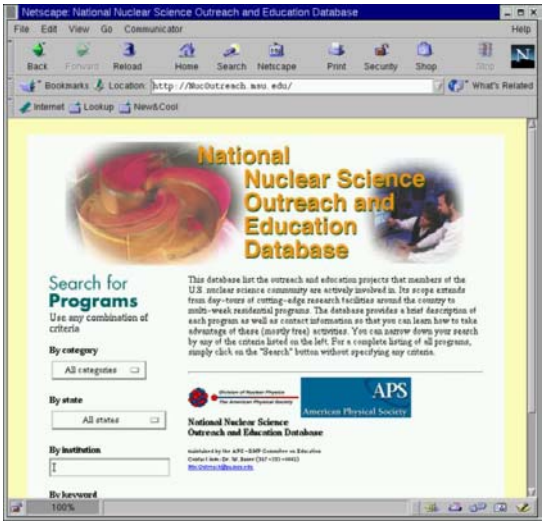
- **Explore the Universe.** The Astronomy Division, in collaboration with the Physics Division and the Office of Multi-disciplinary Activities, is supporting the creation and installation of a major new permanent exhibit, *Explore the Universe*, in the Smithsonian Institution's National Air and Space Museum.[75] This exhibit, opened in September 2001, will provide the 9 million annual visitors to the Air and Space Museum with a perspective on how our understanding of the Universe has changed over time

Entrance to the new Explore the Universe Exhibit at the National Air and Space Museum.

[74] AST-9702484
[75] AST-0083463

as the tools we use to study it have evolved. The exhibition makes use of a selection of artifacts, working models, images, interactive videos and computer programs, hands-on exhibits, and live demonstrations to explore scientists' view of the Universe as well as how they use ground- and space-based technology to study it.

Physics



Nuclear Science Education Web Page. Wolfgang Bauer of Michigan State University[76] has set up an interactive web-based outreach and education database for nuclear science. This site will enable physicists involved with outreach and/or education activities at their institutions to post information about their program, including features and contact information. The database can be queried by subject, geographic region, etc. for various reporting purposes. A key impact of this database will be to make this research community aware of the many activities already taking place but that are otherwise not well publicized.

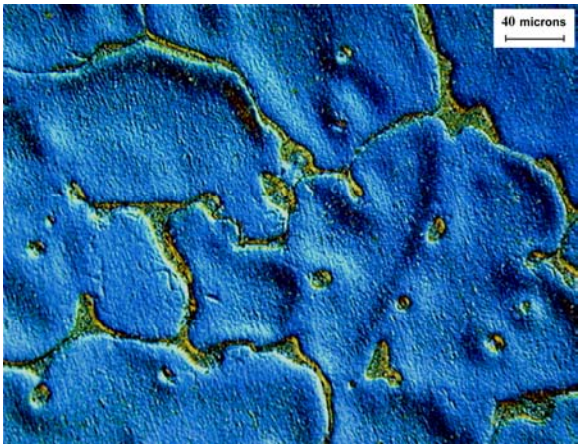
Materials Research

- To bring the nanoworld to everyone, Thomas F. Kuech of the University of Wisconsin MRSEC[77] has developed a series of short web-based 'picture books' accompanied by hands-on demonstrations that illustrate nanoscale materials and devices.[78]. This work is the basis for a lead article in the Smithsonian's *Muse* magazine Spring 2001 issue dedicated to nanotechnology.[79]

- **Macrogalleria.** The Macrogalleria, a pioneering educational polymer web site by Lon Mathias of the University of Southern Mississippi[80] is continuing to garner broad recognition. NSF Director Rita Colwell described it in these terms in one of her speeches: "Many of you have seen the wonderful Web Site called 'Macrogalleria'. It is set up like a shopping mall. The site bills itself as 'the Internet mall where you net surfers can learn all kinds of nifty stuff about polymers and polymer science.' The

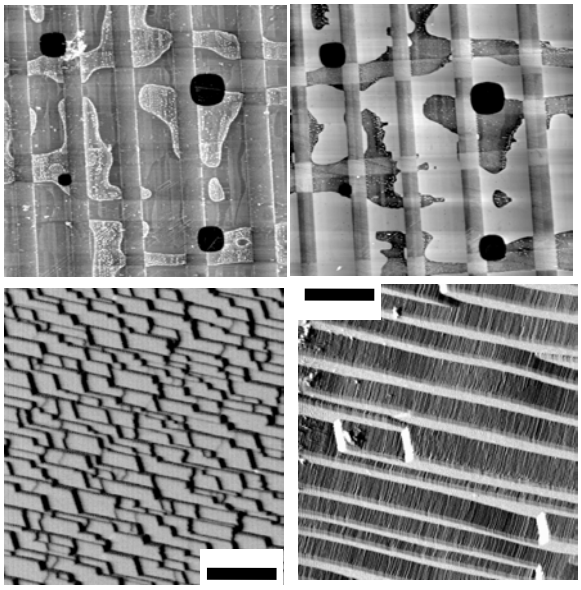
[76] PHY-0085921
[77] DMR-0079983
[78] http://www.mrsec.wisc.edu/edetc/nano/index.html
[79] www.musemag.com
[80] DMR-9950760

student or the Internet surfer clicks on the shops and learns that polymers are everywhere. As he or she ascends to the different levels of the mall, more complex concepts are conveyed." The Macrogalleria was recently selected by *Scientific American*[81] as one of its "50 Top Websites" and only one of five in chemistry. This follows many other distinctions, such as the Education Index Top Site and the Top 5% of Chemistry Sites. The worldwide popularity of the Macrogalleria is so high that it has already been translated into Afrikaans, French, and Spanish, and is being translated into Italian and Portuguese.



- **Prizes for Imagery and Imagination.** Paula Crawford, a Ph.D. student working with Martin Glicksman at Rensselaer Polytechnic Institute[82] was awarded first prize in 'Artistic Microscopy,' and a second prize in 'Engineering Materials' from the American Metallographic Society at the ASM Materials Week in Cincinnati, Ohio. Her elegant micrograph reveals the distribution of a second (intermetallic) phase in a cast aluminum-copper alloy.

- **Prizes for Imagery and Imagination.** Jennifer Giocondi, a graduate student working with Greg Rohrer at Carnegie Mellon University,[83] won two first place prizes for exhibits in the Ceramographic Competition of the American Ceramic Society during its 103rd Annual Meeting and Exposition in March 2001. The stunning images show photochemical decoration of domains in barium titanate (upper) and nanofaceting on the surface of strontium titanate (lower), and demonstrate the ability to deposit materials selectively on a sub-micron scale.



[81] http://www.scientificamerican.com/explorations/2001/051401top50/#ScientificAmerican
[82] DMR-9633346
[83] DMR-0072151

II. OUTCOME GOAL: IDEAS

FY 2001 Annual Performance Goal

NSF is judged successful when

NSF's performance is successful when, *in the aggregate*, results reported in the period demonstrate significant achievement for one or more of the following indicators:

- A robust and growing fundamental knowledge base that enhances progress in all science and engineering areas including the science of learning;
- Discoveries that advance the frontiers of science, engineering, and technology;
- Partnerships connecting discovery to innovation, learning, and societal advancement; and
- Research and education processes that are synergistic.

FY 2000 Areas of Emphasis across NSF

- Appropriate balance of high risk, multidisciplinary or innovative research across all NSF programs
- Investments in three initiatives:
  - Information Technology Research
  - Nanoscale Science and Engineering
  - Biocomplexity in the Environment
- Investments in non-initiative fundamental research
  - Mathematical Sciences Research
  - Functional Genomics
  - Cognitive Neuroscience

Introduction

Discoveries in the mathematical and physical sciences range over an enormous scale: from the very short distances (10^{-33} cm) within which the structure of matter suggested by string theory is thought to exist to cosmological distances (10^{+28} cm). Discoveries also extend over extremes of temperature: at the nano-Kelvin end, the trapping, manipulation, and study of fundamental new types of atom assemblies–Bose-Einstein condensates; and at the other extreme, temperatures that may have existed only shortly after the Big Bang, when free quarks and gluons underwent a phase transition into the confinement regime, which seems to characterize all the matter in the universe today. There is increasing public interest and fascination in these topics.

In the course of pursuing fundamental research, such activities continue to produce exceptionally valuable technological developments. These developments impact medical and biological research, computation, engineering, communications, manufacturing, and more. For example, new tools for medical and biological research include: laser tweezers for probing genetic materials, hyperpolarized MRI imaging for greatly improved whole body imaging, femtosecond lasers for eye surgery (glaucoma treatment, vision correction) with greatly increased effectiveness, and new coherent x-ray sources for imaging.

The broad portfolio of research and educational activities supported by the Directorate has resulted in a number of remarkable discoveries that have attracted the attention of the press and the public, as well as led to the less obvious, but just as critical, development of fuller, more accurate understanding of the universe we inhabit. Progress in the mathematical and physical sciences is, of course, linked to other disciplines, and there are many examples of work jointly supported with other NSF Directorates of other agencies. In addition, the development of technology and progress in all fields of research are closely related. We wish to emphasize, however, that in all the research highlighted here, the education of future citizens and future scientists has been an integral component. The examples below, only a small fraction of the fundamental research that MPS supports, serves to illustrate, in several key areas, how MPS is meeting its goals.

- **Nobel Prize.** The 2000 Nobel Prize in Chemistry was awarded to Alan Heeger of the University of California at Santa Barbara,[1] Alan McDiarmid of the University of Pennsylvania,[2] and Hideki Shirakawa of the University of Tsukuba "*for the discovery and development of conductive polymers*". Alan Heeger has been a grantee in the Division of Materials Research for many years. His research has focused on the photophysics of conducting polymers. The Divisions of Materials Research and Chemistry supported both Heeger and McDiarmid through individual grants since the 1970s when their work on conductive polymers began. Research into electroactive polymers has brought forth plastic transistors, light-emitting diodes, lasers and other photonic devices, as well as applications such as "electronic paper." The work of chemists such as MacDiarmid and others laid the groundwork for the area that is now known as nanoscience, a strategic priority area for the NSF.

- **National Medals of Science.** John D. Baldeschwieler's[3] work in molecular assemblies led to practical pharmaceutical products and instrumentation. He developed Ion Cyclotron Resonance Spectroscopy, an important tool for chemical and biochemical analysis that led to a new scientific field providing unique ways to study molecular structure and reactivity.

Jeremiah P. Ostriker[4] was cited for "his bold astrophysical insights which have revolutionized concepts of pulsars, the 'ecosystem' of stars and gas in the galaxy, the sizes and masses of galaxies, the nature and distribution of dark matter and ordinary matter in the universe, and the formation of galaxies and other cosmological structures."

- **Presidential Award for Excellence in Science, Mathematics and Engineering Mentoring.** Daniel L. Akins of the City College of New York[5] received the *Presidential Award for Excellence in*

[1] DMR-9730126, DMR-0099843
[2] CHE-7702207
[3] CHE-9510443
[4] AST-9318185; AST-9803137
[5] CHE-9872777

Science, Mathematics and Engineering Mentoring. Dr. Akins established the Center for Analysis of Structures and Interfaces (CASI), a major research center and training laboratory for high school students in their junior and senior years, high school chemistry and physics teachers, and undergraduate and graduate students. These efforts have led to City College being one of the nation's leaders in providing Ph.Ds. to minority students. During the 1997-98 Academic Year, eleven underrepresented minority students obtained their Ph.Ds. at City College in chemistry or engineering.

- **National Academy of Sciences Henry Draper Medal.** The National Academy of Sciences presented its prestigious *Henry Draper Medal for 2001* to R. Paul Butler of the Carnegie Institution of Washington and Geoffrey W. Marcy of the University of California, Berkeley "for their pioneering investigations of planets orbiting other stars via high-precision radial velocities. They have proved that many other planetary systems exist in the universe." This work has been supported since its inception by the Division of Astronomical Sciences, first with a Research at an Undergraduate Institution (RUI) award to Marcy while he was at San Francisco State University,[6] and more recently with awards to Butler,[7] Marcy, and Steve Vogt at the University of California at Santa Cruz.[8] The Academy awards the Draper Medal every four years to those who have made a significant contribution to astronomical physics; it was first awarded in 1886.

- **National Academy of Engineering Founders Award.** The National Academy of Engineering presented their *2000 Founders Award* to Charles Townes for his life-long contributions to engineering. Townes developed the maser-laser principle and has most recently been supported through the Division of Astronomical Sciences through work with William Danchi of the University of California at Berkeley[9] for his pioneering work on interferometry that has expanded the technique of high angular resolution interferometry into the 10-micron atmospheric window.

- **American Chemical Society National Awards.** Chemists supported by the Division of Chemistry receiving national awards from the American Chemical Society in 2001 included:

John Ross, Stanford University,[10] *Peter Debye Award in Physical Chemistry*;

Daniel Neumark, University of California at Berkeley,[11] *Nobel Laureate Signature Award for Graduate Education in Chemistry;*

Harry B. Gray, California Institute of Technology,[12] *George C. Pimentel Award in Chemical Education*;

Fred Basolo, Northwestern University,[13] *Priestley Medal*;

William A. Klemperer, Harvard University,[14] *E. Bright Wilson Award in Spectroscopy*;

John D. Roberts, California Institute of Technology,[15] *Nakanishi Prize*;

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[6] AST-9520443, AST-9619418
[7] AST-9988087
[8] AST-9988087
[9] AST-9500525, AST-9819729
[10] CHE-9708567
[11] CHE-0092574
[12] CHE-0111416
[13] CHE-8818696
[14] CHE-9806153
[15] CHE-0104273

Robert F. Pasternack, Swarthmore College,[16] *Award for Research at an Undergraduate Institution*;

David Tirrell, California Institute of Technology,[17] *Polymer Chemistry Award*; and

Tobin Marks, Northwestern University,[18] *Chemistry of Materials Award*.

Twenty-two other chemists supported by the Division of Chemistry received ACS national awards in 2001.[19]

- **American Mathematical Society National Awards.** Mathematicians supported by the Division of Mathematics receiving national awards from the American Mathematical Society in 2000 included:

Michael Aizenman of Princeton University was awarded Netherlands' most prestigious award in mathematics, the *2002 Brouwer Prize of the Dutch Mathematical Society***.**

Elliott Lieb of Princeton University[20] was awarded the *2001 Rolf Schock Prize in Mathematics* of the Swedish Academy of Sciences.

Once every five years the American Mathematical Society awards a Prize for outstanding contributions to geometry. This prize was first given in 1964 and the NSF has supported all sixteen previous recipients. This year the three recipients of the *2001 Veblen prize* are Jeffrey Cheeger of New York University,[21] Yakov Eliashberg of Stanford University,[22] and Michael Hopkins of the Massachusetts Institute of Technology.[23]

Thomas Hou of the California Institute of Technology[24] was awarded the *2001 James H. Wilkinson Prize in Numerical Analysis and Scientific Computing* by the Society of Industrial and Applied Mathematics (SIAM). The prize is awarded every four years at a SIAM Annual Meeting.

Henry Kesten of Cornell University[25] received the *Leroy P. Steele Prize for Lifetime Achievement*.

William Symes of Rice University[26] was awarded the *Ralph E. Kleinman Prize* by SIAM for outstanding research, or other contributions that bridge the gap between mathematics and applications.

C. F. Jeff Wu of the University of Michigan[27] was elected a member of Academia Sinica, only the fifth statistician to have received this honor since its inception in the mid-forties.

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[16] CHE-9510127
[17] DMR-9996048
[18] DMR-9977520, CHE-0078998
[19] CHE-9617544, CHE-9318794, CHE-9300107, CHE-9610493, CHE-9980549, CHE-9873839, CHE-9734430, CHE-0070122, CHE-8822412, CHE-9809856, CHE-0102258, CHE-9875261, CHE-9319512, CHE-0093048, CHE-9909416, CHE-9623828, CHE-9988766, CHE-9408247, CHE-9710504, CHE-9988651, CHE-9819179, CHE-9819652
[20] PHY-9820650
[21] DMS-0104128
[22] DMS-9971965
[23] DMS-9803428
[24] DMS-0073916
[25] DMS-9970943
[26] DMS-9973423
[27] DMS-0072489

David L. Donoho of Stanford University [28] was this year's *John von Neumann lecturer* at the SIAM meeting.[29]

Division of Mathematical Sciences grantees received numerous other distinctions and awards[30].

American Physical Society National Awards

Janet Conrad of Columbia University[31] received the *Maria Goeppert Mayer Award* "for her leadership in experimental neutrino physics, particularly for initiating and leading NuTeV decay channel experiment and the Mini-BooNE neutrino oscillations experiment, which are noted for their timeliness and significance in resolving frontier issues in neutrino physics."

Louis Brus of Columbia University received the *Irving Langmuir Prize* for establishing the field of semiconductor nanocrystals.

Paul Grannis of the State University of New York at Stony Brook[32] received the *W. K. H. Panofsky Prize* "for his distinguished leadership and vision in the conception, design, construction, and execution of the D0 experiment at the Fermilab Tevatron proton-antiproton collider. His many contributions have been decisive in all aspects of the experiment."

Bertrand Halperin of Harvard University[33] received the *Lars Onsager Prize* "for his wide-ranging contributions to statistical physics and quantum fluids, especially the elucidation of the quantum Hall effect and other low-dimensional electronic phenomena; and for his exemplary leadership in bringing theory to bear on the understanding of experiments."

Mildred Dresselhaus of the Massachusetts Institute of Technology[34] was awarded the *Karl T. Compton Medal for Leadership in Physics*.

Klaus Schmidt-Rohr of Iowa State University was awarded the *Dillon Medal.* (Young Investigator Award).

Ellen D. Williams of the University of Maryland[35] received the *David Adler Lectureship Award* for her "elegant experimental exploration of the structures and phase transitions of surfaces and for her effective communication on this subject in lectures and publications."

Henry R. Glyde of the University of Delaware[36] received the *John Wheatley Award* for his "enduring commitment and multifaceted contributions to the development of physics in Thailand, which include innovative creation of scientific links between North American research universities and Chulalongkorn University, inspiring collaboration with leading Thai physicists, and the marshaling of financial and intellectual resources to establish new regional research centers."

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[28] DMS-0072661
[29] http://www.siam.org/meetings/an01/
[30] DMS-0100678, DMS-0040396, DMS-9802773, DMS-0112734, DMS-0072292, DMS-0071408, DMS-0103265
[31] PHY-9733023, PHY-9804051
[32] PHY-9940628
[33] DMR-9416910
[34] DMR-0116042
[35] DMR-0102950
[36] DMR-9972011

Other National and International Awards

George Whitesides of Harvard University[37] received the Materials Research Society *Von Hippel Award* for bringing fundamental concepts of organic chemistry and biology into materials science and engineering.

Rodney Clifton at Brown University[38] received the American Society of Mechanical Engineers *Timoshenko Medal* for seminal contributions to the development of experimental and computation methods for high-strain rate phenomena in mechanics.

Ray Goldstein of the University of Arizona[39] was awarded the *Pnevmatikos Award*[40] in Nonlinear Science for 2000, an international prize that is presented every two years to an outstanding researcher under the age of 40 in an area of nonlinear science. The citation reads "for his contributions to the understanding of pattern formation involving the dynamics of filaments, interfaces and surfaces, combining powerful mathematical methods with penetrating physical arguments, numerical computations and experiments to clarify nonlinear phenomena in a wide variety of physical and biological systems."

Robert Grubbs of the California Institute of Technology[41] was awarded the 2000 *Benjamin Franklin Medal in Chemistry* of the Franklin Institute "for his wide ranging seminal contributions to greatly advance and expand the field of olefin metathesis, a unique carbon-carbon bond breaking/making process, that has enormously added to the chemist's capabilities at making a broad range of drugs and other useful complex molecules, improved rubbers, and plastics for laboratory and commercial applications."

Terence Langdon of the University of Southern California[42] was awarded the *Henry Marion Howe Medal* for 2000 by ASM International, and in 2001 he was awarded a Senior Fellowship by the Japan Society for Promotion of Science for his collaborative research with colleagues at Kyushu University in Japan.

Kristi Anseth of the University of Colorado[43] was awarded the 2001 *Outstanding Young Investigator Award* of the Materials Research Society. Anseth is an NSF CAREER grantee whose work on polymeric biomaterials for tissue engineering is co-funded with NSF's Bioengineering Division. Remarkably, Anseth's student Amy Burkoth won American Chemical Society's Student Award in Applied Polymer Science in 2001.

Kristi Anseth

[37] CHE-9901358
[38] DMR-9724388
[39] DMR-9812526
[40] http://uanews.opi.arizna.edu/cgi-bin/WebObjects/UANews.woa/wa/MainStoryDetails?ArticleID=2898
[41] CHE-9809856
[42] DMR-0093011
[43] BES-9734236

PERFORMANCE INDICATORS FOR IDEAS

A. Summary Comments by the Committee of Visitors for the Division of Chemistry on the Performance of the Division for this Outcome Goal during FY 1998 – FY 2000:

"The Division is successful in its support of discovery across the frontier of science and engineering, connected to learning, innovation and service to society.

The Division places a priority on support for high risk-high potential research, for adequate funding of academic investigators at the beginning of their careers, and for projects integrating research and education. The Division is extensively involved in interdisciplinary and crosscutting NSF-wide programs.

Perhaps the best way to indicate the Division's support for Ideas is to give examples of Division supported research that has been recognized as successful by others. The Division's support of recognized high impact research is well illustrated by recently awarded Nobel Prizes. The 1998 Nobel Prize in Chemistry was awarded to John Pople (Northwestern University, CHE-9629964). Professor Pople has been supported for over 25 years by the Division for discovery and implementation of novel methods for computing the electronic structures of molecules. The 1999 Nobel Prize was awarded to Ahmed Zewail (California Institute of Technology, CHE9526069, 9525756) for his pioneering real-time studies of ultrafast chemical dynamics.

John Ross, Stanford University and Stuart Rice, University of Chicago, were two of the twelve scientists awarded the 1999 National Medal of Science for their discoveries and lifetime achievements. Ross (CHE-9708567) was cited for pioneering studies of chemical reactions in molecular beams and his demonstration of the computational possibilities of chemical kinetics. Rice (CHE-9980363, 9977841, 9807127) was cited for guiding the evolution of modern physical chemistry from statics to dynamics.

The power of multidisciplinary science is extremely well illustrated in the area of glycobiology and by the research of Professor Laura L. Kiessling, an NSF Young Investigator at the University of Wisconsin (CHE-9840499) and Professor Carolyn Bertozzi, a CAREER recipient at the University of California, Berkeley (CHE-9734430). Both Kiessling and Bertozzi were named as 1999 MacArthur Award winners."

B. Summary Comments by the Committee of Visitors for the Division of Mathematical Sciences on the Performance of the Division for this Outcome Goal during FY 1998 – FY 2000:

Performance Outcome: The program is successful when*, in the aggregate*, results reported in the period demonstrate significant progress in achieving one or more of the following indicators:

a. A robust and growing fundamental knowledge base that enhances progress in all science and engineering areas including the science of learning;
b. Discoveries that advance the frontiers of science, engineering, and technology;
c. Partnerships connecting discovery to innovation, learning, and societal advancement; and
d. Research and education processes that are synergistic.

Successful in all categories

Comments:

This is a great strength of the Research Programs of the DMS. Outstanding research projects have been funded; the results are documented in the Programmatic Annual Reports of the DMS for the years 1998, 1999 and 2000. We list some of the outstanding results in Appendix B.

a. Along with world-leading breakthroughs in fundamental mathematics, DMS has supported a wide variety of successful projects addressing critical contemporary issues in science and engineering. DMS has also taken the lead in integrating research and education at K-12, undergraduate, graduate and postdoctoral levels. Combinatorics is a good example: with the help of DMS, this field, formerly criticized for its prevalence of isolated problems and techniques, now boasts a strong common base of concepts and theorems. Broadening to a case where one mathematical field forms a common base for many others, we have the now-ubiquitous presence of dynamical systems throughout applied mathematics. Finally, mathematics as a whole is becoming a universal tool in such areas as biology and materials science.

b. There are many examples of mathematical ideas that have "escaped" the mathematical community and infected various scientific fields or the public in general. Much of the work connected to the Taniyama-Shimura conjecture was funded by NSF, as are new collaborations between number theorists and quantum theorists; and even the public is becoming aware of the role that string-matching and other mathematical techniques is playing in the Genome Project.

c. Most of the core programs contribute synergistically at the level of graduate education. At the undergraduate level, the RUI and REU programs are critical, as well as is support of graduate and postdoctoral students. Support of faculty research programs leads to energized professors teaching classes at all levels, and including new results and points of view in their curricula.

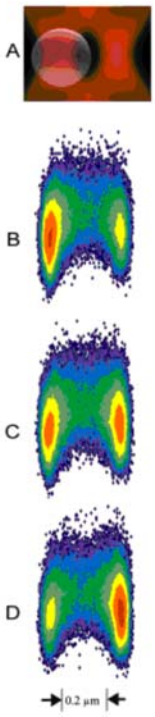
d. Data show that there has been a serious drop-off in the mathematical pipeline between undergraduate and graduate school. The importance of early research experiences in creating interest and in preparing students for further study in mathematics has been widely noted. The Committee enthusiastically recommends continuing and increased support for REU programs as one means of enhancing the pool of potential graduate students.

Examples of MPS Directorate Performance for FY 2001

Indicator 1. A robust and growing fundamental knowledge base that enhances progress in all science and engineering areas including the science of learning

MPS Primary Area of Emphasis: Enhancing Instructional Workforce

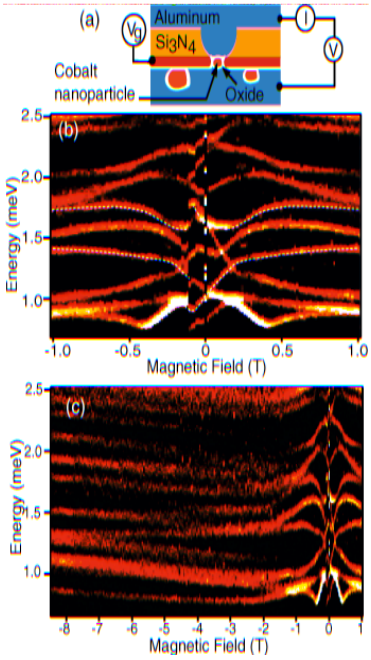
- **Controlling nature's randomness.** Diffusion plays a fundamental role in a remarkably large number of physical phenomena, including crystal growth, molecular processes in living cells, and the formation of galaxies. A particle undergoing diffusion executes a random walk through space. If it were possible to tame the randomness of the diffusive process, it would have enormous impact on virtually all of the physical sciences and in many crucial technologies. Brage Golding and Mark Dykman at Michigan State University[44] use optical tweezers to control the diffusion of a submicron sphere (A) between two normally equally likely sites in an optical trap (C). By changing the modulation phase of light shining on the particle, they can make the particle stay mostly on the left side (B) or the right side (D) of the trap. In effect, they have created an optical orifice that behaves like a controllable pore for particle flow.



- **Observing a Time Before Galaxies Existed.** Another step in probing the early universe and the transition from the hot, smooth early phases and the cool, lumpy universe of today has been taken by the researchers involved in the Sloan Digital Sky Survey (SDSS).[45] Researchers have discovered, in the spectrum of the most distant quasar known, the signature of neutral hydrogen in the intergalactic medium, indicating that their observations are probing redshifts before large numbers of quasars and galaxies formed. At redshifts less than 1000, the universe cooled down enough to allow electrons and protons to combine, making neutral hydrogen, which should cause a complete absence of flux in the quasar spectrum blueward of Lyman alpha. Contrary to this expectation, quasar spectra show a series of narrow absorption lines in this wavelength region indicating that what neutral hydrogen there is in the intergalactic medium is confined to narrow filaments or clouds. Most of the hydrogen (>99.99%) is ionized. Some time between a redshift of 1000, and that of the observed quasars ($z < 5$), the hydrogen of the universe was reionized by the first generation of hot stars and quasars in the universe. Recent observations of the highest-redshift quasar yet discovered, SDSS J1030+0524, at $z=6.28$, shows the Gunn-Peterson effect; it is completely blank in a deep exposure with the Keck telescope over a 300 Angstrom range just blueward of Lyman alpha. This appears to be the signature of a high optical depth of neutral hydrogen; the existence of this neutral hydrogen indicates that the universe has not yet been flooded with a substantial density of ionizing photons from stars and quasars.

[44] DMR-9971537
[45] AST-0096900 and AST-0071091

- **Artificial Atoms.** At the extreme nanoscale limit, artificial atoms and molecules are being fabricated. These have quantized electronic energy levels and it becomes possible to add and subtract electrons from among these levels. The fabricated structures include single electron transistors, quantum dots, etc. Dan Ralph of Cornell University[46] is exploring the fundamental physics processes at work in this new regime, and how individual quantum states can be manipulated for sensor and memory applications. In magnetic cobalt nanoparticles (figures at right), the individual energy levels shift and jump as a magnetic field rotates the direction of the particle's magnetic moment, so that the energy of just one quantum state could be used to measure the orientation of the particle in magnetic memory applications.



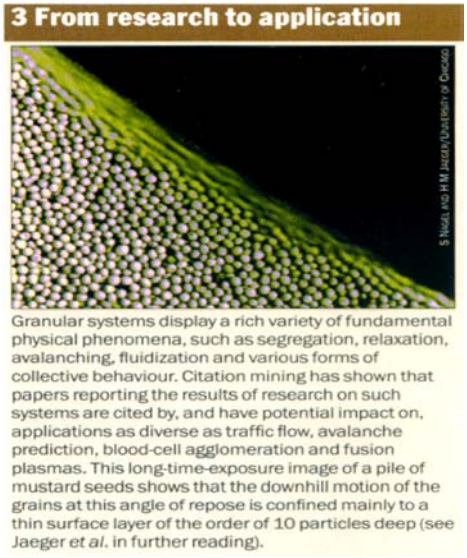
- **Why Flags Wave.** The complicated interaction between a flexible object (such as a flag) and its surrounding fluid is not fully understood. In a project headed by Charles Peskin of New York University, [47] an experiment by Jun Zhang of Rockefeller University, Stephen Childress of New York University, Albert Libchaber of Rockefeller University, and Michael Shelley of New York University has shed new light on how flags flap in a breeze. They observed the periodic flapping of a fine silk thread in a fast-flowing soap film; this is essentially the case of a one-dimensional flag waving in a steady two-dimensional background flow. They found that for a single filament (or 'flag') held at its upstream end and otherwise unconstrained, there are two distinct, stable dynamical states. The first is a stretched-straight state where the filament is immobile and aligned in the flow direction. The existence of this state seems to refute the common belief that a flag is always unstable and will flap. The second is a flapping state where the filament executes a sinuous motion in a manner akin to the flapping of a flag in the wind. This work bears on a host of difficult and unresolved theoretical issues in fluid dynamics and progress in this area is likely to find application in a wide variety of different disciplines. These results were featured in a *Nature* News and Views article.[48]

A silk thread flutters in a watery breeze

- **Quantum Computing.** Siyuan Han and his students at the University of Kansas[49] have demonstrated that macroscopic quantum coherent oscillations between two states can be maintained over many cycles. The states are macroscopic superconducting currents in NbN SQUID devices. They execute about 10,000 oscillations before losing coherence. This is the first demonstration in the solid state of conditions that are a prerequisite to physical realization of *scalable, fault-tolerant quantum computing*.

[46] DMR- 0071631
[47] DMS-9980069
[48] *Nature,* **408**, December 14, 2000, 777-778
[49] DMR-9876874

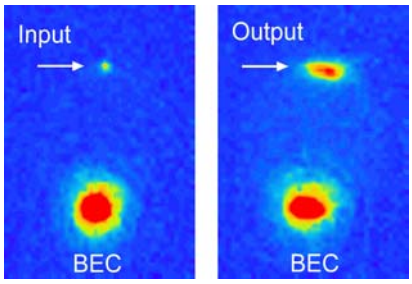
- **High Risk Research-Steps Towards Quantum Computing.** Harold Baranger, Weitao Yang and Shailesh Chandrasekharan of Duke University[50] will study the interplay of electron-electron correlation and quantum mechanical interference in nanostructures, including networks of carbon nanotubes, "nanomolecules," and quantum dots. This award will also focus on spin states of some of these systems and explore entanglement of quantum states in these systems with an eye toward quantum computing.

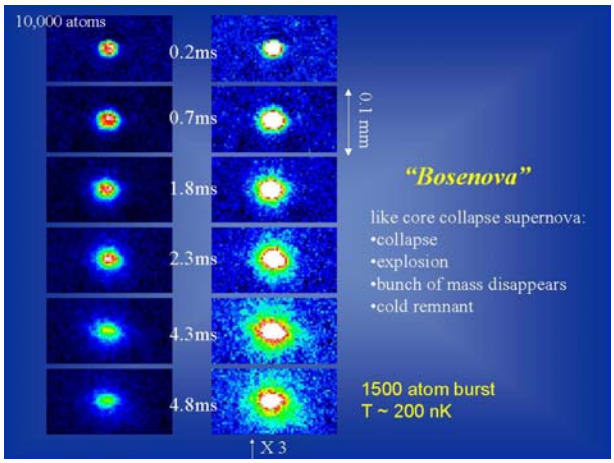


Granular systems display a rich variety of fundamental physical phenomena, such as segregation, relaxation, avalanching, fluidization and various forms of collective behaviour. Citation mining has shown that papers reporting the results of research on such systems are cited by, and have potential impact on, applications as diverse as traffic flow, avalanche prediction, blood-cell agglomeration and fusion plasmas. This long-time-exposure image of a pile of mustard seeds shows that the downhill motion of the grains at this angle of repose is confined mainly to a thin surface layer of the order of 10 particles deep (see Jaeger *et al.* in further reading).

- **The Physics of Granular Materials.** A case study published in the June 2001 issue of *Physics World* analyzes the impact of basic physics research on the wider fields of science and technology. In their case study based on citation mining, the authors highlight the enormous impact of the review article "*The Physics of Granular Materials*," published by Steven Sibener and Leo Kadanoff of the University of Chicago[51] MRSEC in *Science* magazine in 1992. This single article garnered more than 300 citations since publication and helped launch the field of granular dynamics within condensed matter physics. What is particularly noteworthy is that about 20% of the citations of this article are from papers outside basic physics and involve applications as diverse as traffic flow, avalanche prediction, blood cell agglomeration, and fusion plasmas.[52]

- **Bose-Einstein Condensates (BEC) Explosion Resembles Supernova.** Bose-Einstein condensates form coherent matter sources, which can be amplified while maintaining the coherence properties of the source. Such amplified sources are expected to become tools for use in coherent atom optics, exactly as lasers became tools in coherent photon optics. In the figure at left, atom amplification is probed by sending an input beam through the atom amplifier. The output pulse contains many more atoms than the input pulse – with typical amplification factors were between 10 and 100. However, researchers at the Joint Institute for Laboratory Astrophysics at the University of

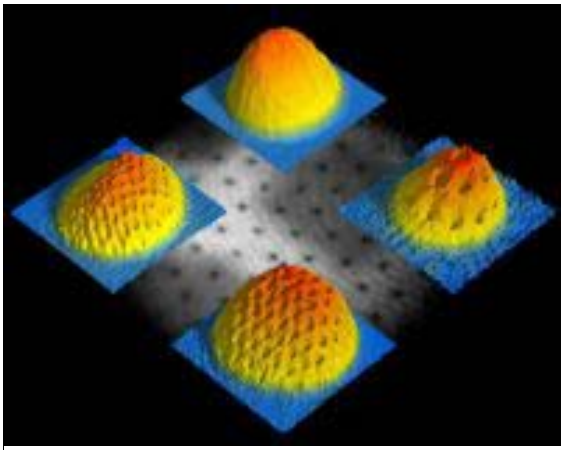




[50] DMR-0103003
[51] DMR-9808595, DMR-9400379 and DMR-8819860
[52] http://MRSEC.uchicago.edu/MRSEC/

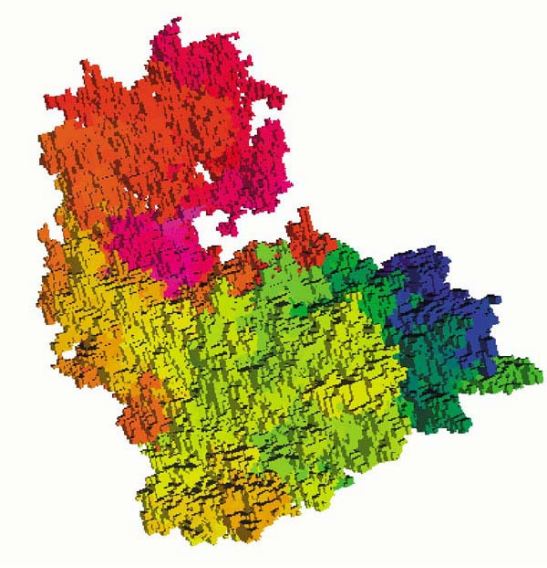
Colorado[53] have shown that an exploding Bose-Einstein Condensate behaves in the same way as an exploding supernova upon collapse. The collapse generates an expanding cloud of gas, leaving a cold remnant behind.

- **Vortices in BECs.** In a further study of the properties of Bose-Einstein condensates, Wolfgang Ketterle of the Massachusetts Institute of Technology[54] has shown that macroscopic vortices are a manifestation of the quantum fluid behavior of Bose-Einstein Condensates. The images show quantum vortices in a rotating condensate of sodium atoms. A condensate 60 micrometer in diameter and 250 micrometer in length was set in rotation by rotating laser beams. It then formed a regular lattice of vortices. The condensate was then allowed to ballistically expand which resulted in a twenty times magnification. The images represent two-dimensional cuts through the density distribution and show the density minima due to the vortex cores. The examples shown at the right contain 0, 16, 70 and 130 vortices. The cloud diameter is about 1 mm.



Vortices in a Quantum Fluid

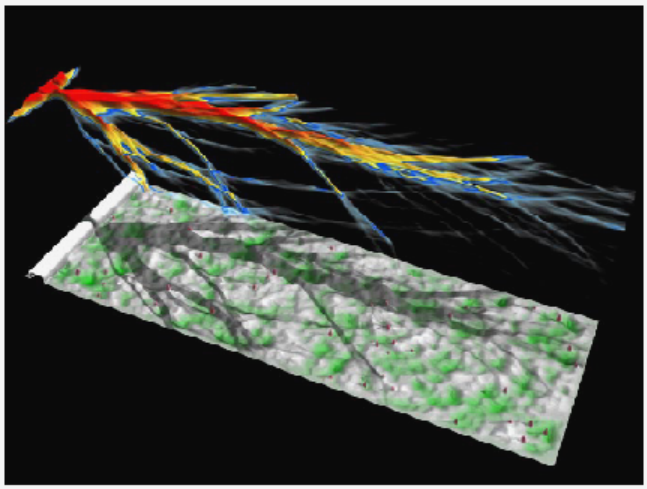
- **Magnetism, Crumpled Paper, and Avalanches.** For a wide variety of systems, the response to an external stress is the production of discrete events with sizes that vary. For example, the Earth responds to stress between tectonic plates, paper emits intermittent sharp noises as it is crumpled, magnetic materials magnetize in jumps in response to an applied field. Tools used to describe second-order phase transitions in equilibrium systems have been extended to describe these events in driven non-equilibrium systems. Many investigators have been involved. These include Daniel Fisher of Harvard University,[55] a



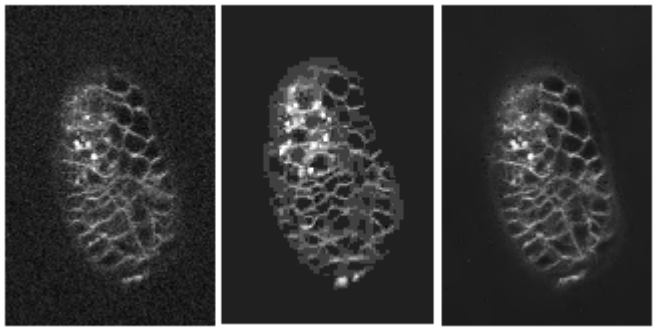
Fractal spatial structure of an avalanche. *Fractal structures, as well as power laws, are characteristic of systems at their critical point. This moderate-sized avalanche involved the flipping of domains in the simulation. The colors represent time: the first domains to flip are colored blue, the last pink. So far, there have been few experiments showing the spatial structure of avalanches. When results become available, a wealth of predictions of the scaling theories can be tested. Other systems display a qualitatively different kind of spatial structure, where the avalanche is made up of many small disconnected pieces, which trigger one another through the waves emitted as they flip. Adapted from J. Sethna et al. Nature,* ***410****, 242 (2001).*

[53] PHY-9512150
[54] PHY-9987902
[55] DMR-9976621

pioneer in the field who studied charge density wave systems, Alan Middleton of Syracuse University,[56] who uses innovative numerical methods to advance the field, Jean Carlson of the University of California at Santa Barbara[57] studying earthquake faults, Jim Sethna of Cornell University[58] who has been studying crackling noise,[59] and Karin Dahmen of the University of Illinois at Urbana-Champagne[60] who has been studying avalanches using a simple model of magnetic systems. These systems exhibit universal behavior on long length and time scales and yield to powerful renormalization group methods developed for phase transitions in equilibrium systems.



- **Electron Flow in a High Mobility Two-Dimensional Electron Gas.** Electron motion through high mobility two-dimensional electron gases is often thought to be nearly ideal. As shown in the figure, Robert Westervelt and his colleagues at Harvard University[61] have discovered that electron flow from a quantum point contact forms narrow channels at distances well below the mean free path. The upper part of the figure shows the computed electron wave flow over the potential shown in the lower part (high potential is white, low is green). These calculations agree well with images of electron flow from a quantum point contact in a GaAs/AlGaAs heterostructure obtained by scanned probe microscopy at low temperatures. Although the statistically averaged parameters – mobility, mean free path – are the same as in traditional pictures, the actual flow through a given nanoscale device shows additional structure. These developments improve our understanding of electron flow, with important effects on nanoscale electronic device design.[62]



Cell Fusion in C. elegans epithelial cells labeled with Fm 4-64, original image and its compressions using JPEG and 3D wavelets at compression level 115, respectively. At this compression rate, the JPEG has failed to retain the structure, while the 3D wavelet compression yields no detectable artifacts.

- **Wavelets.** The Wavelet Center for Ideal Data Representation headed by Amos Ron of the University of Wisconsin at Madison[63] was established in response to the need to develop new basic forms of data representation. For example, Ingrid Daubechies and Ronald DeVore developed analytical techniques that establish the first

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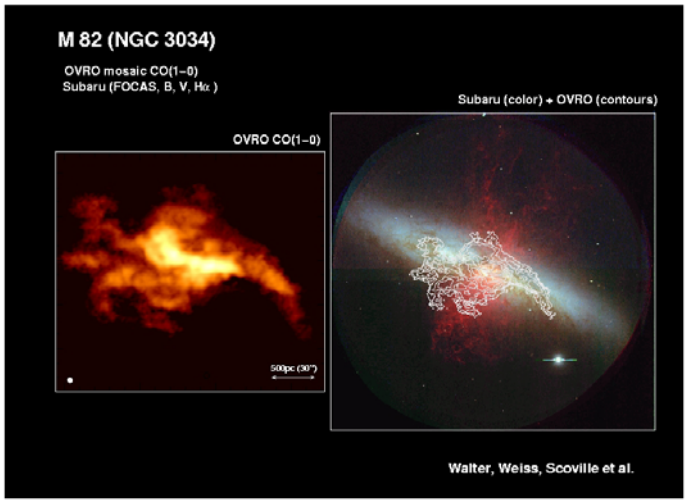
[5υ] DMR-9702242 and DMR-0109614
[57] DMR-9813752
[58] DMR-9873214 and DMR-9805422
[59] http://simscience.org/crackling
[60] DMR-0072783
[61] DMR-9809363
[62] http://www.mrsec.harvard.edu
[63] DMS-9872890

robust error bounds for Sigma Delta modulation. This analysis opened the door to the design of high-order Sigma-Delta schemes that provide better error decay for bit allocation. A patent application has been made for the higher-order schemes. Together with Z. Cvetcovic at AT&T Labs, Daubechies has also worked on another way to use frames, to propose a different approach to A/D conversion. A patent on this approach is pending. For image encoding, universal practical encoders that are optimal and progressive have been developed. They can also be adapted to allow "burn in." One application is important for remotely transmitting large images such satellite and medical imagery.

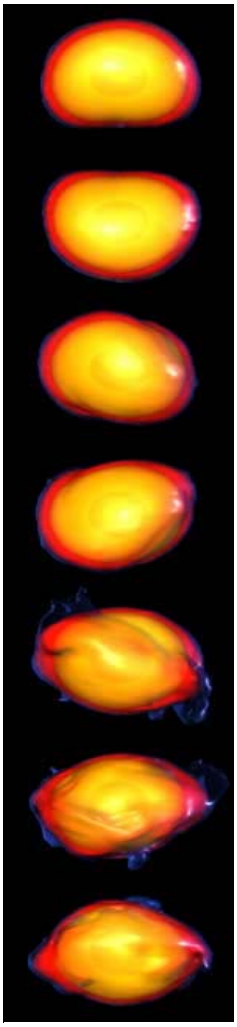


- **A Starburst Galaxy.** Recent radio observations of the prototypical starburst galaxy M82 have revealed a complex and dynamic system. Over the last year, Fabian Walter, along with Nick Scoville and collaborators at the California Institute of Technology,[64] has carried out a major project with the Owens Valley Radio Observatory millimeter-wave array, mapping the large-scale structure of molecular gas in the galaxy M82. The sensitivity and areal coverage of the resulting high-angular resolution data is an order of magnitude better than previous interferometric observations. The figure below includes a color carbon monoxide [CO(1-0)] image of M82, and the same results displayed as intensity contours and overlaid on an optical image of the galaxy from the Japanese Subaru telescope. There appears to be tidal stripping of the molecular gas along the plane of the galaxy, and coincident with the well-known neutral hydrogen (HI) streamers. The distribution of molecular gas also coincides with the dramatic dust features seen in optical absorption. Perhaps most exciting is the discovery of molecular gas in the prominent outflow observed in H-alpha and X-ray emission.

- **Coral Reefs, Sponges, and Chemoprotective Agents.** In the course of their development, plants and slow-moving or immobile animals have often given rise to organic molecules with potent properties, acting as anti-feedants or chemoprotective agents. These molecules frequently display significant pharmacological activity in humans (e.g., antibiotics, anticancer). Such "natural products" can both serve as valuable drugs in their own right (e.g., taxol) and provide important hints for the rational design of new drugs. As John Faulkner, at the University of California at San Diego[65] and the Scripps Institute of Oceanography notes, "When we go to a coral reef and find animals that look like large chunks of food – poorly protected, soft-bodied, sessile or slow-moving and easy to grab – we assume that it has physical protection. The chemicals responsible for the animal's survival are often those that we seek for biomedical research." Through investigations of marine sponges, Faulkner is seeking out potential anti-cancer, anti-fungal and

[64] AST-9981546
[65] CHE-9816169

anti-bacterial agents, inhibitors of HIV-1 integrase, anti-inflammatory agents, and agents to treat tropical diseases such as leishmaniasis.



Giant waves on neutron star.

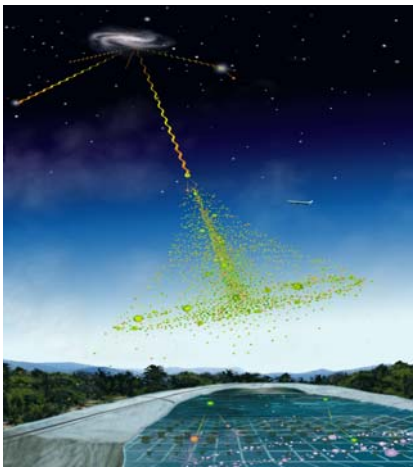
- **Simulating Giant Waves in Newborn Neutron Stars:** Neutron stars are born in supernova explosions when approximately one solar mass of burnt nuclear matter in the core collapses from about the size of the Earth to the size of an average city. The collapse of matter into this dense core can leave the newborn neutron star spinning extremely rapidly, some 1,000 revolutions per second. Now, Lee Lindblom and Michele Vallisneri at the California Institute of Technology[66] and Joel Tohline at Louisiana State University[67] have carried out the most detailed computational modeling ever done of the stability of these stars. In addition to surprising new insights into neutron stars, these simulations are yielding a clear "signature" to search for as the new Laser Interferometer Gravitational-Wave Observatory (LIGO) tries to detect gravity waves directly for the first time in history. Newborn rapidly rotating neutron stars are unlike most very stable stars. If the star is spinning fast enough, gravitational waves will feed growing oscillations on the star. The nonlinear evolution also causes the fluid to develop strong differential rotation, concentrated near the surface and poles of the star. The simulations show that the frequency of the gravitational waves remains almost constant at about 950 Hz. This is important because a stable frequency provides an unusually clear 'signature' or pattern that can be looked for, making this a good source of gravity waves for LIGO to try to detect. A Quicktime movie of this simulation is available.[68]

- **Radiation Induced Instabilities.** Anthony Bloch and his colleagues at the University of Michigan[69] have proved a number of interesting results on the stability of a class of mechanical systems interacting with wave fields. They explored these systems in the context of a gyroscopic oscillating mechanical system coupled to an extended wave system. Due to the coupling, motion within the mechanical system generates waves, which can be carried off to infinity. Such radiation damping has been studied in models arising in the theory of quantum resonances, ionization type problems and nonlinear waves. They consider the case of gyroscopic stability and analyze when the wave equation destabilizes the system. They prove that instability can occur and describe which types of coupling and potential energy in the mechanical system give rise to instability. Since gyroscopic systems may be shown to be the normal form for a large class of physical systems of interest, this provides a fairly widely applicable model for studying the effect of wave coupling on finite-dimensional systems. Stability of interconnected systems is of interest for many different applications including the study of satellite or space station motion, which include a mixture of rigid and flexible components.

- **Four-Dimensional Geometry.** There are only three basic types of geometry for two-dimensional spaces, and just eight types of geometry in three dimensions, but there is as yet no credible conjecture for a similar list for four-dimensional spaces, including those that model space and time in relativity. Clifford Taubes of Harvard University [70] is probing the possibilities for the large-scale structure of four-dimensional manifolds. For the particular case of four-dimensional spaces that are complex (in particular

[66] PHY-9796079, PHY-9900776, and PHY-9907949
[67] AST-0731698 and AST-9987344
[68] http://www.cacr.caltech.edu/projects/hydrligo/final.mov
[69] DMS-9803181
[70] DMS-0104196

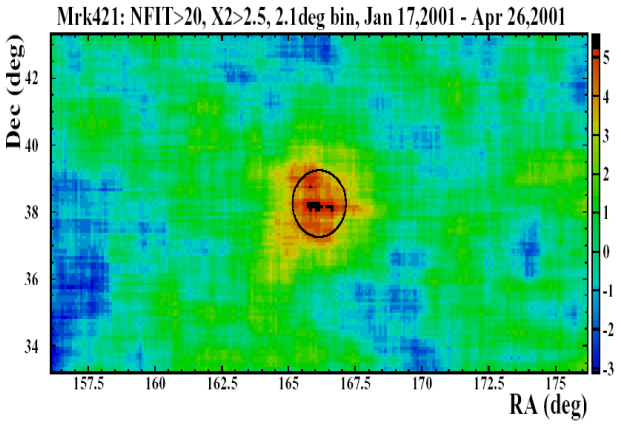
Kahler) surfaces, the investigations of Thomas Parker of Michigan State University [71] address major conjectures in algebraic geometry by gauge-theoretic arguments. His work, largely in collaboration with his student Eleni Ionel of the University of Wisconsin [72] is aimed toward further developing the symplectic gauge theory. Gauge theory originated in the observation that certain coordinate changes preserve important aspects of physical systems. The Maxwell equations for electromagnetic fields are an example. Gauge theory has been the focus of many fruitful interactions between mathematicians and physicists over the past twenty years, including Yang-Mills theory, Seiberg-Witten theory, and geometric aspects of string theory.



Artist depiction of high energy cosmic ray shower development above the Milagro detector

- **Observation of Astrophysical TeV Gamma Ray Sources**: Milagro is the first energetic air-shower detector with an all-sky, high duty-factor capability to be sensitive to gamma rays in the TeV energy range. The Milagro detector was built at a Los Alamos National Laboratory (LANL) remote site by a University of Maryland,[73] Los Alamos National Laboratory, University of California at Irvine, University of California at Santa Cruz, University of Wisconsin, and New York University collaboration. The core of the detector is a 80m x 60m x 8m covered pond filled with water and instrumented with 723 8" photo-multiplier tubes. The pond has been operational continuously since January 2000 and records air showers at a rate of 1-2KHz. Two TeV gamma-ray sources have been observed – the Crab Nebula and Mrk 421 during its flare of Winter 2000-2001. The collaboration has also demonstrated, for the first time in a ground-based array, successful gamma-hadron background rejection. In addition, Milagro continually monitors the northern skies for gamma ray bursts

Aerial view of the Milagro Pond



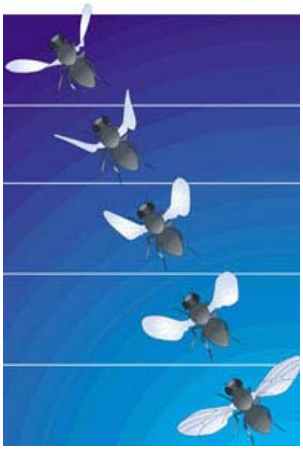
Sky Map centered on MRK421 during the flare of winter 2000-01

(GRBs). The detector is being upgraded to enable a substantial increase in sensitivity in both angular accuracy and background hadron rejection. In addition, Milagro will soon have a trigger processor (designed and built at Maryland) capable of rejecting muon triggers thus allowing a substantial reduction

[71] DMS-0104331
[72] DMS-0071393
[73] PHY-0075326

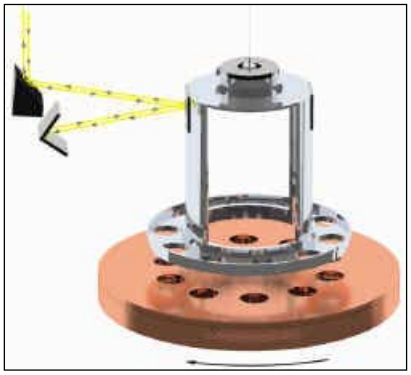
in the threshold. This will dramatically increase the volume of space over which the detector will be sensitive to GRBs.

- **Bumble Bees *Can* Fly.** Z. Jane Wang of Cornell University[74] has developed a theory of how some insects can manipulate the flow of air around them to switch in an instant between darting motions and hovering stillness. Prior studies of insect flight have indicated that rotation of the wings during flapping is a crucial part of the mechanism by which an insect controls lift forces and alters direction during flight. Her theory explains how the rotating motion of insect wings during flapping creates vortices that permit an insect to hover. She found a two-dimensional mechanism for creating a downward dipole jet of counter-rotating vortices that generates lift. The vortex dynamics explained the role of the phase relation between the wing translation and rotation in lift generation. It also gave an intuitive picture of why the instantaneous forces can reach a periodic state after only a few strokes. This, in principle, enables an insect to take off quickly. It showed that a two-dimensional hovering motion could generate enough lift to support a typical insect's weight, thus dispelling the myth that "bumble bees cannot fly according to conventional aerodynamics."



The fruit fly generates impressive lift by beating its wings in a figure-of-eight pattern

- **Short Range Tests of Newton's Inverse Square Law:** Gravity poses one of the biggest mysteries in physics: Why is it so weak compared to all the other forces of nature? Recently, an intriguing solution to this puzzle, involving "extra" space dimensions, has been suggested. String theory requires that there are 10 space dimensions, and it is usually assumed that 7 of these dimensions are curled up in very tiny regions, so small that they cannot be detected with foreseeable technology. The new idea, due to Nima Arkani-Hamed and Savas Dimopoulos of Stanford University and Gia Dvali of New York University, is that the apparent weakness of gravity could be explained if gravity can "leak off" into the extra dimensions while everything else is confined to the usual 3 dimensions of length, width and height. The University of Washington[75] group, consisting of C. D. Hoyle, U. Schmidt, B. R. Heckel, E. G. Adelberger, J.H. Gundlach, D. J. Kapner, and H. E. Swanson, recently measured the strength of gravity at a distance of just 0.2 millimeters and found no deviation in the gravitational pull from that predicted by Newtons' inverse-square law. The current findings are based on results using a ring suspended just above a rotating disk. The ring, which has 10 small holes bored into it, hangs by a tungsten fiber just 20 microns (less than one-thousandth of an inch) thick. The rotating disk, which has 10 similar holes bored into it, exerts gravitational pull on the pendulum, twisting it back and forth 10 times for every revolution of the plate. The amount of twist is measured by shining a laser beam off a mirror mounted on the ring. The active component of the pendulum is a ring with 10 holes bored into it. The rotating attractor situated just below the ring consists of 2 discs. The UW team already is fabricating equipment to test to 0.1 millimeter or less, and has begun planning an experiment to test at even smaller distances.

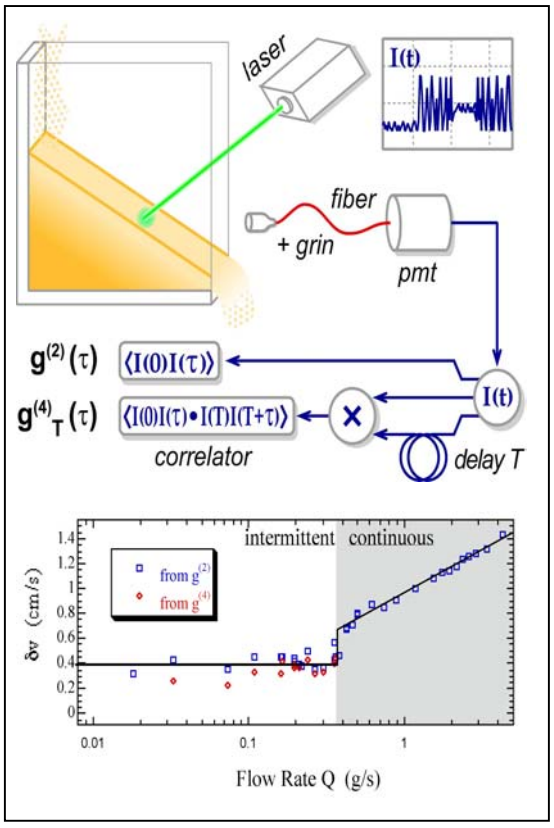


- **LIGO International Collaboration.** A prototype data exchange has been implemented allowing LIGO and VIRGO (the French-Italian gravity-wave detector) scientists to exchange data every 10 minutes for a pre-defined small subset of the respective project channels. VIRGO is a collaboration

[74] DMS-0075510
[75] PHY-9970987

between Italian and French research teams on a three-kilometer interferometric gravitational wave detector located at Cascina, near Pisa, Italy. Initial studies will focus on seismic, electromagnetic, and power line signal correlations. These studies will provide a basis for understanding the remote seismic, electromagnetic, and power grid correlated environments that will affect future gravitational-wave searches using a long-baseline, intercontinental array of detectors.

Granular Media and Aspirin: Granular materials are mysterious. Under small forces they remain at rest, like a solid, while under large forces they can flow like a liquid. In between they tend to flow intermittently, for example by a series of avalanches. Doug Durian of the University of California at Los Angeles[76] has developed a new experimental tool capable of resolving grain dynamics across this entire range of behavior. He exploits extra information in higher-order correlations in the intensity fluctuations of light multiply scattered from the sample, allowing for unprecedented study of the transition from smooth to intermittent flow. They find that fluctuations inside avalanches are a bit slower than in smooth flow just above the transition. They also find that the avalanches are quasiperiodic, less random than telegraph noise. This challenges current theoretical ideas, which are limited to the extremes of very slow or very rapid flow. Such work may eventually help prevent unwanted jamming that unpredictably plagues the transport of granular materials in so many industries. Similarly, it may help solve the familiar problem of how to pour exactly two pills from that bottle of aspirin….



[76] DMR-0070329

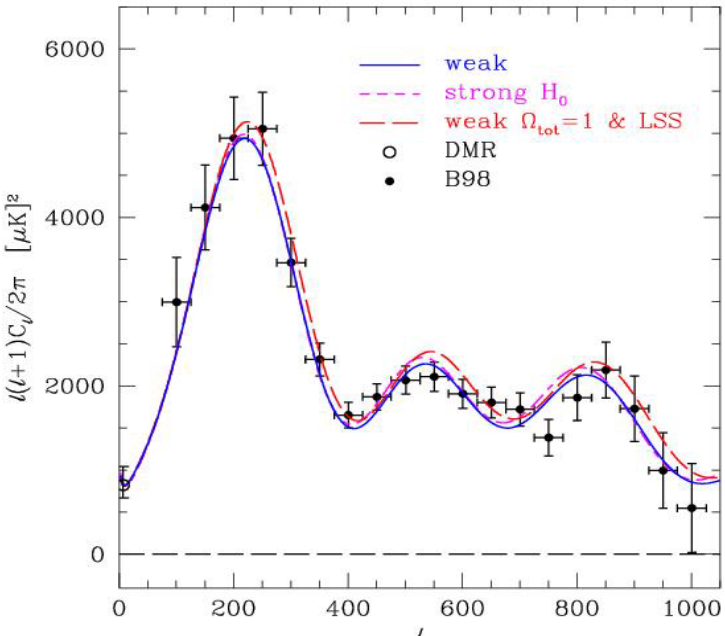
Examples of MPS Directorate Performance for FY 2001

Indicator 2. Discoveries that advance the frontiers of science, engineering, and technology

MPS Primary Area of Emphasis: Enhancing Instructional Workforce

- **Cosmic Microwave Background.**

- The Cosmic Microwave Background radiation (CMB) is the remnant radiation from the Big Bang. The CMB allows us to look back billions of years to a time when the early universe was only a few hundred thousand years old. This was before the first stars and galaxies were formed but after most of the more complex, high-energy, elementary particle interactions ceased to have any large-scale impact. CMB measurements offer a powerful tool for examining basic properties of the universe such as its geometry, expansion, dark matter and energy content, age, and evolution. CMB observational data is usually presented as an angular power spectrum, and the location and magnitude of these peaks enable scientists to determine these quantities. Last year the NSF-supported BOOMERanG telescope measured the very faint temperature fluctuations in the microwave radiation and confirmed earlier indications that the geometry of the universe is Euclidean. The BOOMERanG experiment mapped the CMB using highly sensitive arrays of microwave detectors with a balloon-borne telescope that circumnavigated Antarctica. Since then, a number of NSF-supported teams have published additional measurements that have strengthened and extended the initial conclusions. Andrew Lange of the California Institute of Technology[77] and John Ruhl of the University of California at Santa Barbara,[78] reporting on further analysis of the BOOMERanG measurements, John Carlstrom of the University of Chicago[79] reporting new data taken at the South Pole with the DASI experiment, and Andrew Jaffe of the University of California at Berkeley[80] reporting data taken with the Maxima-1 balloon experiment all described measurements that provided new information on the magnitude and location of the higher-order (smaller angular-scale) peaks in the spectrum. Both the BOOMERanG and Maxima-1 experiments



Plot of the BOOMERanG data by angular scale. The peaks occur at scales of roughly 1degree (l= ~200), 20 arc minutes (l=~550), and 15 arc minutes (l=~850). The colored curves are several models that produce fits to the data.

[77] AST-0098737, AST-9729121, and OPP-9729121
[78] AST-9813920
[79] AST-0096913, OPP-9940455
[80] AST-9872979

received support from the NSF Center for Particle Astrophysics of the University of California at Berkeley.[81]

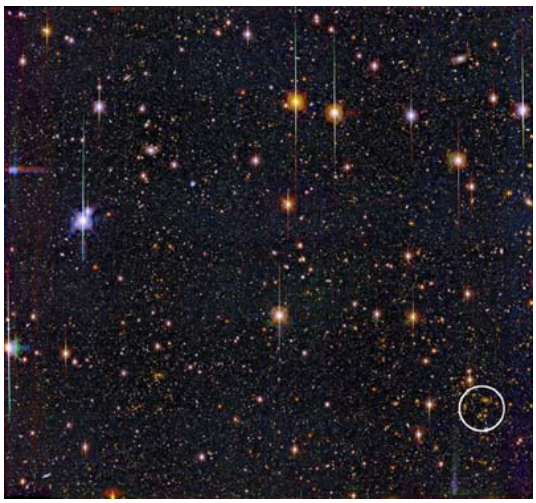
- **Cosmic Background Imager.** The BOOMERanG, DASI, and Maxima instruments are all designed to measure scales of ~30 arc minutes (roughly the size of the full Moon). Results obtained by Anthony Readhead of the California Institute of Technology[82] using the Cosmic Background Imager (CBI) in the Chilean Atacama Desert complement these data by being sensitive to fluctuations at smaller angular scales of 4.2 arc minutes or 1/7 the size of the full moon. The CBI observations show a sharp decrease in the fluctuations at small angular scales, out to roughly 8 arcminutes (l=1500). Such a decrease in power at high l is one of the fundamental predictions of the standard cosmological model, and these are the first observations that cover a broad enough l-range to show this decrease in a single experiment. Further information is available on the web sites for BOOMERanG,[83] MAXIMA,[84] for the CBI,[85] and for DASI.[86]

- **Alternative Interpretations.**. The fits to the CMB measurements all agree that models of the Universe which have a "flat" geometry, are dominated (by up to 90%) dark matter, and fit the standard nuclear physics models for the generation of the hydrogen and helium during the Big Bang are consistent with the observations. However there are also other theoreticians working on alternative interpretations of the measurements. Max Tegmark of the University of Pennsylvania[87] has proposed several more exotic cosmologies and McGaugh of the University of Maryland[88] has proposed that a Universe with no dark matter content can explain the observations.[89] Support of these researchers illustrates the effort to balance appropriate high risk and innovative research with more conventional community-endorsed approaches of most investigators.

- **Nanoporous diamond.** Yuri Gogotsi of Drexel University[90] and Michael McNallan of the University of Illinois at Chicago[91] reported the conversion of silicon carbide to crystalline diamond-structured carbon at ambient pressure and temperatures at or below 1000ºC, without plasma activation. This technique involves placing silicon carbide into glass tubes, heating it, and exposing it to a mixture of chlorine and hydrogen gases. A form of pure carbon almost identical to both natural and conventional synthetic diamond, but built of nanocrystals (just a dozen atoms in cross-section), is produced. The transmission electron micrograph shows regions of both graphite and diamond. Like natural or other synthetic diamond, each carbon atom is tightly bonded to four neighbors, but the arrangement of these groups can be slightly different. *This method allows for synthesis of very hard, stiff, nanoporous, and ultra-light diamond and/or diamond-graphite nanocomposites*.

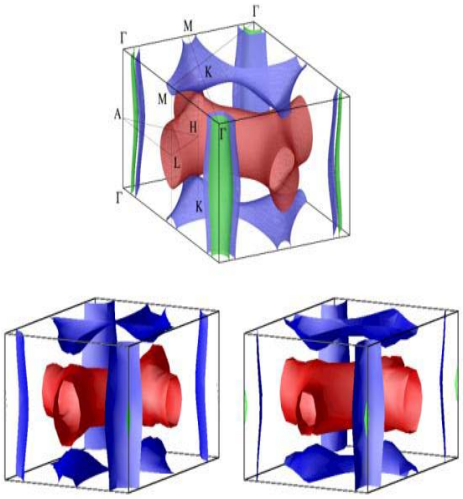
[81] AST-9120005
[82] AST-982989 and AST-0098734
[83] http://www.physics.ucsb.edu/~boomerang/new_press_images/index.html
[84] http://cfpa.berkeley.edu/group/cmb/
[85] http://www.astro.caltech.edu/~tjp/CBI/
[86] http://astro.uchicago.edu/dasi/
[87] AST-0071213
[88] AST-9901663
[89] http://www.astro.umd.edu/~ssm/mond/
[90] DMR-9874955
[91] CMS-9813400

- **Discovering Galaxies Without Using Their Light.** CTIO 4-meter Blanco Telescope observations made by J. Anthony Tyson and David Witten of Lucent Technologies have used the distorting effects of a weak gravitational lens to discover and locate a dim cluster of at least 15 galaxies at a significant distance from Earth. This discovery was made using only the mass properties of the cluster, not its visible light. This first-time accomplishment raises prospects for a powerful technique called 3-D mass tomography to conduct large-scale searches for dark matter. This approach may provide a valuable independent check of current theories about the accelerating expansion of the Universe. In the figure, the circle in the lower right-hand corner of the image encloses the galaxy cluster.



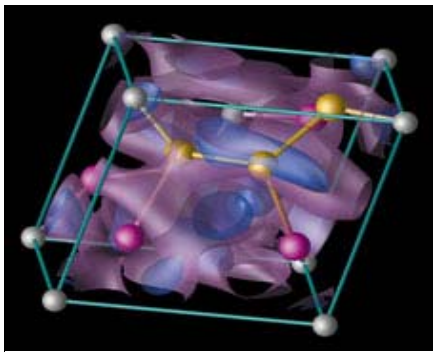
- **The Superconductor MgB_2.** In January 2001 superconductivity was discovered in the commonly available material MgB_2. This material exhibited a "high" transition temperature of 40K. Amy Liu of Georgetown University,[92] in collaboration with researchers at the Naval Research Laboratory (NRL), used density functional theory to calculate the electronic structure and Fermi surface of MgB_2 and electron-phonon coupling strengths, a measure of the strength of the contribution of a particular phonon

Tthe electronic structure calculations of the Fermi surface of $MgB_{2\ for}$ the undistorted crystal (top) and for two B bond-stretching phonon patterns of opposite sign (left and right). Opposite distortions induce opposite changes in the 3D sheets (tubular networks) but the same changes in the 2D sheets (cylinders) show the nonlinear coupling of this mode to the electrons in the 2D sheets. This nonlinearity may help explain the way the transition temperature depends upon the isotopic mass of the constituent elements.



mode to the "glue" that binds the electrons into pairs in the conventional theory of superconductivity. The model is supported by currently available tunneling and thermodynamic data, and may help explain the high transition temperature and the puzzling way it depends upon the isotopic mass of the constituent elements. The exploration of superconductivity in MgB_2 and related materials and their possible technological applications has only just begun.

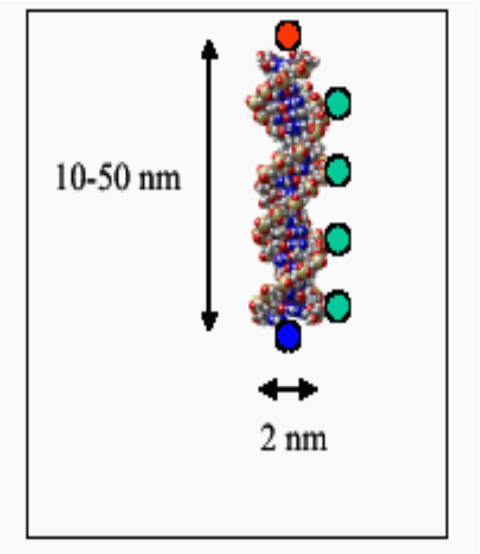
[92] DMR-9973225



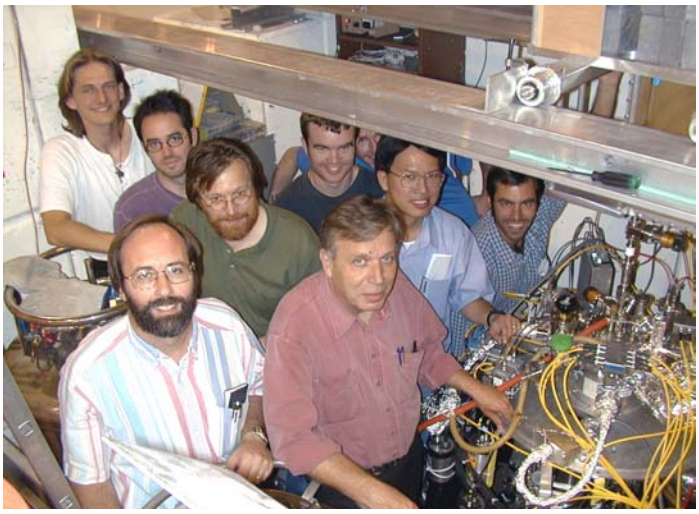
Calculated electronic density of a candidate direct band-gap material CSn_2Si_2. The results suggest that a good interface with silicon based electronic circuits can be made.

- **Properties of Materials.** We continue to develop the ability to predict, from fundamental theory, the properties of materials not found in nature or not yet synthesized. Motivated in part by the desire to construct a new material to improve the interface between electronic and photonic devices, Vincent Crespi of Pennsylvania State University[93] and Steven Louie and Marvin Cohen of the University of California at Berkeley[94] worked in collaboration with materials scientists to design optoelectronic materials that could actually be fabricated. Electronic structure calculations using density functional theory together with a many-body perturbation theory method were used to determine candidate alloys involving only group IV elements which have desirable features: a lattice constant that matches well with that of silicon, a direct bandgap in the range of 0.7 to 1.0 eV that is optimal for optical transitions, and well-defined synthesis strategies that potentially enable production of bulk quantities of material. Two candidate materials were predicted, one of which is shown in the Figure.

- **Unconventional Wisdom Concerning Nano-Lightpipes.** Everyone knows that it is impossible to propagate light through structures smaller than the wavelength of light. Julia Kornfield and her colleagues at the California Institute of Technology[95] have belied this conventional wisdom, showing that light can propagate along waveguides whose lateral dimensions are only a few nanometers, or a few percent of the wavelength of light. The key is to exploit the tendency for electromagnetic excitations to "hop" between electric dipoles (such as fluorescent dye molecules or metal nanoparticles). The Caltech researchers demonstrated light propagation through two types of sub-wavelength-scale waveguides. The first is a DNA waveguide in which a fluorescence excitation hops from an optical donor molecule bound to one end of the DNA backbone to an acceptor molecule at the other end through dye molecules tethered at intervals in between (see figure). These fluorescence resonant energy transfer waveguides have so far shown that light can take several hops between molecules bound to DNA, and this can be extended to many hops along a longer waveguide. The second nanoscale waveguide structure is called a "plasmon wire," which is a chain of metal nanoparticles along which light hops from one particle to another. Light can even propagate around sharp corners and through nanoscale networks – all of which is impossible in conventional optical waveguides.



[93] DMR-9876232
[94] DMR-0087088
[95] DMR-0080065



Jubilant ATRAP collaborators next to the apparatus that first trapped, electron-cooled and stacked 4.2K antiprotons

- **ATRAP Collaboration Announces Cooled Positrons and Antiprotons in Same Trap: Major Step Toward the Production of Cold Antihydrogen.** CERN's unique new antimatter factory, the Antiproton Decelerator (AD,) first delivered antiprotons to experiments in July - November of 2000. The ATRAP experiment, led by Gerald Gabrielse at Harvard University,[96] is attempting to make cold antiprotons interact with cold positrons (the antimatter counterpart of electrons) in order to form cold antihydrogen atoms for the first time. An antihydrogen atom, a positron orbiting an antiproton, is the simplest atom formed entirely of antimatter. Several very rapidly moving antihydrogen atoms were first observed at CERN in 1995, demonstrating that these atoms can be formed. With CERN's newly dedicated facility the quest begins to make antihydrogen atoms that are cold enough to be trapped. Once such atoms are trapped, lasers can probe for tiny differences between antihydrogen and hydrogen. In May 2001 the ATRAP Collaboration announced the first use of cold positrons to cool another type of particle – antiprotons. ATRAP now has both of the ingredients of cold antihydrogen in the same trap structure at the same time – both 4.2 K antiprotons and 4.2 K positrons – and they are interacting. This is the closest that anyone has been to producing cold antihydrogen.

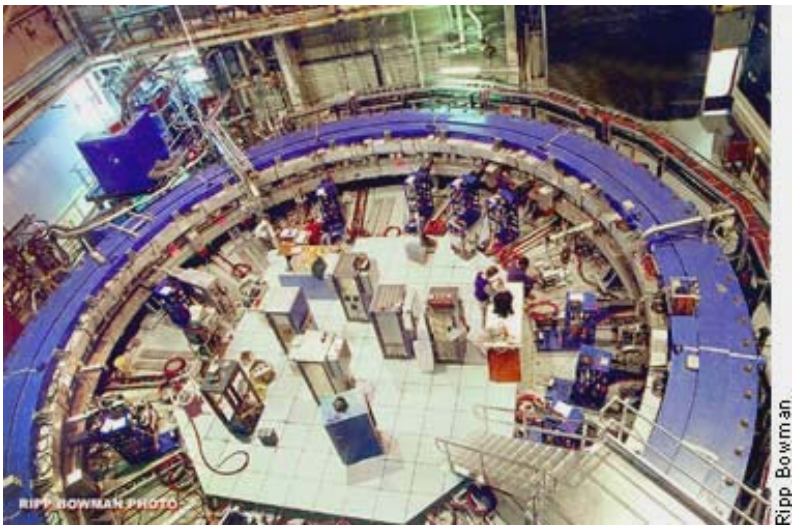
- **Schrodinger's Cat and Quantum Computing.** Research at the frontier of classical and quantum mechanics continues to excite many scientists. This field presents major experimental challenges and typically involves research at ultra-low temperatures. One area of focus is quantum coherence. The challenge is to measure or control the "coherence" of a quantum state for multiple cycles, – the more cycles the better. This turns out to be exceeding challenging in solids owing to normally strong interactions between the quantum state and its environment. It becomes even more challenging when the states involve large numbers of electrons, approaching macroscopic proportions. In such cases, a situation analogous to the famous Schrödinger cat conundrum is approached. James Lukens at the State University of New York at. Stony Brook[97] has been able to create a superconducting device in which two Josephson junction SQUID circuits with oppositely circulating currents are coherently maintained in the same quantum state. This is the largest system in which these strange effects predicted by quantum mechanics have ever been seen.

[96] PHY-9722595
[97] DMR-9876850

There are ramifications of such experiments both for fundamental measurement theory of quantum mechanics and for possible creation of qubit elements for quantum computing.

- **Quantum Cosmology and Polymer Geometry.** Most physicists believe that general relativity ceases to provide a good description of the physical reality in the vicinity of the Big Bang itself. On general physical grounds it is clear that such a theory must incorporate effects not only of general relativity but also of quantum physics. Over the last two years the research program on quantum gravity that was initiated by Martin Bojowald, Abhay Ashtekar and others at Pennsylvania State University,[98] attempting to unify general relativity and quantum physics, has found that at the tiniest scale conceivable today, called the Planck length (10^{-33} cm), the continuum picture of space breaks down and has to be replaced by a precise 'polymer-like geometry'. While at the laboratory scales (10^{-18} cm and above) this true geometry can be approximated by a continuum, the approximation fails miserably near the Planck scale. As the universe expands, its volume does not change continuously but only in discrete steps. Near the Big Bang one must abandon the use of differential equations on which most of physics is based and replace them by more fundamental difference equations describing the 'true' time-evolution. Once this is done, infinities disappear and regular physics is restored without any ad-hoc assumptions. While general relativity is an excellent approximation for today's universe, space-time 'dissolves' near the Big Bang. Einstein's deterministic, geometric universe has to be replaced by a specific, probabilistic universe built from polymer geometry.

- **Muon Anomalous Magnetic Moment and New Physics Beyond the Standard Model.** A collaboration working at the Alternating Gradient Synchrotron at Brookhaven National Laboratory, involving B. Lee Roberts of Boston University[99] and Alan Nathan and David Herzog of the University of Illinois,[100] has reported its initial findings on the g-2 experiment after several years of data taking and analysis. The experiment, which measures the magnetic moment anomaly of the muon to a precision of 1.3 parts per million, has yielded a result that is at variance with calculations from the standard model of particle physics. More data remain to be analyzed; however, if the variance with the standard model holds up, it can mean there is new physics (symmetries, particles, etc.) yet to be explored that gives rise to this small, but very significant, discrepancy.

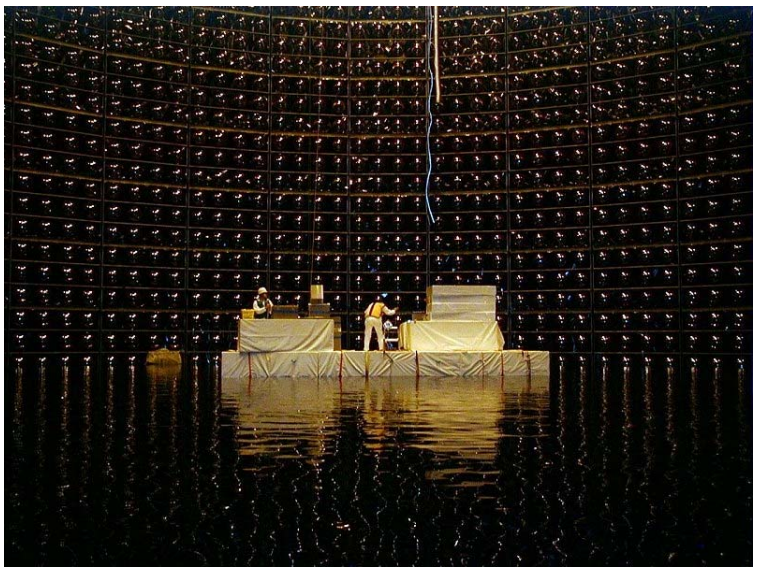


- **HiRes Sees Highest Energy Cosmic Rays.** Researchers led by P. Sokolsky of the University of Utah,[101] using the University of Utah's HiRes cosmic ray detector, have found clear evidence of the pile-up associated with the GZK cut-off, an energy limit beyond which particles from sources at cosmological distances should not occur due to interaction with the cosmic microwave background radiation left over

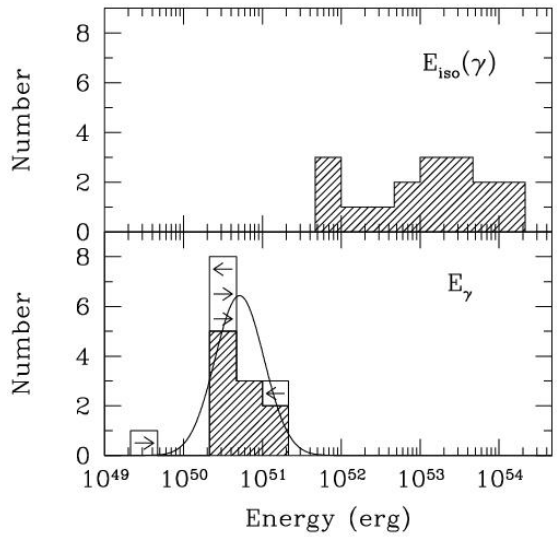
[98] PHY-0090091
[99] PHY-9722600
[100] PHY-9420787
[101] PHY-9943497

from the Big Bang. The highest energy event observed is found at 2 x 10^{20} eV. This group has now performed four independent experiments and analyses. These new results challenge our understanding of the most energetic particles in the observable universe. A documentary video of HiRes and the search for high-energy cosmic rays has been made by associates of the HiRes group in order to introduce fundamental physics concepts to K-12 teachers and students.

- **Super-Kamiokande Neutrino Detector Observes Flavor Oscillations.** Super-Kamiokande is a 50-kiloton water-Cerenkov detector located at a depth of 1500 meters in the Kamioka-Mozumi mine of Japan. The detector was designed to explore neutrino properties by making high statistics measurements of neutrinos produced in the atmosphere by high-energy cosmic rays and neutrinos produced in the nuclear reactions of the sun. It is also the world's most sensitive detector for proton decay. The first era of operations, which began in April of 1996, has come to a close in July of this year for detector upgrades and repair. Results of this experiment have included the first convincing evidence for neutrino oscillations and non-zero hence neutrino mass. In addition, the most precise measurements to date of solar neutrinos using neutrino-electron elastic scattering was performed. This measurement in combination with the Sudbury Neutrino Observatory (SNO) charged current measurement of solar neutrinos has yielded better than 3-sigma evidence for solar neutrino oscillations.



Repair work in the Super-K detector - August 2001



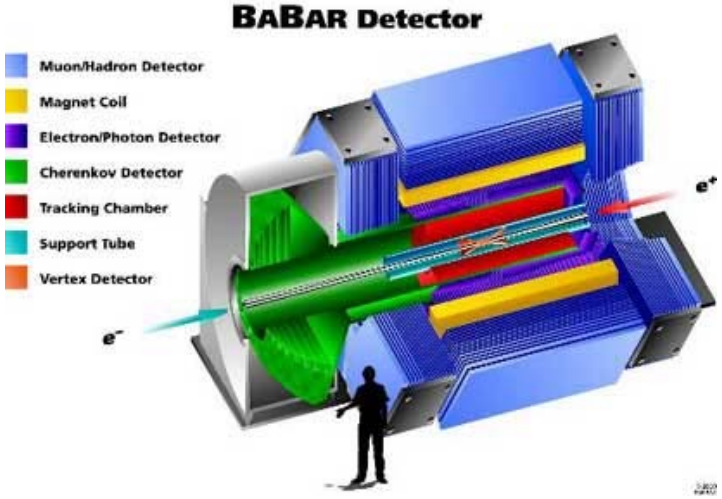
Gamma-ray Bursts. Gamma-ray bursts (GRBs) are mysterious flashes of high-energy light that are detected about once a day somewhere on the sky. They are now known to be the most brilliant, transient events in the Universe. Their power, the energy per unit time, is so immense that for a brief moment the power of a GRB can compete with the power emitted by the rest of the Universe. However, their origin remains unknown. Most believe GRBs are enormous explosions that occur at great distances and that there is a powerful "central engine" which powers the burst.

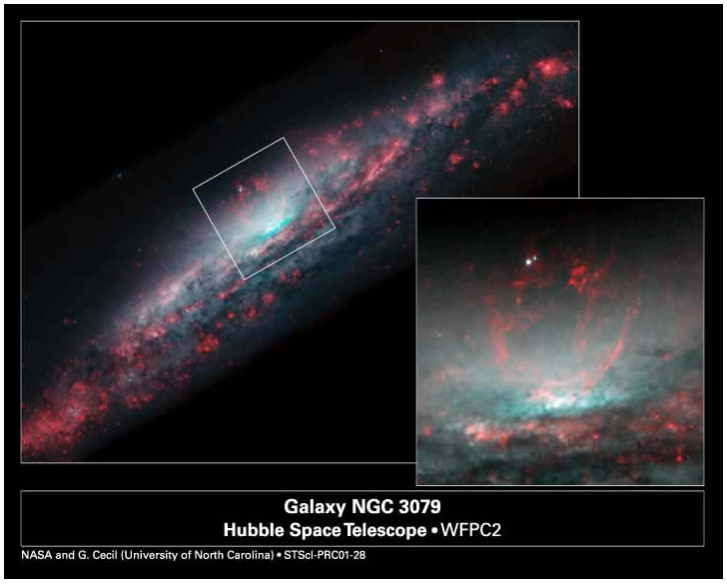
Sri Kulkarni of the California Institute of Technology[102] and collaborators, using the Very Large Array (VLA) and a number of ground-based optical telescopes, have now established that the central engines appear to release a fixed amount of

[102] AST-0098676 and AST-9803157

energy which comes out in the form of a 2-sided jet. This is one of the first clues about the nature of the central engine – the true energy is about 10^{51} erg – similar to that of supernovae. This hints at a fundamental connection between GRBs and supernovae. In the figure, the top panel shows the apparent energy of a GRB, assuming isotropic emission. The bottom panel shows the effect of incorporating estimates of the opening angles of jets to obtain estimates of the actual energy release.

- **The Matter-Antimatter Asymmetry Puzzle Continues.** Why is the universe full of matter, rather than equal amounts of matter and antimatter? There must be some fundamental asymmetry in nature that favors matter over antimatter. An international collaboration of physicists conducting experiments at the Stanford Linear Accelerator Center[103] (SLAC) has discovered a new, fundamental difference between the behavior of matter and that of antimatter. Using a 1,200-ton detector named BABAR, they observed this intriguing phenomenon – known as charge-parity (CP) violation – in decays of heavy, short-lived subatomic particles called B mesons. This is the second observed case of CP violation, a process first seen decades ago in experiments with K mesons (for which the Nobel Prize in Physics went to Val Fitch and James Cronin). The detector records subtle distinctions between decays of B mesons and those of their antimatter counterparts, called anti-B mesons. Both are more than five times heavier than protons and live for just over a trillionth of a second. Physicists employed the detector to observe an unmistakable difference, or asymmetry, between the rates at which B and anti-B mesons decay into a special set of specific final states. Until the BABAR discovery, no subatomic particles other than K mesons had clearly exhibited this exceedingly rare phenomenon.



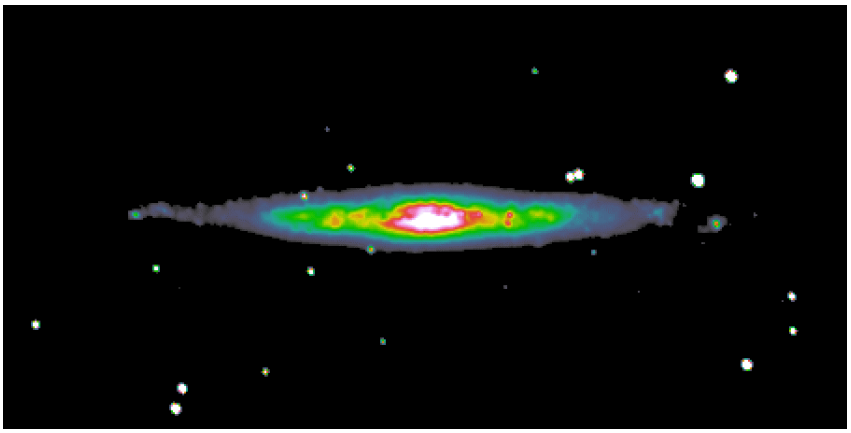


- **Superwinds.** Studies on superwinds in active galaxies and galactic fountains in normal galaxies have been made in the optical by CAREER awardee Sylvain Veilleux of the University of Maryland[104] to determine the extent, origin, and source of the ionization of the material that is seen well out of the plane in normal spiral galaxies. The mass and extent of the warm extra-planar material is correlated with the local star formation rate in the disk, and photoionization by normal hot, massive OB stars appears to be the primary source of the ionization. It appears that an additional source

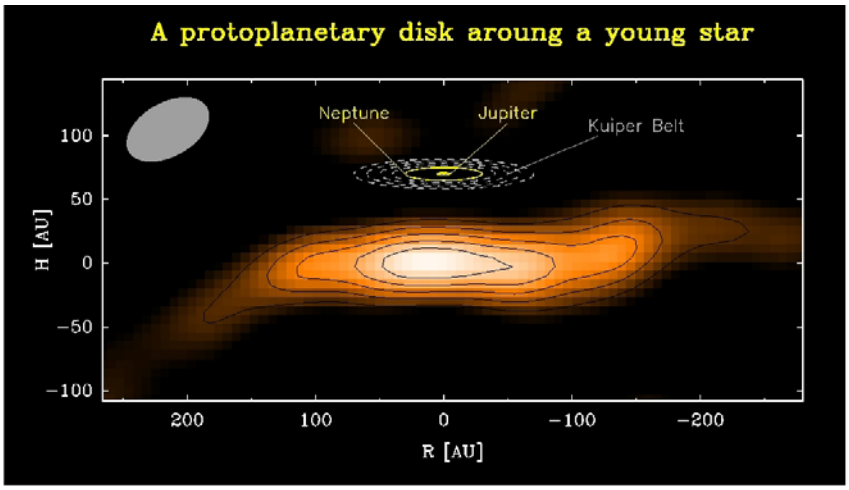
[103] P.Burchat of Stanford University (PHY-9876867) and B. Meadows, University of Cincinnati (PHY-9901568)
[104] AST-9874973

previously thought necessary, is required in only a few galaxies. The work on superwinds in active galaxies looks at the effects these powerful events have on the host galaxies and the surrounding environment. Ground-based Fabry-Perot data are combined with radio and X-ray data and Hubble Space Telescope images to track the energy flow through various gas phases. The data show spectacular ionized filaments on the outskirts of the host galaxies, as in this image of NGC 3079. These filaments occasionally extend well beyond the HI extent that normally defines the galaxy extent.

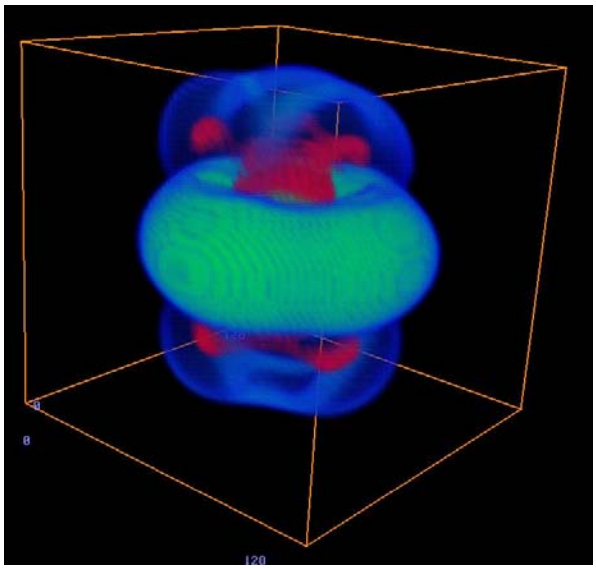
- **Thin Galactic Disks.** The nearby disk galaxy NGC 4244 looks unremarkable, but its simple structure holds a puzzle. Astronomers find that the model of hierarchical structure formation successfully describes the formation of structure in the early universe: structures first form in small clumps and then merge to make larger galaxies. But when disk galaxies merge, the very flat, kinematically cold disks are destroyed. Recent work by Heather Morrison of Case Western Reserve University[105] and collaborators shows that NGC 4244 has only a thin disk, down to some of the most sensitive limits on surface photometry ever achieved. How did this disk galaxy escape the ubiquitous merging activity for many billions of years and survive as such a cold, fragile structure?



- **Protostellar Core Fragmentation.** Postdoctoral scholar, R. Launhart, and Anneila Sargent of the California Institute of Technology have done observations of protostellar core fragmentation and binary star formation.[106] A total of 13 sources have now been observed. Molecular line images can be constructed for six of these sources. They identify two extended sources, probably protostellar cores, three protobinary systems, and one putative preplanetary disk. Based on the continuum morphology – the emission is elongated along a direction perpendicular to the axis of the associated bipolar nebula – and the Keplerian velocity pattern, CB26 appears to be surrounded by a preplanetary disk. An image of this disk is shown.

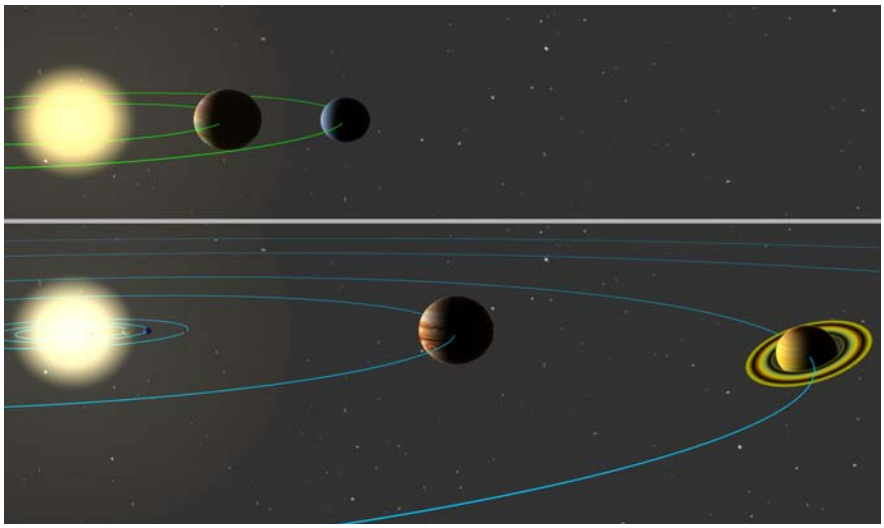


[105] AST-9624542
[106] AST-9981546



- **Stellar Outflows.** Adam Frank of the University of Rochester[107] is using his CAREER grant to model outflows that mark the birth and the death of stars. Outflows take the form of fast streams of gas (100 to 1000 km/s) blown off the surface of a star and interacting with surrounding matter. The combination of violent shock waves (formed at the interaction region) along with ionizing stellar UV fluxes combine to produce observable outflows in the form of luminous clouds of plasma. The outflows offer important clues to unknown processes occurring at the extremes of stellar evolution and serve as fossil imprints of the obscured central star's history. Frank and his collaborators produced a series of supercomputer simulations aimed at understanding the nature of these outflows. The figure to the left shows the result of a fully 3-D simulation of a stellar wind expanding into a pre-existing doughnut or torus of ambient gas. The outflowing wind is constrained to flow out the top and bottom of the holes of the torus producing a "bipolar" stellar outflow.

- **Extra-solar Planets.** A major impetus to the observational and theoretical studies of the formation of stars and their planetary disks has been provided in the last few years by the discovery of extra-solar planets. The most recent discovery, by the team of Geoff Marcy of the University of California at Berkeley,[108] Dennis Butler and Deborah Fischer of the Carnegie Institute of Washington, and Steve Vogt of the University of California at Santa Cruz, finds a planet three-quarters the mass of Jupiter in a circular orbit around the solar-like star 47 Ursa Majoris. Although 70 extra-solar planets have been found thus far, this is the first system with two planets in circular orbits, and at distances that make the planetary system similar to our own.

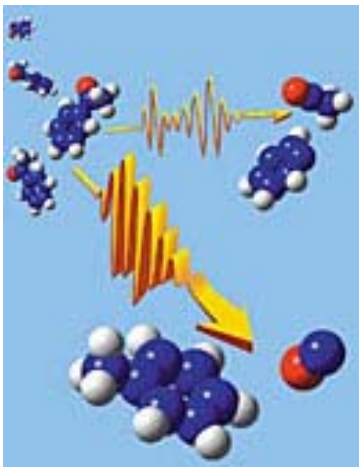


Artist's conception of the 47 UMa planetary system, by comparison to our solar system. In a striking parallel to our solar system (bottom), both Jupiter-size planets are in nearly circular orbits around their star (top). The diameters of the sun, the star and the planet orbits are not to the same scale.

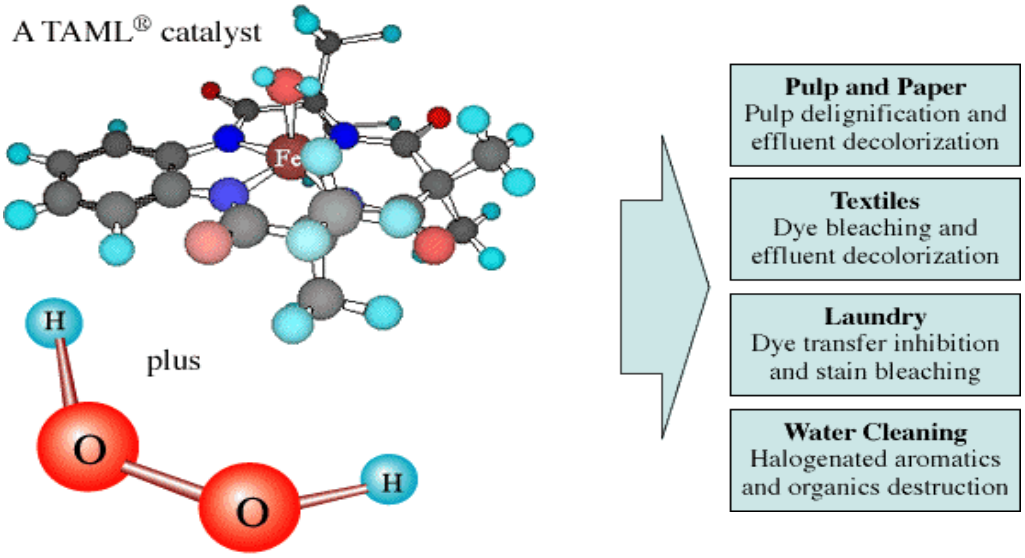
- **Quantum Control.** One of the "holy grails" of chemistry is the use of carefully tailored laser pulses to cause photochemical reactions to proceed along one of a number of parallel reaction pathways. This concept of influencing reaction dynamics and product distributions, known as quantum control, is

[107] AST-9702484
[108] AST-9988087, AST-9988358

becoming more of a reality as laser pulse-shaping technology advances. The rapid re-equilibration of excited state energy has, to date, thwarted efforts to tune product distributions selectively. Progress in achieving quantum control of reactions has accelerated in the past year as illustrated by the work of Robert Levis of Wayne State University[109] and by Herschel Rabitz of Princeton University.[110] These researchers have combined Monte Carlo sampling and chemical analysis of reaction products to develop practical techniques for tuning laser pulse combinations for the production of desired products. As an illustration of the method of strong field quantum control, acetophenone molecules (upper left hand corner of the figure) can interact with intense, tailored laser pulses to produce selective bond rearrangement and cleavage. The upper pulse is amplitude and phase shaped to cleave the phenyl-carbonyl bond producing C_6H_5 and CH_3CO. The lower pulse is tailored to rearrange the parent to produce toluene and CO. The optimal laser pulses are derived through an automated closed-loop feedback learning process in the laboratory.



- **Household Laundry and Green Oxidation Processes.** Terrence Collins and colleagues at Carnegie-Mellon University[111] have developed catalysts for the activation of hydrogen peroxide in water for green oxidation processes that might substitute for polluting processes that currently utilize chlorine. They have made important discoveries in homogeneous oxidation and in bleaching chemistry that have significant commercial implications. Catalytic activators of hydrogen peroxide known as *TAML activators* (TAML = Tetra-Amido Macrocyclic Ligands) were developed. TAML molecules are broadly useful homogeneous catalytic activators of hydrogen peroxide in water. The trademark is now registered in both the USA and Europe. Ten US patents have been obtained claiming their unique catalytic properties in conjunction with hydrogen peroxide and scores of international applications have been filed. TAML activators offer a significant technology breakthrough in the laundry industry, which is searching for cost-effective, environmentally benign alternatives to prevent dye transfer in household laundry processes. TAML activators provide the most potent dye transfer inhibition technology yet discovered. They work under mild



[109] CHE-9976476
[110] CHE-9807443
[111] CHE-9612990

conditions in neutral to basic pH. They effectively activate hydrogen peroxide in minute concentrations (nanomolar to millimolar). They work to prevent dye transfer throughout the entire temperature range used in laundering, and show extremely high selectivity for fugitive dye molecules over fabric-bound dye. The non-toxic catalysts decompose into inactive products while performing the bleaching task. These discoveries are expected to conserve water by facilitating the move of laundering to smaller volume washing machines. These TAML activator catalysts are also being explored and exploited for use in pulp bleaching, a process that employs chlorine-bleaching technologies that have caused major pollution of rivers. As a result of his work, Collins received the Presidential Green Chemistry Challenge Award and the Annual Award of the Society of Pure and Applied Coordination Chemistry of Japan.


Courtesy of University of Wisconsin

- **Chemistry, Astronomy, and Antibiotics.** In studies that highlight the broad conceptual context of organic chemistry, Robert McMahon at the University of Wisconsin at Madison[112] is carrying out fundamental research in mechanistic organic chemistry that is leading to a deeper understanding of the organic chemistry and spectroscopy of dense and diffuse interstellar clouds. Interstellar clouds are the birthplace of new stars and planets. The existence of complex organic molecules in the interstellar medium may have profound implications concerning origins of life. McMahon has recently prepared and characterized highly reactive species modeling the carbon-chain compounds postulated to serve as diffuse interstellar band carriers, including propadienylidene ($H_2C=C=C:$) and *cis*-hex-3-ene-1,5-diyne (HCC-CH=CH-CCH). The latter not only provides a link between the open-chain hydrocarbons known to exist in interstellar clouds and the aromatic compounds thought to exist there, but also addresses fundamental questions about the reactivity of a powerful new class of pharmaceutical agents, the "enediyne" antibiotics.

- **Molecular Computing and Chirality.** Many molecules of biological importance such as amino acids, nucleic acids, carbohydrates and their metabolic products are chiral, i.e. mirror image molecules are not identical. The structural, metabolic and functional control, modulation, and responses of these molecules are controlled by the chirality. Because chiral phenomena are common in living systems, most medicinal agents are chiral. However, application of chirality in the design, synthesis, and utilization of materials is rather limited in non-medical fields. Recent studies on the development of chiral materials have led to systems with strong chiroptical properties in circular dichroic and polarimetric measurements. James Canary and coworkers at New York University[113] are currently studying copper coordination complexes and their derivatives with electrochemical and chiral properties. In a recent publication the investigators have reported light-activated interconversion of thioxanthenes, where lights at two different wavelengths activate the forward reaction and reactions. These studies indicate that the chirality a molecule and its properties and

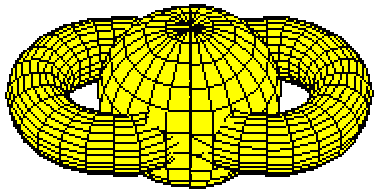
[112] CHE-0110769
[113] CHE-0079072

applications may be controlled by changing the wavelength of the light, opening up the possibility of optically modulated molecular computing.

Investments in Non-Initiative Fundamental Research (NSF Areas of Emphasis)

1. Mathematical Sciences Research

- **Tiled Surfaces.** A tiling of a Riemann surface is a covering by polygons, without gaps or overlaps, of a two-dimensional surface. Now if the surface has genus higher than 2, say as in the picture shown, then the geometry will be hyperbolic. What that means is that if we cut apart the surface, flatten it and try to join together replicates to tile a plane, we will end up with a tiling of the hyperbolic plane. Thus the edges of the tiling will follow the curved lines of hyperbolic geometry. To the right is an example of an unwrapped tiled surface giving a tiling of the hyperbolic plane by (4,3,3) triangles. Now it is more than a coincidence that we don't have a picture of a hyperbolic surface here. That is because it is quite difficult to draw them, and since it is impossible to have a geometrically true 3D realization of these surfaces. One of the goals of the REU site led by Allen Broughton at the Rose-Hulman Institute of Technology [114] was to obtain reasonable renditions of many such surfaces. They began with the unwrapped versions of the tilings as tilings of the hyperbolic plane and some recipe for abstractly constructing such a surface and understanding its geometry. The icosahedral tiling yielded the answer. The 120 triangles in the icosahedral tilings are all congruent to each other by means of a rotation or reflection of the sphere that preserves the tiling. The same is true of higher genus surfaces with highly symmetric tilings, i.e., there will be a "tiling group" of the surface that will move any tile congruently onto another. The groups can be almost any finite group, and therefore they use the methods of computational group theory.



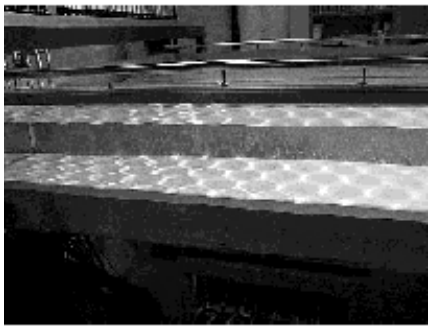
180o/l + 180o/m + 180o/n < 180o.

- **Random Matrix Theory and Integrable Systems.** Through investigations begun in the theory of random matrices, Craig Tracy of the University of California at Davis[115] discovered fundamentally new and important distribution functions that have application in several areas of mathematics and physics. These Tracy-Widom distribution functions are the simplest examples in a hierarchy of distribution functions, in the same way that the Korteweg-deVries equation is the first in a hierarchy of integrable partial differential equations. From the perspective of probability and statistics, the distribution functions describe the extreme statistics of a sequence of strongly dependent random variables. For a sequence of independent random variables, it is known that a small class of universal distribution functions describes the possible limiting distributions of the maximum. It now appears that the same is true for the Tracy-Widom distribution functions. The Tracy-Widom distribution functions were first discovered in the context of random matrix theory, where they appear as the limiting distribution of the largest eigenvalue in certain Gaussian random matrix ensembles. There is a growing literature establishing that the same is true for other random matrix ensembles. The distributions also appear in combinatorics as the limiting distribution of the length of the longest increasing subsequence in a random permutation; in the theory of stochastic growth processes as the limiting distribution of fluctuations about the shape of an interface; in statistics as the limiting distribution of the largest principal component of certain covariance matrices; in

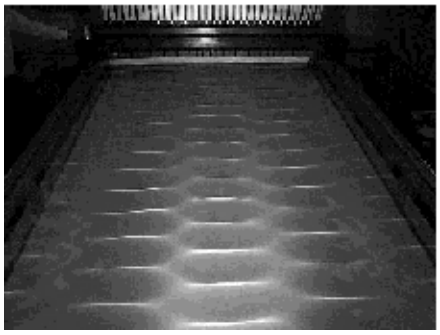
[114] DMS-0097804
[115] DMS-9303413 and DMS-9802122

the theory of superconductivity as the distribution of fluctuations of the excitation gap in a metal grain or quantum dot induced by proximity to a superconductor, and in queuing theory and the theory of random tilings. Originating from a purely mathematical construction, the Tracy-Widom distribution functions have turned out to be ubiquitous in descriptions of random processes and are now being observed in low-temperature physics experiments.

- **Water Wave Patterns**. Diane Henderson[116] of Pennsylvania State University and her colleague Joseph Hammack constructed a precise three-dimensional wave basin with a segmented wave maker and various associated instrumentation. They have also conducted related experiments in a two-dimensional wave basin and in a parametrically excited wave facility. Using the three-dimensional wave basin they observed that the two-dimensional wave patterns in deep water are significantly different from the corresponding patterns in shallow water. Nichols and Craig, using numerical experiments of the full Euler equations, predicted this result. Harvey Segur[117] of the University of Colorado conjectured that the patterns could be described by sn-solutions of either the scalar or vector nonlinear Schrödinger (NLS) equation. They observed that, consistent with the numerical results of Nichols and Craig, and with the sn-solutions of NLS, the pattern contains lines of constant height in the x direction and in the y direction. This is different from the hexagonal patterns observed in shallow water waves. Their group worked out the topological structure of the wave fields that allows for the visual appearance of hexagons, but with the wave gage measurements of lines of constant amplitude. These lines of constant height are critical to understand the patterns in deep water. The photographs below show two wave fields created by carrier waves that are modulated with a cosine modulation in the y-direction. The left photograph shows a definite hexagonal structure to the wave field. The right photograph shows a different view of a longer y-wavelength modulation.

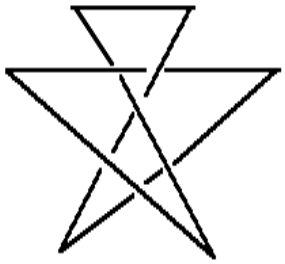


Side view showing hexagonal patterns.



View from downstream showing a zigzag pattern. Wave gage measurements show lines of constant height in this region.

- **Geometric Group Theory.** The Focused Research Group (FRG) award to Jonathan McCammond of Texas A&M University,[118] Laura Anderson of SUNY at Binghamton,[119] Noel Brady of University of Oklahoma,[120] and Robin Forman of Rice University[121] is one of several awards made this year in support of research on geometric ideas in group theory. The motivating idea for this subject is that a sufficiently large group of symmetries for a geometric



A polyhedral unknot that cannot be unknotted by rigid moves (Cantarella and Johnston).

[116] DMS-9972210
[117] DMS-9731097
[118] DMS-0101506
[119] DMS-0124326
[120] DMS-0124344
[121] DMS-0124201

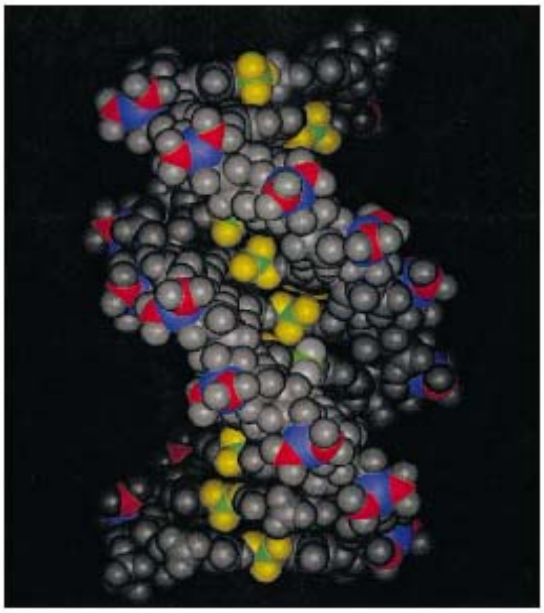
object should reflect some of the curvature-related aspects of that geometry, at least when viewed at large length scales. The four-campus FRG will explore combinatorics modeled on the geometric theory of fiber bundles and a version of the Ricci curvature that is derived from properties of the combinatorial Laplacian, imitating the Hodge theory of elliptic differential operators.

- **General Relativity.** Over the past few years there has been important progress in General Relativity. Major work has been done on the Penrose conjecture, which is a quantitative version of the positive mass theorem for spacetimes with black holes. For curved spacetimes in general relativity, there is no natural mass-energy density which can be assigned to the gravitational field, so it has been proposed to measure the gravitational mass of a region in a spacetime by minimizing the total mass of all physical spacetimes which contain this region as a subset. This minimal mass spacetime, if it can be shown to exist, will be a static solution of Einstein's equations. One of the goals of the proposal by Richard Schoen of Stanford University [122] is to find a way to construct such static solutions. Other new awards in this area include Gregory Galloway[123] and three co-funded proposals with the Gravitational Program in the Physics Division: Lars Andersson of the University of Miami,[124] James Isenberg of the University of Oregon,[125] and Vincent Moncrief of Yale University.[126]

- **Convex Geometry.** Erwin Lutwak, Deanne Yang and Gaoyong Zhang of the Polytechnic University of New York[127] focus their research on establishing sharp geometric inequalities that are invariant under linear or affine transformations and using them to obtain new analytic inequalities. This research could prove to be useful in more applied areas such as robot vision, information theory, and stereology.

2. Functional Genomics

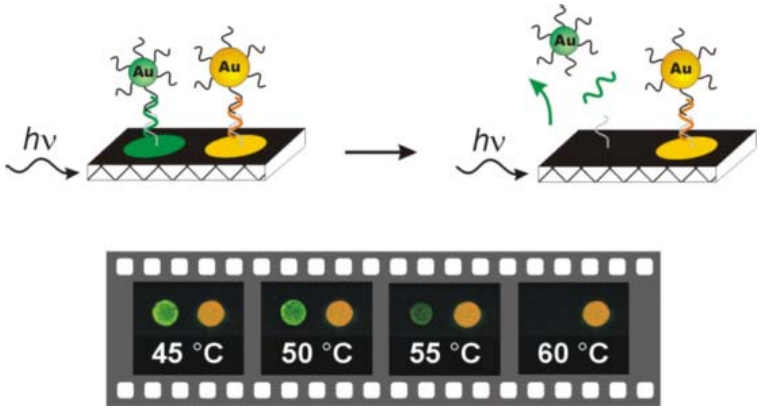
- **The Materials Science of Genetic Information.** Activities linking solid-state chemistry with the study and exploitation of biological and environmental processes are beginning to emerge. For example, double-stranded (ds) DNA has been shown to be a one-dimensional semiconductor. Anisotropic conduction in the one-dimensionally ordered solid double-stranded DNA films is attributed to the concerted movement of cations in the direction of the main axis of the ds-helices when an electric field is applied. Such movement raises the high-frequency longitudinal polarizability and thereby makes the resolved component of the high-frequency dielectric constant high. In a very significant development Adam Heller of the University of Texas at Austin[128] has determined that the biological function of the insulator-to-semiconductor transition upon parallel alignment of the ds-DNA is protection against reversible chemical change by oxidation or reduction.



[122] DMS-0104163
[123] DMS-0104042
[124] DMS-0104402
[125] PHY-0099373
[126] PHY-0098084
[127] DMS-0104363
[128] DMR-9801070

In an insulator, removing or adding an electron produces a localized reactive radical. Adding a hole or electron to a band of a semiconductor (which extends over a large number of atoms) does not make any atom in the ensemble uniquely reactive. The organization of ds-DNA in aligned, polarizable arrays may prove to be a central evolutionary strategy for preserving genetic information. Alignment is expected in the life cycle of cells and organisms when their DNA is exposed and when it becomes vulnerable in a changed environment.

- **Labeling and Detection of DNA Sequences.** Chad Mirkin and coworkers at Northwestern University[129] have recently developed a new arrayed method for multicolor labeling and detection of DNA sequences using nanoparticle probes. The method uses the array as an internally reflecting waveguide, and the size-dependent scattering properties of gold nanoparticles as a method of orthogonally



tagging different DNA targets with different colored (in this case, green and orange) labels. Imaging the labels requires only the light source and an ordinary microscope or the naked eye. Because nanoparticle-tagged DNA conjugates melt more sharply from array elements than DNA alone, the sequence selectivity of this system is higher than that of multicolored, fluorescently tagged arrays. The technique devised in Mirkin's laboratory involves 50-nm and 100-nm gold particles, which serve as the colored probes to selectively detect two different DNA sequences in a single solution. The method also involves co-hybridizing oligonucleotide-modified particles and oligonucleotide targets to arrays of DNA attached to glass slides. Light scattered from the particles is imaged as bright spots on a dark background; the 50-nm particles scatter green light, and the 100-nm particles appear orange. The group assessed the method's selectivity in temperature-dependency tests using targets with a single base-pair mismatch. Slightly mismatched targets (green) dissociate over a narrow range (55 to 60 C) as indicated by a color change that is readily visible in real time. The technique will be extended to additional colors using nanoparticles of various sizes and compositions. The method's selectivity should also be suitable to examine single-nucleotide polymorphism and genetic disease mutations. This novel technology has been licensed to Nanosphere Inc., a small start-up company. They hope to commercialize this gold nanocrystal technology for DNA diagnostics in the very near future.

- **Undergraduate Research.** At the Research Experiences for Undergraduates site at Iowa State University[130] three students worked on a project with James Cornette in the area of computational molecular biology. In cellular manufacturing of proteins, messenger RNA (mRNA) is transcribed from nuclear DNA and transported across the nuclear membrane to the ribosome where the mRNA information

[129] CHE-9871903
[130] DMS-9732061

is translated into protein. Scientists can extract mRNA directly from cells and can sequence segments of the mRNA that are some 400-600 nucleotides of length. By examining cells from a specific tissue type (liver, kidney, leaf, root, etc.), the scientist can gain information about the proteins important to that cell type. They may get some 5,000 protein sequences of length 400-600 nucleotides from proteins from a particular cell type. The challenge to the mathematician is to interpret the information.

- **Unique Protein Structures.** The recent completion of numerous genomics projects, including those of bacteria, yeast, *C. elegans,* and humans, has revealed the presence of between 6000 and 35,000 potential open reading frames in each genome. As the focus now shifts to understanding the function of these genes, this influx of information has placed unprecedented demands on efforts to determine structures and functions of the new proteins predicted from these sequences. Deciding which sequences among these numerous proteins may represent unique protein structures remains a largely unsolved problem. Rodney Guy and colleagues at the University of California at San Francisco[131] are working to create the tools to address this problem by the development of high-throughput methods for the determination of moderate resolution protein structures. This approach utilizes a combination of chemical crosslinking, mass spectrometry, and computational analysis.

3. Cognitive Neuroscience

- **Mapping Brain Function.** De Witt Sumners at Florida State University[132] and Kenneth Stephenson of the University of Tennessee Knoxville[133] are investigating methods of mapping brain function using conformal mapping algorithms and other geometric ideas. A conformal map of one region to another preserves angles between intersecting curves, a property that is especially valuable in the study of regions such as the visual cortex. Monica Hurdal of Florida State University has been supported by earlier Computational Mathematics grants to Sumners for work on this project, and her efforts at brain mapping have been described in several widely-read accounts, such as a piece in the August 2001 issue of *Scientific American*.

- **Population Rhythms and Wave Propagation in Networks of Coupled Neurons.** Under a Mathematical Sciences Postdoctoral Research Fellowship, Jonathan Rubin[134] collaborated with David Terman and Carson Chow in the analysis of patterns of activity in conductance-based ordinary differential equation models of synaptically coupled neurons, using and developing techniques of geometric singular perturbation theory. This has enhanced understanding of how inhibition, either coming from a global source or applied more locally, can act to synchronize or desynchronize cells or to sustain localized activity. These results are particularly relevant to the interactions of excitatory and inhibitory of cells in the thalamus.

[131] CHE-0118481
[132] DMS 0125000
[133] DMS 0101324
[134] DMS-9804447

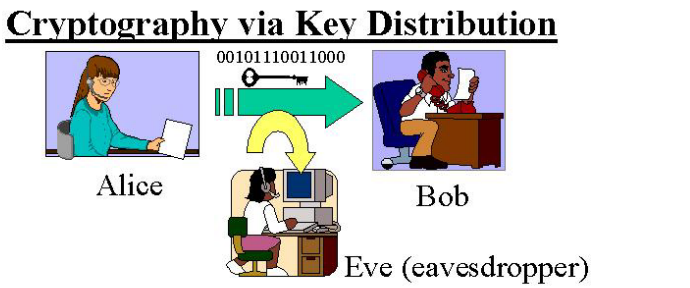
Examples of MPS Directorate Performance for FY 2001

Indicator 3. Partnerships connecting discovery to innovation, learning, and societal advancement

MPS Primary Area of Emphasis: Information Technology Research (NSF Initiative and Area of Emphasis)
Nanoscale Science and Engineering (NSF Initiative and Area of Emphasis)
Biocomplexity in the Environment (NSF Initiative and Area of Emphasis)

1. Information Technology Research (NSF Initiative and Area of Emphasis)

- **Quantum key Distribution with Macroscopic Light Pulses.** Quantum key distribution (QKD) is a technique to transmit a random number secretly from one party to another for the purpose of encrypting sensitive data. Any eavesdropper will necessarily be detectable by the quantum properties of measurement. Until work carried out by researchers at the University of Oregon, it was believed that QKD could be done efficiently only by using single quantum particles, such as photons. PhD student Andrew Funk, working with PI Michael Raymer of the University of Oregon,[135] has discovered a way to use macroscopic light pulses (containing one to ten million photons) to implement QKD. Besides being a novel physical idea, the technique has some advantages: it allows encoding many bits onto a single pulse; it is insensitive to stray background photons; and it does not require single-photon sources, which are presently unavailable.



- **Random Matrices and Random Permutations.** It is well known that a large percentage of computer time is devoted to the rearrangement of the data used in the course of computations. How many data, after a complete reshuffling, are statistically still in order? This question of random permutations in the work of Mark Adler and Pierre Van Moerbeke of Brandeis University[136] also applies to statistical mechanics, the basis of thermodynamics, and to questions of polymers.

[135] PHY-9876608
[136] DMS 0100782

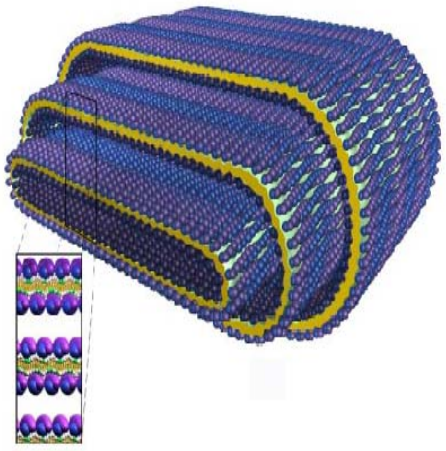
- **National Virtual Observatory.** FY 2001 saw the beginning of coordinated efforts to realize the 'National Virtual Observatory.' The first concept of the virtual observatory was developed with the help of a Small Grant for Exploratory Research (SGER) award to Alexander Szalay of the Johns Hopkins University.[137] This grant enabled fuller discussions in the community and the creation of a white paper on the concept. This year's Information Technology Research (ITR) competition saw the culmination of this effort with the support of a large collaborative project to build the framework for the NVO. NASA and NSF will be cooperating in this activity. This project, which received a strong recommendation from the recent National Academy of Sciences Decadal Survey, will federate astronomical data sets and establish them as a common resource for both researchers and the public. The project will focus not only on the archives, but also on establishing the protocols, standards, and tools that will permit the large astronomical datasets of the future to be fully utilized. Coordinated efforts are also underway at collaborating institutions to develop archives, visualization tools, and related resources.

- **Data Analysis.** Analysis of large data sets has been identified as one of the major challenges of the coming century. A Focused Research Award to Stanford University[138] includes a topologist, Gunnar Carlsson[139], probabilist Persi Diaconis[140], statistician Susan Holmes[141], and psychologist Joshua Tenenbaum, and develops flexible topological methods for the analysis of data that is difficult to handle using classical linear methods. These investigations in the new field of Statistical Algebraic Topology will be most useful when data are obtained by sampling with noise from highly curved or singular algebraic varieties embedded in Euclidean space. Examples arise routinely in visual perception, astronomy, geophysics, genetics, and other natural sciences. The group is developing topologically-based software for dimension reduction and parameterization of high dimensional data sets, homological recognition techniques for locating and analyzing singular points in data sets, and tools for estimating dimensions when standard methods do not work well. Another Focused Research Group award to Anau Srivastava, David Banks, Gordon Erlebacher, and Eric Klassen of Florida State University[142] includes investigations that use techniques from differential geometry to analyze problems in recognition theory.

- **Adaptive Mesh Refinement.** William Allard and John Trangenstein of Duke University[143] are developing algorithms for problems involving diffusion. By locally refining meshes, significant savings in computer time can be achieved. For example, they report that explicit adaptive two-dimensional computations for electrical wave propagation in the heart were five times faster than the corresponding uniform grid computations.

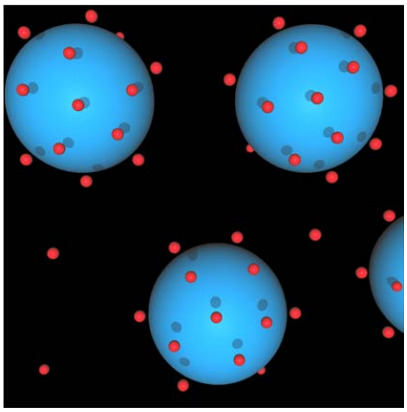
2. Nanoscale Science and Engineering (NSF Initiative and Area of Emphasis)

- **Nanostructured Tubules for Chemical and Drug Delivery.** Anthony Cheetham and his colleagues at the University of California at Santa Barbara[144] MRSEC have made use of the hierarchical self-assembly of proteins and lipids to create a three-layer membrane at equilibrium. The synthetic capsules resemble bacterial cell walls constructed *out-of-equilibrium* and containing two to five layers. The



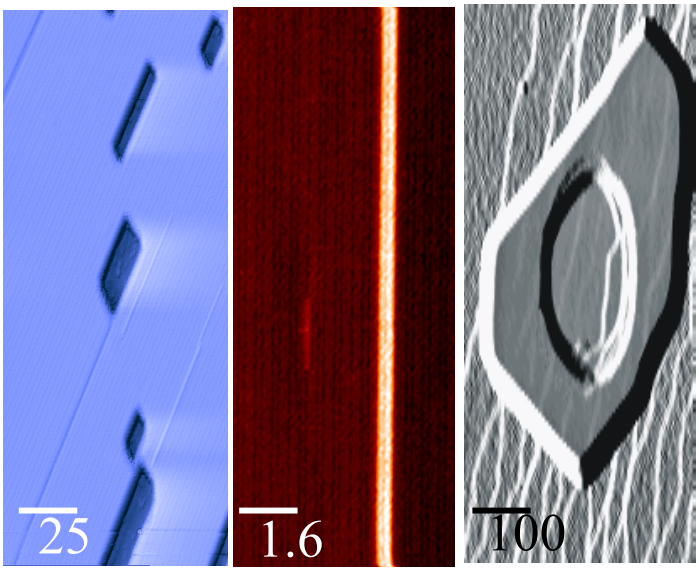
[137] AST-9876645
[138] DMS-0101364
[139] DMS-0104162
[140] DMS-0072360
[141] DMS-0072569
[142] DMS-0101429
[143] DMS-9870384
[144] DMR-0080034

nanostructured tubules and tubule-networks thus realized have potential applications for chemical and drug delivery. The governing concepts for this biological supramolecular assembly are general; future challenges include constructing 4- and 5-layer "functional" composite membranes.[145]



- **Colloidal Microspheres.** Jennifer Lewis of the University of Illinois at Urbana-Champaign[146] has shown that negligibly charged colloidal microspheres (blue in the figure) aggregate in aqueous solution, but undergo a stabilizing transition upon addition of highly charged nanoparticles (red). This type of self-organization, or haloing, provides a new method for tailoring the behavior of complex fluids. The cover image at left is from *Proceedings of the National Academy of Sciences*.[147]

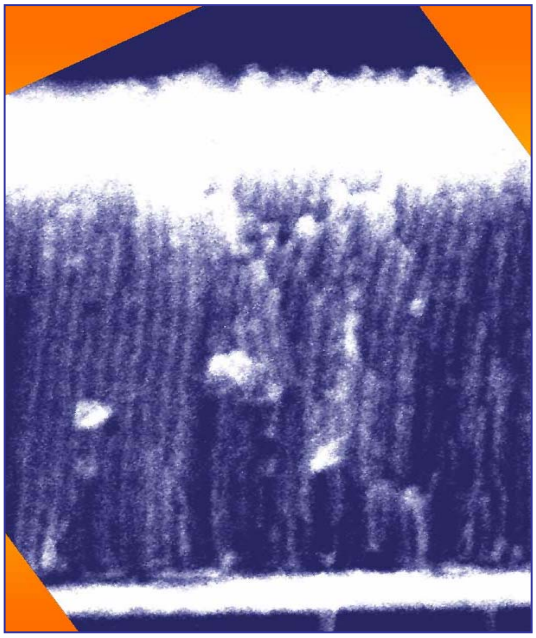
Quantum Engineering of Nanostructures. In nanostructures, where the length scale is near or smaller than the de Broglie wavelength of the electron, quantum confinement plays an important role in determining electronic structure. Because of this the ability to control the size and geometry of nanostructures provides a means to engineer and manipulate physical properties. Recently, C. K.Shih et al. of the University of Texas[148] discovered that quantum mechanically confined electronic states have a strong influence on the formation and stability of nanostructures, thus giving rise to a new meaning for the words "quantum engineering." This Focused Research Group project explores both aspects of "quantum engineering" of nanostructures with different dimensionalities, illustrated by the three examples in the figure (dimensions are in nanometers). At the left an atomically flat silver film has been grown on a gallium arsenide substrate. The stability of the film is governed by electronic states arising from electrons confined in a 2-dimensional quantum well whose properties are determined by the film thickness.[149] The group is also exploring quantum engineering of nanostructures of other dimensionalities. A stable silver nanowire that evolved from the flat silver film is shown in the middle figure. Remarkably, the diameter of such wires is quantized, perhaps as a direct consequence of the quasiperiodic superstructure of the silver film that follows



Ag/GaAs film **Ag nanowire** **Pb/Si**

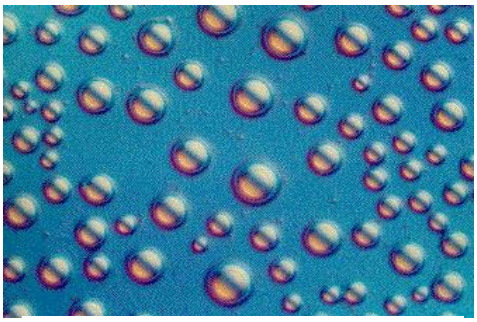
[145] http://www.mrl.ucsb.edu/
[146] DMR-0071645
[147] *Proc. Nat. Acad. Sci.*, **98** (16), 8923 (July 31, 2001)
[148] DMR-0071893
[149] *Phys. Rev. Lett.* **85**, 5158 (2000), *Science* **292**, 1131 (2001)

a Fibonacci sequence.[150] The third panel shows an engineered circular 'nanowell' in a metallic lead nanoterrace, this time on a silicon substrate. In this example atomic rearrangement following an STM pulse has been controlled to produce features with a predetermined diameter (120 nm) and precise depth (8 atom layers) even though the structure involves millions of atoms.

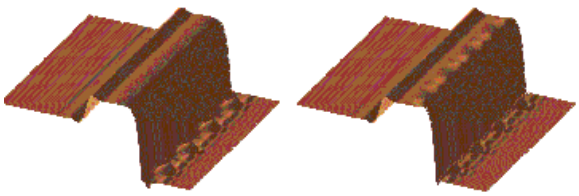


- **Nanotemplates.** Mark Tuominen and Thomas Russell of the University of Massachusetts at Amherst[151] are supported through the Nanoscience Initiative on a project to generate novel block-copolymer nanostructural architectures. They recently succeeded in developing a new nanofabrication technique that allowed them to create magnetic nano-wire arrays from diblock copolymer templates. Through phase separation of these copolymers and field-effected orientation they obtain densely packed lattices of nanocylinders perpendicular to the substrate; these are then etched and filled with cobalt, thus generating arrays of nanowires 14 nm in diameter. The research also included collaboration with IBM, which resulted in licensing of the nanowire arrays for magnetic storage to a new company named Paramount Capital.

- **Thin Liquid Films**. The FRG awarded to Andrea Bertozzi of Duke University[152], Michael Shearer of North Carolina State University,[153] and their colleagues involves the investigation of the stability and dynamics of self-similar rupture, blow-up, and spreading in a class of fourth-order degenerate diffusion equations that includes many problems arising in the modeling of thin liquid films. Thin liquid films have a broad range of applications in areas such as spin coating microchips, de-icing airplanes, paint design, lung surfactants, nanoscale fluid coatings, and gene-chip design. Instabilities in thin liquid films can lead to rupture and complex pattern formation. One of the group's results concerns bifurcations and concentrations in van der Waals driven dewetting. Their work has important ramifications for the use of certain mathematical models in understanding and predicting experiments. Another result concerns undercompressive shocks in two-dimensional thin film flows. Experimental and computational studies of Marangoni-gravity driven films have shown that undercompressive/compressive shock pairs can develop from suitable initial conditions. The investigators considered nonlinear stability of these shock structures



Polystyrene and PEA film: Can we understand the dewetting dynamics using lubrication theory?



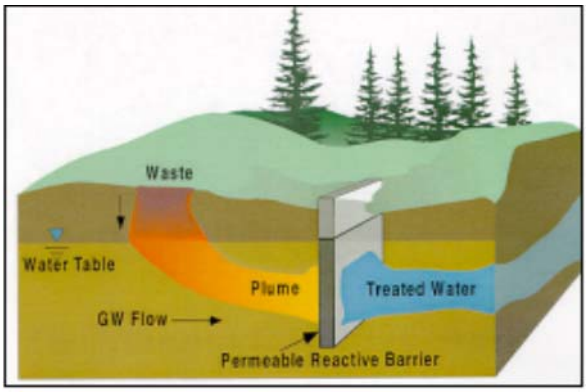
Undercompressive waves and fingering in liquid films

[150] *Phys. Rev. Lett.* **83**, 3222 (1999)
[151] CTS-9871782
[152] DMS-0074049
[153] DMS-0073841

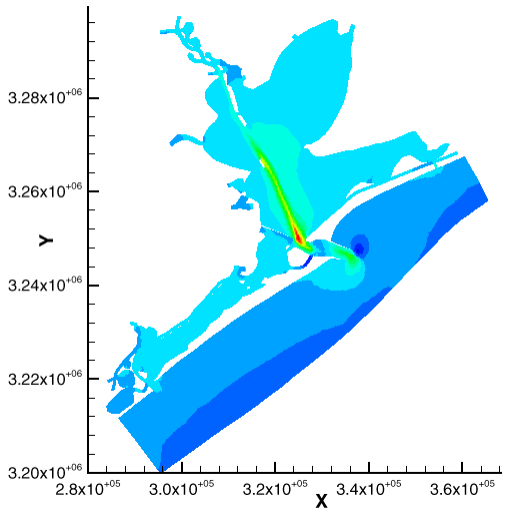
in two dimensions. Numerical simulations illustrate how perturbations ahead of the advancing front pass through the leading undercompressive shock front and collect on the compressive shock.

3. Biocomplexity in the Environment (NSF Initiative and Area of Emphasis)

- **Organohalide Pollutants.** An example of work supported in this area is the Collaborative Research Activities in Environmental Molecular Science (CRAEMS) at Johns Hopkins University. Five Johns Hopkins University[154] investigators and their collaborators from National Laboratories and industry are exploring fundamental mechanistic aspects of dehalogenation chemistry. Motivation for this research stems from the challenges posed by organohalide pollutants. Of the top 25 organic contaminants found in ground water in U.S. urban cities, 17 are organohalides. Shown on the right hand side is an EPA pictorial representation of the technology currently utilized to remove organohalide pollutants from ground water (GW). A permeable reactive barrier, comprised of zero-valent iron particles, intercepts the flow of contaminated GW. The halogenated pollutants present in the GW react with the iron catalysts in the permeable reactive barrier to form environmentally friendly products and treated water. One investigation pertains to selectivity and reactivity of bimetallic reductants, comprised of iron and a second metal, towards catalyzing reductive dehalogenation reactions. These modified catalysts are in some cases orders of magnitude more reactive than are conventional Fe(0) particles. The present work is directed towards applying bimetallic catalysts to decontaminate polychlorinated pollutants present in gas phase waste streams as well as ground water. This work may provide a useful means of decontaminating soils polluted with organohalides as recalcitrant as polychlorinated biphenyls (PCBs).



- **Computational Fluid Dynamics.** Clint Dawson, Mary Wheeler, and Vadym Aizinger of the University of Texas at Austin[155] have developed a discontinuous Galerkin (DG) finite element method for the two-dimensional, depth-integrated shallow water equations. This method is based on formulating the shallow water equations as a system of conservation laws, or advection-diffusion equations. It allows greater flexibility and the ability to handle high gradient flows on unstructured meshes. Numerical results have been computed for several test cases, including supercritical flow, river inflow and standard tidal flow in complex domains, and a contaminant transport scenario where they have coupled the shallow water flow equation with a transport equation for a chemical species. The resulting computational methods have been used in the development of a complex shallow water simulator,



A Discontinuous Galerkin solution for two-dimensional flow and transport in Galveston Bay

[154] CHE-0089168
[155] DMS-9805491, DMS-9873326

called UTBEST (University of Texas Bay and Estuary Simulator). The figure is of a simulated contamination event in the Houston Ship Channel with the domain modeled being all of Galveston Bay.

- As part of the Environmentally Benign Chemical Synthesis and Processing Activity, John W. Frost at Michigan State University[156] seeks to establish alternatives to benzene-based synthetic chemistry. Rather than use non-renewable petroleum and carcinogenic benzene, Frost and his colleagues employ nontoxic carbohydrates derived from plant sources. Examples include the syntheses of hydroquinone, catechol, and adipic acid. A central feature of these synthetic routes is the elaboration of chemical catalysts and synthetic organic methodology suitable for converting microbe-synthesized metabolites into industrial chemicals.

- The Science and Technology Center on Environmentally Responsible Solvents and Processes[157] is developing new modes of collaboration and co-operation for academic research centers, enhancing their effectiveness through the integrated use of collaboration training and collaboration technologies. The STC, a collaboration among the University of North Carolina - Chapel Hill, North Carolina State University, North Carolina A & T, and the University of Texas at Austin, incorporates best practices identified from social science research and the latest from successful corporate management teams. In addition the nature of the collaborations in the Center are being studied by social scientists to develop a clearer idea of what works and what doesn't work in collaborative activities.[158]

- **Ocean Circulation.** Support provided to Robert Higdon of Oregon State University[159] is part of a continuing project on the computer simulation of ocean circulation where the ultimate objective is an understanding of the global climate system. Specifically, his project has focused on time stepping schemes for numerical models of ocean circulation. A standard method used in geophysical fluid dynamics is the leapfrog method, which unfortunately allows a highly oscillatory non-physical mode that can severely contaminate the computed solution unless it is filtered by some means. Higdon developed and implemented a two-level method that does not admit this mode and that allows a time step longer than the one allowed by leapfrog. The framework established by this method is also well suited for incorporating nonoscillatory advection schemes to solve the momentum equations.

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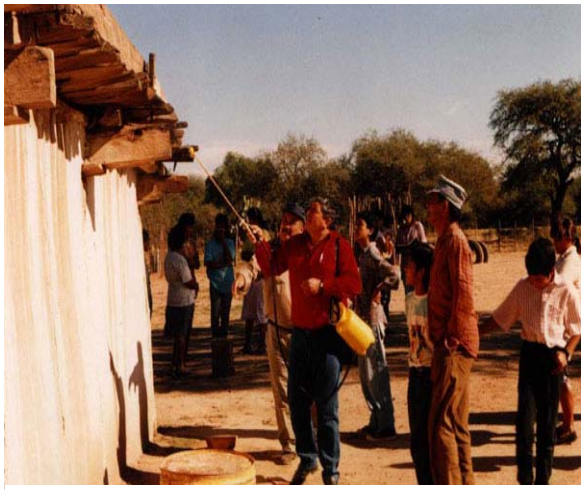
[156] CHE-9906786
[157] CHE- 9876674
[158] See "*Of High Priests and Pragmatists,*" *The Economist*, June 23, 2001
[159] DMS-9803331 (co-funded by Physical Oceanography)

4. Health

- **Laser Technology.** In an Interdisciplinary Grants in the Mathematical Sciences (IGMS) project led by Jerome Spanier of Claremont Graduate University,[160] a novel method was developed based on the combined use of perturbation Monte Carlo and differential Monte Carlo methods for solving a wide variety of inverse problems at the Beckman Laser Institute. An efficient algorithm was implemented for applying this method to the successful reconstruction of optical properties in heterogeneous tissue typical of cervical lesions and other anomalies in human tissue.

- **Mathematical Model of Chagas Disease.** Joel Cohen of Rockefeller University[161] and Columbia University and his colleague Ricardo Gürtler of the Universidad de Buenos Aires have identified improved control tactics for a vexing public health problem. American trypanosomiasis, or Chagas disease, caused by the protozoan parasite Trypanosoma cruzi and transmitted by blood-feeding triatomine bugs, is a chronic, frequently fatal infection that is common in Latin America. Neither adequate drugs nor a vaccine are available. A mathematical model, developed by these researchers, calibrated to detailed household data from three villages in northwest Argentina, shows that householders could greatly reduce the risk of human infection by excluding domestic animals, especially infected dogs, from bedrooms, removing potential refuges for bugs from walls and ceilings and using domestically applied insecticides. The mathematical model makes it possible to do computational experiments that could not be done ethically in a real household and shows how simple and inexpensive methods for disease prevention can be provided. This research was featured in an article in *Nature*.[162]



People being shown how to spray to reduce the bugs.

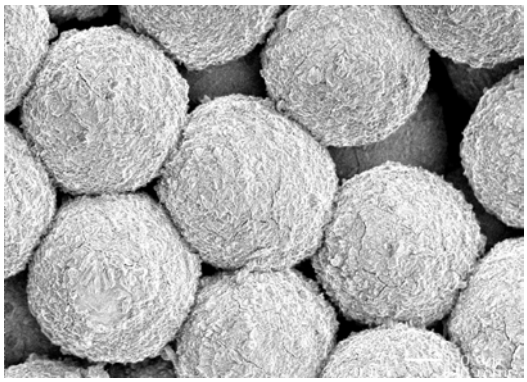
- **Breast Cancer Prognostication.** A POWRE project headed by Mousumi Banerjee of Wayne State University[163] has led to the development of tree models for breast cancel prognostication. The models have enriched the understanding of breast cancer epidemiology and treatment. Specifically, findings from the project have provided possible explanations to the apparent racial disparity in breast cancer survival, and uncovered a previously unrecognized but potentially important mechanism of Tamoxifen treatment resistance in diabetic patients.

- **Medical Imaging and Robotics:** Two senior topologists are using their knowledge to investigate theoretical problems in medical imaging and in robotics, geographic information systems, and biological applications, respectively. James Damon of the University of North Carolina[164] is currently developing geometric methods for computer imaging by developing a scale-based geometry with special applications to medical image processing and analysis. John Harer of Duke University,[165] a recent recipient of an

[160] DMS-0075117
[161] DEB-9981552 (Co-funded by Applied Mathematics and Computational Mathematics)
[162] *Nature,* **293**, July 27, 2001, pp. 694-698)
[163] DMS-9973410
[164] DMS-0103862
[165] DMS-0107621

IGMS[166] award, is investigating new approaches to computational problems that arise in robotics, geographic information systems, and in biological applications. The primary goal of the project is to use techniques from Morse theory, homology theory, geometric group theory, and combinatorics to study problems of shape, configuration, motion planning, and structure in computer science. Applications include computer graphics, visualization of scientific data, computational analysis of molecular docking problems and robotics.

- **Understanding Surface Coatings for Implants.** Jody Redepenning of the University of Nebraska[167] works on the development of new hydroxyapatite/biopolymer composites and is determining the influence of deposition conditions on chemical and physical characteristics of electrolytically produced calcium phosphate coatings. One provisional patent has been filed. Shown is a scanning electron micrograph image of an electrolytically prepared hydroxyapatite coating. The coating covers the surface of titanium beads such as those found on the exterior of hip and knee implants. The non-line-of-sight procedure used produces a relatively uniform coating on irregularly shaped objects.



- **Optimization Theory and Chemotherapy.** Urszula Ledzewicz of Southern Illinois University at Edwardsville [168] and Heinz Schaettler of Washington University produced a unified theory of first- and higher-order necessary conditions for optimality of normal and abnormal processes in optimal control. A local version of a generalized local maximum principle has been completed. A new direction in their research is the investigation of an optimal synthesis for mathematical models for cancer chemotherapy; they have analyzed singular controls and showed that the controls are not optimal both for a two- and three-compartment model.

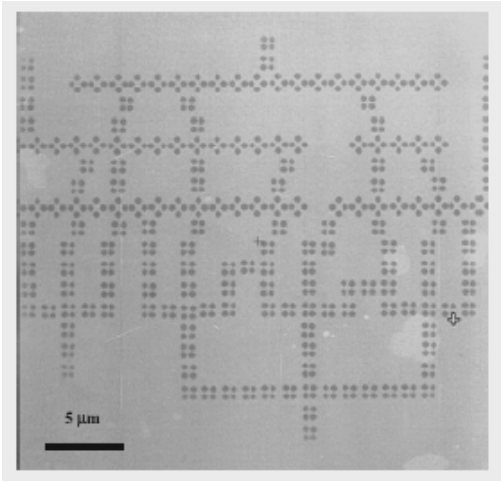
[166] DMS-9721428
[167] DMR-9972587
[168] DMS-9971747

Examples of MPS Directorate Performance for FY 2001

Indicator 4. Research and education processes that are synergistic

- **Undergraduate Research.** Undergraduates attending the Research Experiences for Undergraduates (REU) site at Hope College[169] modeled evolutionary change in the European corn borer. In the Midwest, this insect has been a major pest to the corn crops. Recently, scientists have developed a genetically altered corn that is resistant to the borer. Natural farmers would like to plant this new corn exclusively. However, there is concern about the borer evolving to one that will eat the new corn. The model describes how population of the borer will grow depending on the ratio of the new and old corn planted.

- **MRSEC-PUI Collaboration.** The MRSEC at the University of Virginia,[170] in partnership with Notre Dame University, has established a collaboration with Longwood College, a four-year college in rural Virginia. Through this collaborative program students and faculty from Longwood, a predominantly undergraduate institution (PUI), undertake research projects at the University of Virginia. Academic credit is given at Longwood to the students for these activities and there is a formal Longwood – University of Virginia transfer program at the senior and Masters levels. Under this collaboration, Longwood students and faculty have been doing research on "nanoprinting" of project-related structures. The initial focus has been on patterning of "Quantum Cellular Automata (QCA)" circuits, a concept developed by Center participants at Notre Dame. Initial results of a focused ion beam – fabricated QCA adder circuit are shown in the figure. The feature diameters are on the order of 200 – 300 nm, about an order of magnitude greater than ultimately needed for practical QCA operation at elevated temperatures, but the techniques are scaleable to substantially smaller sizes. The researchers are currently attempting to transfer these structures into magnetic thin films, to explore magnetic analogs to the QCA concept.[171]



- **Brown Dwarfs and High Risk Research.** Brown dwarfs continue to yield surprises, the most recent to come from the observations by REU students at National Radio Astronomy Observatory. Using the VLA for a collaborative observing project they designed and carried out, they discovered the first radio emission ever detected from a brown dwarf. "What is so cool is that this is research that probably nobody else would have tried to do because of its low chance of success. That made it ideal for summer students – we had almost nothing to lose," said Kate Becker, a student at Oberlin College in Ohio. Strong radio emission from brown dwarfs is unexpected because, according to conventional theories, they are not supposed to have magnetic fields strong enough to generate the radio emission. The students' surprising discovery is forcing experts to re-think their theories about how brown dwarfs work. Not only were the radio bursts from the brown dwarf much stronger than those from Jupiter, but follow-up observations

[169] DMS-9820280
[170] DMR-0080016
[171] http://www.mrsec.virginia.edu/education/mrsec_education.htm)

showed that the object's magnetic field was surprisingly weak. These observations promise new understanding of the difference between true stars and brown dwarfs.

- **Chaotic Attractors.** Clifford Reiter of Lafayette College[172] developed techniques for creating chaotic attractors with three-dimensional crystallographic symmetry. The project employed six undergraduates who were able to engage in all aspects of the research including study of and production of the theoretic results. They helped with the writing of several papers, talks and web resources.

- **Materials Modeling Techniques.** As part of his CAREER award, Andrew Rappe of Pennsylvania State University[173] has developed instructional JAVA applets and HTML tools to aid in teaching advanced general chemistry and to expose undergraduates to modern materials modeling techniques. He is collaborating with Prof. Charlotte Zales of Immaculata College. Resources are publicly available on the Web. Two functional applets are currently available: (1) Maxwell-Boltzmann distribution which simulates the motion of a gas of Argon atoms and is designed to reinforce ideas in probability distributions and randomness, and (2) Atomic quantum mechanics which shows the calculation of "atomic wavefunctions" using density functional theory. Applets under construction address surface science, kinetics of greenhouse gases, and molecular dynamics simulations of biomolecules.

[172] DMS-9805507
[173] DMR-9702514

III. PERFORMANCE OUTCOME: TOOLS

FY 2001 Annual Performance Goal
NSF is judged successful when
in the aggregate, results reported in the period demonstrate significant achievement in one or more of the following indicators: • Shared-use platforms, facilities, instruments, and databases that enable discovery and enhance the productivity and effectiveness of the science and engineering workforce. • Networking and connectivity that take full advantage of the Internet and make science, mathematics, engineering and technology information available to all citizens. • Information and policy analyses that contribute to the effective use of science and engineering resources.

FY 2001 Areas of Emphasis across NSF

• Investments in Major Research Equipment
• Continue investments in:
  • Terascale Computing System
  • Major Research Instrumentation
  • S & E information/reports/databases
  • New types of scientific databases & tools for using them

Introduction

Over the years discoveries made through MPS–supported research have become part of the fabric of U.S. industry and society.

Technology and research in mathematics and the physical sciences have a symbiotic relationship to one another. Technology makes possible the development of new tools that enable discovery. On the other hand, it is discovery that reveals new properties of the physical world that we use in the development of new tools. It is becoming increasingly evident that tools for discovery are becoming increasingly more expensive, and, in the case of major instrumentation, are often beyond the means of individual universities or even countries to develop on their own. As a result, there has been an increasing trend towards collaborative activities and sharing in the development of major instrumentation.

PERFORMANCE INDICATORS FOR TOOLS

A. Summary Comments by the Committee of Visitors for the Division of Mathematical Sciences on the Performance of the Division for this Outcome Goal during FY 1998 – FY 2000:

Successful in all categories

The major-shared facilities of the mathematics communities are the three research institutes supported by DMS: MSRI, IMA and IPAM. These institutes have important and distinct roles to play in creating opportunities for communication among mathematicians and between mathematicians and the larger scientific community. They provide databases, internet use, streaming video and other elements that enhance the capability of the mathematics and engineering workforce. For example, they provide computing platforms for mathematicians who come to visit. Web sites are used by high school teachers and students. Computing infrastructure in many math departments, unfortunately, is not up to par; but the availability of web resources in mathematics can help change that. NSF provided a seed grant to develop MathSciNet, which is one of the most used mathematical databases.

SCREMs provide an important source of funds for the acquisition of computer equipment and software for individual departments and groups. The DMS has been a leader in sponsoring programs for the design of numerical methods and algorithms that are the core of simulation software. Algorithms are described in important articles in the mathematical literature and have made their way into systemic inclusion in the scientific and engineering simulation codes at universities, industry and the national laboratories. Historically, many numerical methods developed over the last fifty years have cited the National Science Foundation for support. The DMS also supports the development of many software packages that are distributed over the internet and facilitate the entry of new research efforts into existing fields. This can lead to the formation of new collaborations.

B. Summary Comments by the Committee of Visitors for the Division of Chemistry on the Performance of the Division for this Outcome Goal during FY 1998 – FY 2000:

The Division is *successful* in it support of broadly accessible, state-of-the-art information bases and shared research and education tools.

Through the Division's Chemistry Research Instrumentation and Facilities (CRIF) program and equipment funds in individual investigator awards, the Division uses 15% of its funds to support state-of-the-art tools. The CRIF program provides support to chemistry departments for the purchase of shared instrumentation, the development of new instrumentation and for instrumentation facilities. The Division supports, jointly with the Department of Energy, a synchrotron beamline at the Advanced Photon Source (CHE-9522232) and a high field Fourier transform ion cyclotron resonance/mass spectroscopy facility at the National High Magnetic Field Laboratory at Florida State University (CHE-9909502). In addition, the Division manages chemistry-related awards for the NSF-wide Major Research Instrumentation (MRI) program. This program brings additional funds into the chemistry program for the support of shared departmental instrumentation. In FY1998, the Federal Government supported $60M of instrumentation in chemistry departments. This should be compared with a total CRIF/MRI program in FY2000 of $12M. The Division's programs can be seen to be a substantial fraction of all Federal Government funds going to chemistry departments for the support of shared instrumentation. This support is critical for the integration of research and education.

Examples of MPS Directorate Performance for FY 2001

Indicator 1. Shared-use platforms, facilities, instruments, and databases that enable discovery and enhance the productivity and effectiveness of the science and engineering workforce

MPS Primary Area of Emphasis: Investments in Major Research Equipment
Continue investments in: Major Research Instrumentation
New types of scientific databases & tools for using them

Mathematics

Statistics and probability play a crucial role in society by providing the tools for quantifying the uncertainty faced by regulators and policy makers. Indeed consumers need to understand the uncertainty associated with almost all research findings and reports to respond in an intelligent fashion consistent with their individual level of risk aversion. In the research domain, statisticians and probabilists play a critical role in efficiently collecting research data and in correctly modeling and providing the appropriate analysis of data, necessary for many other scientific disciplines to make advances. These models must incorporate uncertainty in a quantifiable manner in order to understand and communicate the basis for rejecting hypotheses and advancing new theories.

- **Likelihood Theory and Finance.** Likelihood is one of the basic approaches to statistical inference, and one that has very special and desirable properties when it comes to quantifying the uncertainty in estimates. Per Mykland of the University of Chicago[1] has created a further understanding of how these properties come about, and how they can be implemented in statistical situations where likelihood inference is not available. Options trading, when seen as trading of bets on underlying securities, provides a substantial extension of how to think of such problems. Derivative securities – options, futures, and similar instruments – have emerged as a major feature of the contemporary economic environment. They are a versatile and efficient mechanism for trading risk, thus lowering its cost. There is little knowledge on how to use statistical results based on historical data to quantify the risk associated with derivatives. The Principal Investigator on this project has developed two new methodologies for using empirical results to quantify the risk in derivative securities. One is based on prediction intervals, and gives guidance on the amount of contingency reserves needed for a portfolio of derivatives. The other suggests a way of hedging against statistical uncertainty.

- **Human Genome Data, Image Analysis, and Pattern Recognition.** At the University of Pittsburgh[2] David Stoffer has developed an automated and computationally fast method to discover whether two long DNA sequences contain similar patterns. This technology is important for studying the human genome data. The technology was made feasible by building on the ideas used in discovering the spectral envelope for a qualitative-valued time series. Expansions on the spectral envelope is also at the core of Stoffer's other contributions. Motivated by problems in image analysis and pattern recognition, he developed methodology for automatic retrieval systems and pattern analysis in massive archives of images. This is important in medical image queries, and is expected to have impacts on robotics and automation technologies in industrial manufacturing systems.

[1] DMS-9971738 and www.stat.uchicago.edu/~mykland
[2] DMS-9703720 and www.stat.pitt.edu/~stoffer/dss.html

- **Tracking Missiles.** Stochastic differential equations (SDEs) and stochastic partial differential equations (SPDEs) are used in problems of filtering and in studying finance. Solving them numerically is difficult and time consuming, making them difficult to use in 'real time.' Phillip Protter of Purdue University[3] and his associates have developed a purely probabilistic approach, now known as particle methods, which uses Monte Carlo simulation to solve problems. This avoids the need to numerically solve PDEs, and the resulting solutions can be obtained much faster than before. This may be useful in such areas as radar tracking of missiles.

- **Soil Contaminants Simulator.** Jianping Zhu of Mississippi State University[4] and his associates have developed a Web-based simulation system for transport and retention of dissolved contaminants in soil.[5]

- **Spatial Modeling of Count Data on a Lattice.** As part of her work on a POWRE grants, Mary Christman of American University[6] developed a method of importance particularly to conservation biologists. The method predicts the size of the region in which either a species or a community is found. The methods use either geostatistical or conditional autoregressive methods.

Physics

- **Large Hadron Collider (LHC) Project.** The LHC will be the frontier particle accelerator in the world when it comes on line in the second half of this decade. It will have a factor of seven gain in energy compared with Fermi Lab. There is now preliminary experimental evidence that the Higgs particle, the key to understanding why everything in the universe has mass, can be detected with the LHC. The recent work at the Brookhaven National Laboratory on the magnetic moment of the muon, (the recently reported results from the "g-2" experiment) provided results not predicted by the Standard Model. Further tests of the Standard Model will be done at the LHC. The U.S. ATLAS and CMS projects continue to meet their goals and are reliable and influential partners in the construction of the ATLAS and CMS detectors of the LHC machine. CERN expects to complete construction of the LHC in 2005 and initiate collider commissioning. The U.S. schedules are consistent with this goal. The ATLAS and CMS performing institutions have done an excellent job of meeting cost and schedule. It is noteworthy that Hampton University, a Historically Black University, is among this group.

A segment of the Construction Tunnel in the LHC. Parts of the ATLAS Detector will be assembled here.

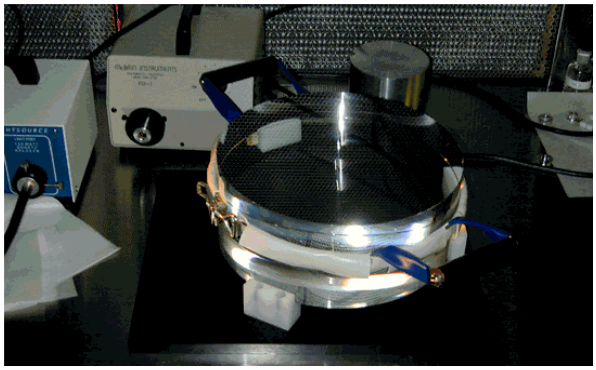
- **RET and CERN.** Ten U.S. undergraduates and four high school teachers have been at CERN to work alongside senior scientists investigating the building blocks of matter and the fundamental forces of nature. This Research Experiences for Undergraduate (REU) site is now in its third year. This summer, the site included 5-10 African American students. In addition, under the Research and Education for Teachers Program, four mathematics and physics teachers were able to be at CERN. These teachers were able to compare and contrast their experiences with 24 European counterparts from 18 other countries.

[3] DMS-9971720
[4] DMS-0075009
[5] http://www.erc.msstate.edu/~alarcon/mrtm/mrtm.html
[6] DMS- 9806051

- **QuarkNet.** QuarkNet, a joint NSF/DOE research-based physics education program, will enable teachers to enhance their knowledge and understanding of science and technology research through association with the LHC. The program is expected to involve 720 high school teachers and nearly 100,000 students. QuarkNet will provide sustained support for teachers to do science and apply what they've learned to the inquiry-based method of teaching. Teachers from Africa are joining QuarkNet.

- **LIGO – First Lock at Hanford.** At 10:00 AM, Friday, October 20, 2000, leaders of the LIGO Laboratory announced that "First Lock" had been achieved with the two-kilometer long interferometer at the Hanford Observatory. This marked achievement of a major LIGO milestone. All mirrors were "locked" into their proper positions to atomic-scale precision using a sophisticated computer-based control system. First lock validated many aspects of the control system design for the initial LIGO detectors, but it had even greater significance the beginning of the process of tuning the interferometer to its full sensitivity. Most importantly, this achievement brought LIGO closer to its real goal – the first true gravitational-wave observations.

- **LIGO Sapphire Development, Military Viewports, Abrasives, and Semiconductor Substrates.** Planning for the advanced LIGO detector has involved research and development in sapphire optics. Sapphire experiences less heating and thermal distortion at high laser power levels than conventional fused silica optics. The LIGO laboratory has undertaken the development of sapphire substrates suitable for detector optics with two vendors: Crystal Systems Inc. (CSI), in Salem, Massachusetts, and the Shanghai Institute for Optics and Fine Mechanics (SIOM) in Shanghai, China. The figure above shows a 25-cm diameter by 10-cm thick substrate that was grown, cut, and mechanically polished by CSI. The LIGO requirements on crystal growth size and uniformity will be pushing the state-of-the-art capabilities of both sapphire vendors. The expertise gained is expected to find application in various common commercial applications of sapphire, including military viewports, abrasives, and semiconductor substrates.

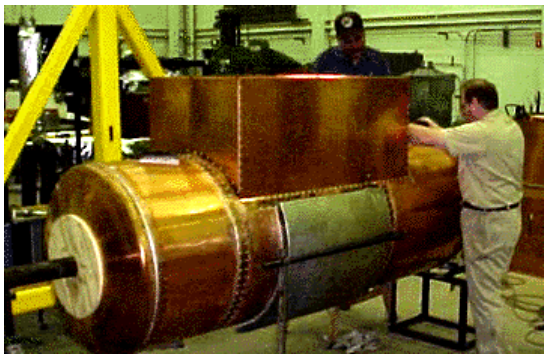


- **MSU/NSCL Coupled Cyclotron Project.** This NSF project, under the direction of C. Konrad Gelbke of Michigan State University[7] will enable the National Superconducting Cyclotron Laboratory (NSCL) to generate a number of beams of radioactive isotopes with intensities many orders of magnitude above present capabilities. This will make it possible to conduct experiments exploring the physics of element generation in the universe and supernova explosion dynamics. The upgrade is now entering its initial period of operations. A dedication ceremony was held on July 27, 2001. The NSCL has a very active REU site program, as well as several outreach activities for teachers and the public.

- **Indiana University Cooler Program.** The Indiana University Cyclotron Facility (IUCF), directed by J. Cameron of Indiana University,[8] in its final year of NSF support, has focused on an aggressive program of measurements at its Cooler facility. The cyclotron, supported in prior years by NSF, is now operated for medical use and is supported financially by other means. The Cooler is operating with a new, operational injector that supplies it with much more intense beams than did the cyclotron. A new polarized source providing beams with an order of magnitude higher intensity is now operational. These features will enable IUCF to study details of few-body systems (such as three-nucleon forces) that will be

[7] PHY-9528844
[8] PHY-9602872

Internal view of new Germanium gamma ray detector array for study of structure of radioactive ions



Installation of superconducting beamline quadrupole for the upgraded radioactive ion beam facility

needed for a reliable understanding of the interplay between the basic strong interaction and the dynamics of two and three nucleons. The Cooler is also used for experiments in beam dynamics, including the effects of space charge, and the dynamics of chaos in beam behavior. The IUCF cyclotron, which became independent of NSF funding in 1998, is in the midst of a new construction phase after which it will emerge as the centerpiece of the Midwest Proton Radiation Institute, providing proton therapy for patients from a wide area of the Midwest. A full patient treatment program is expected in 2003.

- **CESR/CLEO Focus on (b- and c-) Quark Mixing and the Matter-Dominated Universe.** A major focus of the field of high-energy physics is a research area that the CLEO collaboration – associated with the Cornell Electron-positron Storage Ring (CESR) – is very much engaged in. It involves detailed studies of the properties of the heavy charm and bottom quarks, two of the fundamental constituents of matter. Detailed studies of their properties allow one to address why there is an absence of antimatter in the universe. Another major area is to determine whether precision measurements can reveal the existence of effects due to phenomena taking place at higher energies than can be accessed by our current machines. By making precision measurements, we can often see the effects of these phenomena at much lower energies and thereby open windows on new interactions and new particles. Research highlights included a new measurement probing how different quark flavors can mix into one another, a crucial link to understanding why the universe is made of matter and not antimatter. CLEO made the first observation of several rare so-called 'penguin' and 'color-suppressed' decays modes of the B meson. These measurements help to constrain possible sources of new physics that might be turning on at energies well above the reach of current accelerators.

- This summer 16 REU students and two RET secondary school teachers worked at the Wilson Laboratory under the guidance of CESR and CLEO physicists.[9] Other CLEO collaborators participating in this program include Wayne State University and University of Rochester. Women and other underrepresented minorities constituted 25% of the REU program student population, 50% of the RET program.

[9] PHY-9809799

Chemistry

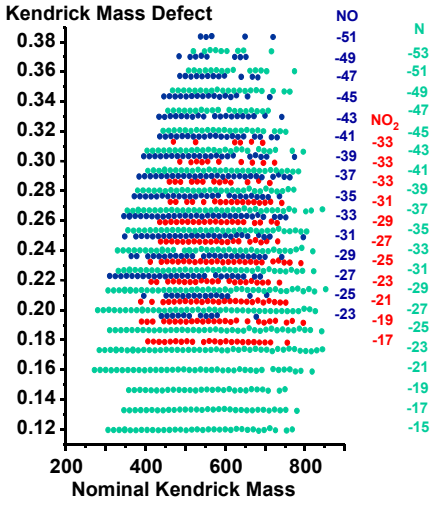
- **Life in Extreme Environments.** Isotopic indicators are extremely useful for the study of life in extreme environments, particularly ancient environments that can only be examined indirectly. Isotopes of iron are of special interest because iron is a critical nutrient and because iron-bearing phases, including well-known biominerals, are widespread in nature and readily preserved in the geologic record. Ariel Anbar and his group at University of Rochester[10] have recently developed and applied MC-ICP-MS methods to examine fractionation of Fe, Cu, Zn and Mo isotopes in the laboratory and in nature. Studies of metal isotope fractionation are likely to be useful in examining the biogeochemical cycling of transition metals. Such research may be particularly valuable if fractionation is associated with metabolic use of these elements. In addition to providing information about biological use of transition metals in modern environments, metabolic fractionations could provide novel "biosignatures" for the study of life in the geologic records of Earth or Mars. Fractionations of key metabolic metals might also help map evolutionary relationships inferred from phylogenetic studies to the geologic record, because changing redox conditions during Earth history undoubtedly led to changes in the availability of metals to the biosphere and, hence, in the use of metals in biology.

Can Fe isotopes tell us about biological use of Fe in the Earth's past? Vast Fe-oxide deposits, such as the Australian Brockman iron formation shown here, are widespread in the geologic record before ca. 1.8 billion years ago. They are all but absent since. A microbial role in their formation is often speculated. Such deposits probably formed when O_2 was scarce in the atmosphere and oceans. Water rich in Fe (II), upwelling from anoxic ocean depths into shallow, mildly-oxygenated basins, could have produced insoluble ferric oxide sediments. Was this redox gradient, typical of the ancient oceans, exploited by microbes for metabolic energy?

Photo Credit: A. D. Anbar and the NASA Astrobiology Institute (MtEE Focus Group)

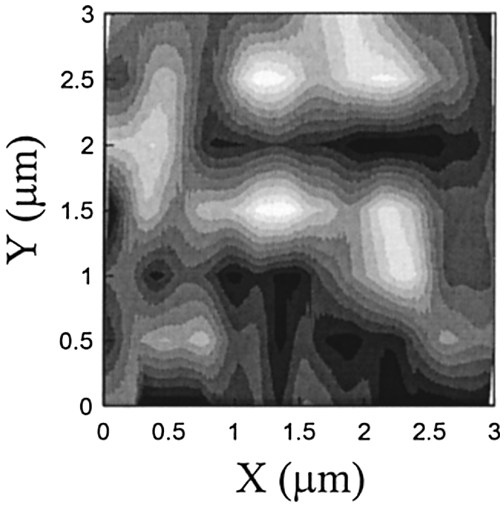
- **ChemMatCARS.** The Division supports the development of a synchrotron beam line facility at the Advanced Photon Source ("ChemMatCARS: A National Chemistry and Materials Synchrotron Research Facility at the Advanced Photon Source").[11] This activity is supported jointly by the Division of Chemistry, the Division of Materials Research, and the Office of Basic Energy Sciences at the Department of Energy The high brilliance of the ChemMatCARS undulator beamline, coupled with a large-area CCD detector allows complete structures to be solved from single crystals too small to measure on a lab-based x-ray source.

[10] CHE-9714282
[11] CHE-0087817



- **Behavior of Biomolecules.** Alan G. Marshall, Christopher L. Hendrickson and Mark R. Emmett of Florida State University (FSU) and John R. Eyler of the University of Florida direct the operation of the Fourier-Transform Ion Cyclotron Resonance/Mass Spectrometry (FT-ICR/MS) Facility, housed in the National High Magnetic Field Laboratory (NHMFL) at FSU.[12] This facility is a unique national resource that provides state-of-the-art analytical instrumentation and mass spectral analysis to chemists and biochemists in US academic and industrial institutions. Studies carried out at the facility lead to a better understanding of the behavior of biomolecules and the structure of biomolecules, complex mixtures important in environmental chemistry, and petroleum products. An example of the use of this facility is in the unraveling of complex mass spectroscopic measurements on petroleum products. Ultrahigh-resolution FT-ICR mass spectrometry can separate and identify thousands of chemically distinct components (e.g., in petroleum heavy crude oil) from a single mass spectrum. Unfortunately, it is difficult to visualize the data, because it would be necessary to expand such a spectrum to a length of more than 200 meters to be able to see all of the individual spectral peaks. Fortunately, high-resolution mass spectra are inherently two-dimensional. Thus, it is possible to slice the mass spectrum into 1 mass unit segments, turn them sideways, and then stack them next to each. Different molecular "classes" (i.e., molecules containing a specified number of heteroatoms, such as N, O, and S) are then separated as shown by the different colors in the Figure. For each molecular “class”, species of different molecular "type" (i.e., different number of rings plus double bonds) are then further separated by their different vertical displacements.

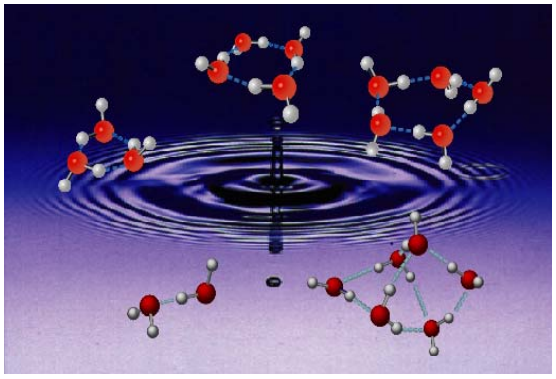
- **Surface Analysis of Living Cell Membranes.** Alan Bard and his group at the University of Texas[13] are developing new methods in the combined areas of electrochemistry and scanning probe microscopy for the purpose of surface analysis of nanostructures and living cell membranes. In the past few years, this group has converted the scanning probe from a simple physical probe into an active element of an electrochemical cell and then increased sensitivity by adding an optical detection scheme for the electrochemistry. With a newly developed 172 nm electrode probe tip, the electrogenerated chemiluminescence source size is comparable to that of a typical near-field scanning optical microscope, but with the added advantage of electrochemical sensitivity. Images of a test sample show resolution of ~230 nm while monitoring the ruthenium complex chemiluminescence at 645 nm. The images show submicrometer holes in a 100 nm thick aluminum film. This work was recently highlighted in the research profiles of *Analytical Chemistry*. There are clear prospects for applications to molecular electronics and ion-transport systems in biological systems.



Electrogenerated chemiluminescence scanning probe microscopy images of a test sample, an aluminum film with submicrometer holes.

[12] CHE-9909502
[13] CHE-9870762

- **Creating Liquid Water.** Richard J Saykally of University of California at Berkeley[14] is exploring the connection between individual water molecules and liquid water in which 99% of all chemistry on Earth takes place. The approach has been to build up to liquid water one molecule at a time, investigating the structure at each stage, as determined by "tetrahedral hydrogen bonding." So far the structure and spectral signature of up to the hexamer has been identified. The hexamer is especially significant since it is the smallest cluster that exhibits a three-dimensional structure; the trimer is the smallest to show chirality. With the requisite theory, the situation is being approached where a force field for liquid water can be constructed from the spectra of these small clusters. The figure illustrates perspective views of a dimer, trimer, tetramer, pentamer, and the hexameric cage structure.



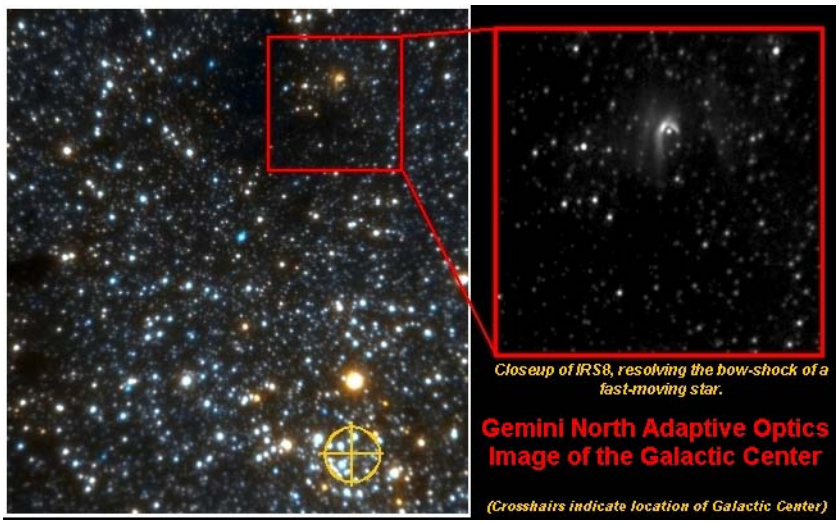
Astronomy

- **National Astronomy Facilities.** The National Radio Astronomy Observatory, the National Optical Astronomy Observatory, the National Solar Observatory, the National Astronomy and Ionospheric Center, and the Gemini Observatories provide access on the basis of scientific merit to a broad scientific user community. Over 2400 scientists and students use these facilities annually; each provides unique capability that enables research and training. More than half the PhD degrees granted in astronomy each year utilize the facilities and the data they produce. Much of the astronomical research highlighted in the "Ideas" area of this report was carried out using the national astronomy centers. Over 900 papers were published last year citing the use of NOAO and NRAO facilities. Scientific results from the national facilities have a significant impact – typically 6 to 10 papers published by NRAO users each year are invited to be cover articles for the journals Nature, Science, and Scientific American. The observatories also issue press releases and maintain web sites with the latest news.[15]

- **NOAO Deep Wide Field Survey.** The centers also generate substantial databases and archives of observational data, often through coordinated surveys that enable research beyond the scope of a single researcher. A recent example was the NOAO Deep Wide-Field Survey, an extensive, multi-year multicolor survey using the 4-meter telescopes. The first results, covering an area of 1.15 degrees square, and with it over 300,000 faint galaxies and stars, were released in January 2001. The full area will be 15 times this size, and will provide deep images in both the visible and infrared over 18 square degrees when it is completed in spring 2002. With it, astronomers will be able to study large-scale structure in the Universe, the formation and evolution of galaxies and quasars, rare stellar populations, and the structure of the Milky Way.

[14] CHE-9727302
[15] http://www.noao.edu/news/

- **Bow-Shock near Galactic Center.** The newest of the large facilities available to the US astronomical community, the Gemini Observatories, passed from commissioning and construction into early science operations in this fiscal year. With both telescopes obtaining data, astronomers have full sky coverage with identical 8-meter class telescopes for the first time ever. Results from Gemini North are already appearing in the press. The first demonstration data of the galactic center have been released to the public. Using an adaptive optics system that was funded by NSF and built by the University of Hawaii, these images represent the sharpest images ever obtained over such a large area of our Galaxy's center. The images, one of which is shown to the right, clearly reveal the morphology of a previously unresolved object called IRS-8 as a 'bow-shock' from a star moving rapidly relative to a gas cloud.

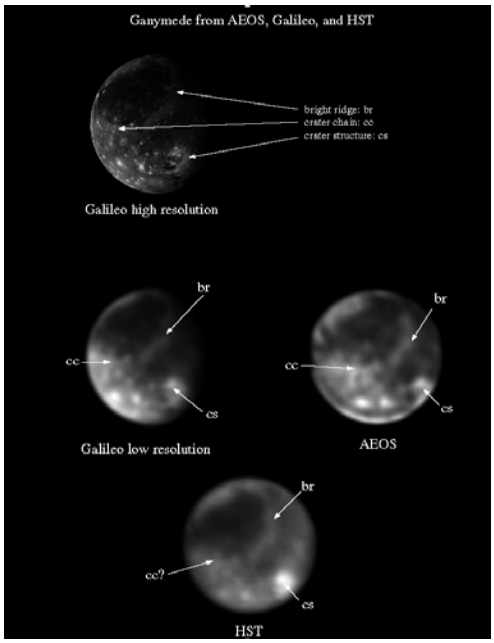


- **University Radio Observatories.** In addition to these national centers, AST supports five university-based radio astronomy observatories that operate their own instruments, play critical role in training the next generation of radio astronomers and instrumentalists, and serve as foci for research groups in radio astronomy and instrumentation. Each of these programs has an active program of instrument development and technical upgrades that improve the capability of their facilities and enhance the productivity of their users. An example is the program of upgrades at the Caltech Submillimeter Observatory (CSO), which is designed to optimize the study of distant galaxies, as well as to provide better mapping capability of star forming regions. Their program of upgrades involves improving the telescope surface, developing long wavelength (BOLOCAM) and short wavelength (SHARC II) cameras (shown on the telescope to the right), and upgrading heterodyne receivers to be tunerless and controlled remotely.

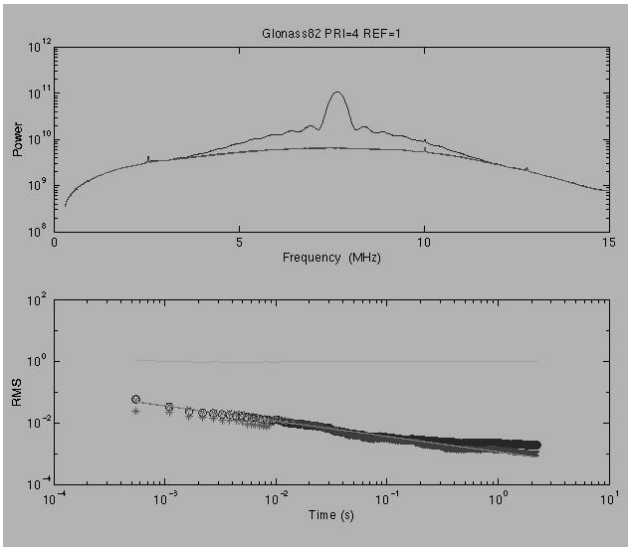
- **Instrumentation Programs.** The Division of Astronomical Sciences also supports the development of instrument systems and advanced technology through its Advanced Technologies and Instrumentation (ATI) Program and the NSF-wide Major Research Instrumentation Program. Grants in the ATI program enable research instruments for existing telescope facilities as well as advanced technology required for the development of next generation telescopes and instruments. Integral to all these efforts is the training and education of students in observational techniques and instrumentation.

- **Optical Interferometry.** Among the areas of development supported by the ATI program is optical interferometry that will enable diffraction-limited imaging using aperture synthesis methods to create images from telescopes with effective apertures up to one kilometer in diameter. Recent results from the Infrared Stellar Interferometer under development by Charles Townes of the University of California at

Berkeley,[16] show the potential of such instrumentation – measurements of nearby stars indicate that our previous understanding of stellar sizes has been confused by the dust and gas surrounding evolved stars. New measurements with ISI show stellar radii some 10 to 25% larger than previous measurements, changes that have implications for our models of stellar structure and atmospheres, temperature, and ultimately distance scales.



- **Adaptive Optics.** Increasing access to state-of-the-art facilities has been the goal of the joint activity with the Air Force Office of Scientific Research (AFOSR) which makes available to the US astronomical community observing time at the Advanced Electro-Optical System (AEOS) telescope, on Maui, Hawaii. The capability of this 3.76-meter advanced technology telescope for scientific research is illustrated with its recent observations of Jupiter's satellite Ganymede. Images obtained with AEOS resolve details only 270 km in size, performing significantly better than the Hubble Space Telescope.



- **Cancellation of Radio Interference.** As an example of work that contributes to the effective use of science and engineering resources, AST supports a new area of technological development in the field of radio astronomy that involves the real-time adaptive cancellation of unwanted radio interference using adaptive digital filters and special signal processing algorithms. This work is bringing together researchers at NRAO, Brigham Young University,[17] Ohio State University, and the University of California at Berkeley, and requiring a close collaboration between scientists and research engineers in an interdisciplinary effort. To characterize these unwanted signals, they have begun a program of recording high-speed data samples of signals that are known to cause interference to radio astronomical observations. With these samples in hand, tests of canceling algorithms are underway, and have proven to be very successful for certain kinds of well-characterized and predictable signals, as is shown below in the cancellation of a signal from the GLONASS satellite.

- **The Atacama Large Millimeter Array (ALMA).** The project is preparing to move into the last year of design and development before project construction, which will take approximately nine years. Construction of ALMA is envisioned as an equal U.S.-European partnership, with the likelihood of Japan as a third equal partner. The scope proposed for the U.S.-European project – an array of 64 12m antennas, with 4 receiver bands extending into the submillimeter – represents a careful balance between

[16] AST-9819729
[17] AST-9987339

an optimized, cutting-edge radio telescope and responsibility to build within cost. The cost for ALMA– and in particular the North American contribution to it–has remained contained since the detailed cost audit was carried out in July 1999. As currently envisioned, ALMA will bring to millimeter and submillimeter astronomy the aperture synthesis techniques of radio astronomy, enabling precision imaging to be made on sub-arcsecond angular scales.

Materials Research

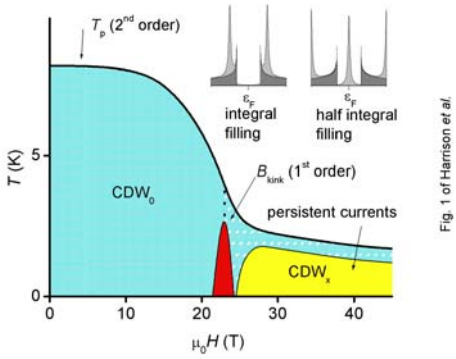
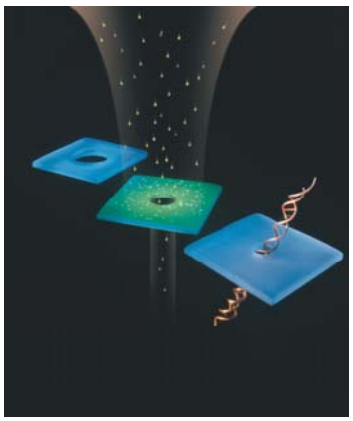


Fig. 1 of Harrison et al.

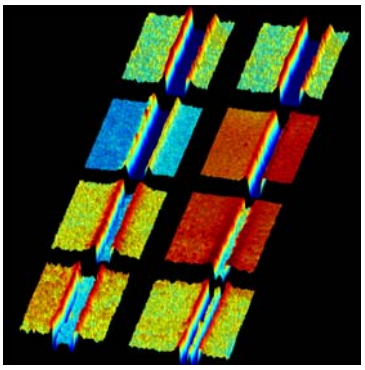
- **Observation of Frohlich Superconductivity in High Magnetic Fields.** In 1954 Frohlich described a type of superconductivity caused by the motion of charge density waves. Charge density waves arise when electrons bunch up into wave-like oscillations and are one of the few macroscopic quantum phenomena observed to date. Some organic materials are known to have charge density waves which establish themselves only at very low temperatures (about one degree above absolute zero) and high magnetic fields (a half-million times stronger than the Earth's magnetic field). Such fields are available at the National High Magnetic Field Laboratory.[18] Recent experiments by NHMFL scientists, in collaboration with an Oxford University scientist, have found compelling evidence of 'persistent currents' in this charge density wave. Persistent currents are electrical currents that travel without friction, just as in a superconductor. Frohlich-style superconductivity has never before been convincingly proven, but conditions in these materials in extremely high magnetic fields strongly suggest that this may be the long-awaited discovery.

- **Scientists Create 'Molecular Rulers' Enabling Precise Construction of Nanoscale Structures.** Paul Weiss and his colleagues at Pennsylvania State University[19] have discovered an effective and precise way to make ultra miniature metal wires in very close proximity to each other. The results, published in the 9 February 2001 edition of *Science*, describe the use of organic molecules as "molecular rulers" that permit the fabrication of extremely thin wires from 15 to 70 nanometers wide and a few micrometers long. The wires are spaced 10 to 40 nanometers apart. Their work is important because nanoscale construction methods have been limited to structures with larger, less controlled spacing than is expected to be useful in the continuing efforts to miniaturize electronic and opto-electronic devices used for circuits, high-density data storage, and sensors. In addition, their work is expected to serve as a test bed in the rapidly developing field of molecular electronics. The National Science Foundation's Major Research Instrumentation Program, the Army Research Office, DARPA, and the Office of Naval Research supported this research. It was conducted at Pennsylvania State University's node of the National Nanofabrication Users' Network.[20]

[18] DMR-0084173
[19] CHE-0111366
[20] CTS-9732194



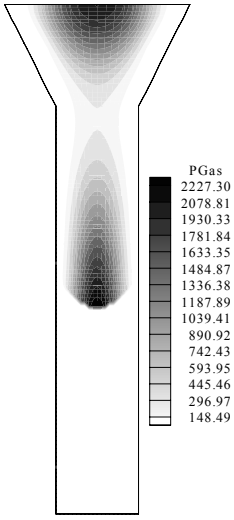
- **Manipulating Matter at the Nanoscale.** Several DMR research themes, such as spintronics, optics, nanoscience, etc. relate directly to emerging or mainstream technologies. However, and somewhat more typically, many awards are pioneering entirely new tools and techniques. An example is the work of Jene Golovchenko of Harvard University.[21] Golovchenko is using an ion beam to poke holes in thin films to produce structures that in turn are used to manipulate nanoscale matter. Manipulating matter on the nanometer scale is important for many electronic, chemical and biological advances. However, available solid-state fabrication methods do not reproducibly achieve nanometer-scale dimensional control.

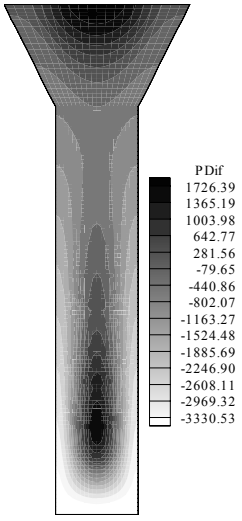


Field emission scanning electron microscopy images depicting stages of a nanostructure reduction process.

Golovchenko and co-workers have discovered how to fashion matter at these dimensions by means of low energy ion beams. The processing reveals surprising atomic transport phenomena that occur in a variety of materials and geometries. They call their method "ion beam sculpting" and apply it to the problem of fabricating a molecular scale hole, or nanopore, in a thin insulating solid-state membrane. This is schematically illustrated in the figure above. Nanopores localize molecular scale junctions and switches and act as masks to create other small structures. Nanopores also function as membrane channels in all living systems, where they are extremely sensitive electromechanical devices that regulate electric potential, ionic flow and molecular transport across cellular membranes. They have used "ion beam sculpting" to fabricate an analogous solid-state device: a robust electronic detector capable of registering single DNA molecules in aqueous solution. Such detectors may find utility in extremely rapid sequencing of DNA for medical diagnostics of genetic diseases and rapid drug design for large populations.

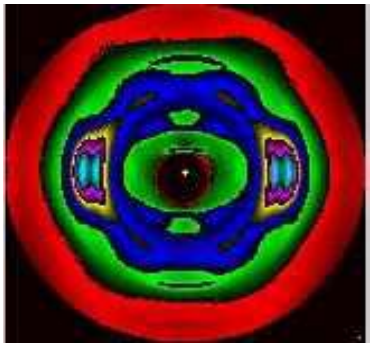
- **Simulating Porosity in Metal Castings**. At a very different length scale, David Poirier at the University of Arizona[22] is simulating the formation of porosity in a nickel-base superalloy (IN718) plate casting. Porosity evolves because the alloy contains gaseous impurities, hydrogen and nitrogen, which are dissolved as atoms in the melt. The concentrations of the atomically dissolved hydrogen and nitrogen are only 20 parts per million each, but as the casting cools and solidification proceeds they become more concentrated in the remaining liquid and generate hydrogen and nitrogen gases in their familiar molecular forms. The total pressure of the hydrogen and nitrogen is shown as *PGas* (right). When the total pressure exceeds the



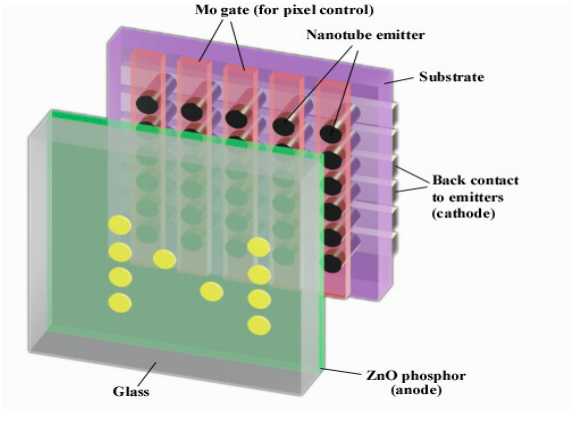


[21] DMR-0073590
[22] DMR-9901290

pressure in the liquid, porosity occurs. In the figure, porosity is predicted where *PDif* is positive. Industry is interested in the simulator as a tool for making casting processes more energy-efficient and cost-effective. Currently Pratt and Whitney, a major producer of jet engines, and Howmet Castings are attempting to verify the simulation.



- **In-situ X-ray Scattering System.** Prof. Benjamin Hsiao of the State University of New York at Stony Brook[23] has developed an *in situ* synchrotron wide-angle and small-angle X-ray scattering system, which allows him to study simultaneously and in real time the structural and morphological development in solidifying polymers. He has applied this to the understanding of shear-induced crystallization, to the study of orientational development during flow, to the isothermal crystallization of blends of different molecular weights, and to the analysis of crystallizing bio-absorbable polymers. His experimental system has been set up at Brookhaven National Laboratories and has been used widely in collaborative work with a large number of academic and industrial institutions.



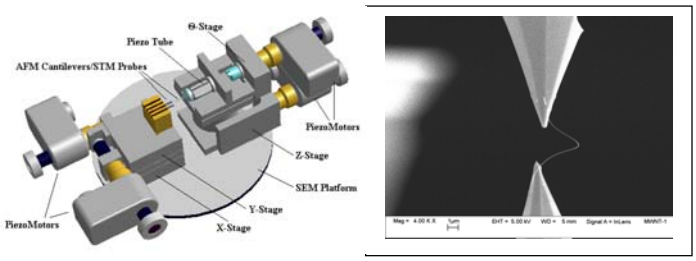
- **Display Technology.** R.P.H. Chang of Northwestern University[24] has made a significant development in the use of nanotubes in fabricating a flat panel screen display.[25] The prototype screen uses hundreds of thousands of stationary nanotubes, which emit electrons to light up pixels on the screen. Unlike a standard CRT screen, in which one electron beam emitted from a hot filament beam moves rapidly back and forth to light the pixels, each pixel is lit by its own electron beam. The screen can be slim, the emission steady, and the resolution is extremely high. Once nanotubes can be manufactured in bulk, large screens could be fabricated very cheaply without expensive lithographic techniques.

- **Neutron Scattering Studies of Nanodroplet Aerosols.** Barbara Wyslouzil et al. of Worcester Polytechnic,[26] Rinehard Strey of the University of Cologne, Gerry Wilemski of the University of Missouri-Rolla and John Barker of the DMR-funded Center for High-Resolution Neutron Scattering (CHRNS) made the first definitive scattering measurements on the nucleation and growth of binary fluid nanodroplets. By continuously forming droplets *in situ* by expansion in a supersonic nozzle inserted in the sample chamber, they have obtained data on the internal structure of the droplets needed to test current theories in atmospheric physics. For example, their measurements on deuterated alcohol/water mixtures clearly show that the alcohol concentrates in the surface regions of the droplets before they reach 100 nm in size, a result that will help refine realistic models for chemical reactions in the atmosphere.

- **Development of Nanocalorimetry.** L.H. Allen and his colleagues at the University of Illinois at Urbana[27] have developed a calorimeter for nanoscale materials. This unique nanocalorimeter is over 1000

[23] DMR-9732653 and 0098104
[24] DMR-0071737
[25] http://www.nsf.gov/od/lpa/news/tips/tipsrel.htm
[26] DMR-9986442
[27] DMR-9726458

times more sensitive than conventional differential scanning calorimeters. The technique has been used successfully (1) to measure heat capacity of liquid/biological samples with droplets ranged in size from about 2 to 100 nL; (2) as a new *in situ* sensing tool for monitoring thin film growth via heat capacity measurements and scanning nanocalorimetry; and (3) to study nanoscale calorimetry of isolated polyethylene single crystals. A silicon "bio-box" sample holder for nanoliter liquid samples has been developed. Initial exploration of this concept was supported by a Small Grants for Exploratory Research (SGER) grant.[28]



- **A New Tool for Nanotechnology.** Rodney Ruoff, Tomasz Kowalewski, James Huettner, and collaborators at Northwestern University[29] have developed a nanomanipulator (schematic left). The tool has been used inside a scanning electron microscope to pick up, mount, and tensile load carbon nanotubes such as the individual multi-walled carbon nanotube shown attached between AFM cantilever tips (right image). Studies on the breaking mechanism and tensile strength of multi-wall carbon nanotubes, the tensile strength of single wall carbon nanotube ropes, and "shell sliding," in which the outer shell of a multi-walled nanotube is displaced relative to the inner shell adjacent to it, have been reported in a number of scientific journals.[30]

- **Inorganic Crystal Surfaces.** Gary Drobny of the University of Washington[31] has developed solid state nuclear magnetic resonance (NMR) as a tool unique in its ability to provide high-resolution information on the structure and dynamics of biopolymers at materials interfaces. He has provided the first high-resolution NMR structural and dynamical studies of proteins on inorganic crystal surfaces.

- **Leapfrogging the Microcircuit Pattern-size Barrier: X-ray Phase Masks for Next Generation Semiconductor Lithography.** James Taylor and his associates at the University of Wisconsin-Madison and at the Center for NanoTechnology (CNTech) have used radiation from the Synchrotron Radiation Center (SRC) at the University of Wisconsin[32] in a unique way for a new approach to next generation lithography. The Bright Peak Enhanced Phase Mask (BPEXPM) approach uses the X-rays from the storage ring to demonstrate printing of 50 nm to 30 nm features that correspond to the years 2007 and 2011 in the International Technology Roadmap for Semiconductors. They have found a new way to apply the principle of phase masks to enhance the intensity that is produced from a mask structure that can be fabricated with normal semiconductor processing. The new lithographic approach truly opens the possibility for leapfrogging the Roadmap in the fabrication of microprocessor and low-density microcircuit applications. It also opens the field to higher-speed microwave communication devices.

[28] DMR-9419604
[29] DMR-0196399
[30] *Science*, **287**, 637,2000; *Phys. Rev. Lett*.,**84**, 5552, 2000; *Phys. Rev. Lett.*, **85**, 1456, 2000; *Phys. Rev. Lett.*, **86**(1), 88, 2001; and *J. Phys. Chem. B*, **104**, 8764, 2000.
[31] DMR-9616212
[32] DMR-0084402, jwtaylor@nanotech.wisc.edu

Examples of MPS Directorate Performance for FY 2001

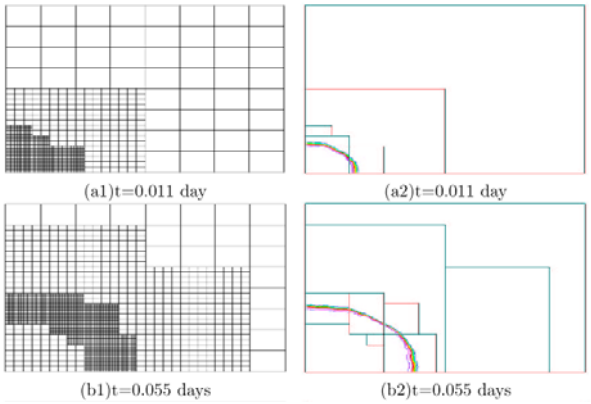
Indicator 2. Networking and connectivity that take full advantage of the Internet and make science, mathematics, engineering and technology information available to all citizens

MPS Primary Area of Emphasis:
Continue investments in: S & E information/reports/databases

Mathematics

- **Numerical Methods for Partial Differential Equations.** Randall LeVeque of the University of Washington [33] and his postdoctoral associate Sorin Mitran wrote a new package BEARCLAW, which stands for "Boundary Embedded Adaptive Refinement for Conservation LAWs". The code will allow the use of immersed interface techniques with Cartesian finite volume methods.

- **LOQO.** David Shanno of Rutgers University[34] and Robert Vanderbei of Princeton University[35] have jointly developed a highly competitive computer software package, LOQO, for solving large-scale optimization problems of various kinds. Developed initially for linear and convex quadratic programs, the software has been extended to compute nonconvex problems. The code LOQO has been tested comparatively with several state-of-the-art codes such as the trust-region interior-point code NITRO and the sequential quadratic programming code SNOPT and has been shown to perform very well, with the performance of LOQO increasing as problem size increases.



Mesh and tracer concentration contours at different times.

- **Homotopy Continuation Methods**. Homotopy continuation methods are reliable and powerful methods to compute numerically approximations to all isolated complex solutions of polynomial systems. Tien-Yien Li of Michigan State University[36] has developed the computer code HOM4PS, based on the polyhedral homotopy approach, that has exhibited excellent performance on a large collection of polynomial systems in a wide variety of applications. In his new award,[37] Li proposes to further develop this methodology and to enlarge the scope of its applications to practical models that do not yet have a satisfactory line of attack. Jan Verschelde of the University of Illinois, Chicago, who was a co-Principal Investigator in Li's on his previous grant, developed the general-purpose polynomial solver PHCpack that appeared as Algorithm 795 of ACM TOMS. This algorithm was used recently by Bertrand Hass to verify a counterexample to Koushnirenko's conjecture concerning the number of positive real roots in a system of k polynomials in k variables. Verschelde has teamed up with an algebraic geometer, Andrew Sommese

[33] DMS-9803442
[34] DMS-9805495
[35] DMS-9870317
[36] DMS 9804846
[37] DMS 0104009

of the University of Notre Dame, in a joint effort to investigate the decomposition of algebraic sets and to develop software for such decomposition.

Hilbert Class Library. Together with their graduate students, William Symes of Rice University[38] and Mark Gockenbach of Michigan Technological University [39] are developing the Hilbert Class Library (HCL), which is a collection of C++ classes defining the fundamental mathematical objects required to represent partial differential equation (PDE) constrained optimization problems, such as those arising from applications in seismic inversion. A specific class implements the adjoint state method to compute the gradient of an objective function defined by a simulation, which is notoriously difficult to implement correctly by hand and is sufficiently complicated to be beyond the reach of state-of-the-art automatic differentiation tools. The resulting software makes available a computational technique that was previously too expensive to apply to many large-scale problems, and does so (semi-) automatically. The first version of the software deals with explicit, fixed time-step schemes. An extension of adjoint state software to adaptive time-stepping schemes in a high-frequency asymptotic code is currently being designed and implemented; adaptivity is essential to achieve both accuracy and efficiency in the principal investigators coherent noise suppression technique for seismic velocity inversion.

- **Factorization Algorithms.** Van Hoeij of Florida State University[40] has developed algorithms for solving linear recurrence equations. In particular, he has drastically improved the factorization algorithm for polynomials. The new algorithm, now implemented in MAPLE is 500 times faster than the previous version. Because of such efficiency, the computer algebra community has adopted the algorithm very quickly: Within a few months others implemented it in at least three more computer algebra systems. The source code is also available online.

- **MCLab.** As part of his CAREER project, Michael Holst of the University of California at San Diego,[41] has developed MCLab (MC in MATLAB), which is an adaptive finite element MATLAB package for general second-order nonlinear elliptic equations on 2-manifolds. The CAREER Award support has allowed him to put some effort into packaging MCLab as a completely self-contained finite element toolkit for teaching finite element methods to advanced undergraduate and beginning graduate students. In addition, he developed the FEtk (The Finite Element ToolKit), which is a general adaptive multilevel finite element toolkit for solving a large class of partial differential equations using finite element methods. The toolkit consists primarily of the finite element kernel MC (Manifold Code), the finite element mesh viewer and manipulator SG (Socket Graphics), the low-level programming abstraction layer MALOC (Minimal Abstraction Layer for Object-oriented C), the prototyping and teaching tool MCLab (MC in MATLAB), and the extension library MCX (MC eXtensions). The five parts of FEtk are used cooperatively to adaptively solve a PDE and then visualize the solution. Most of FEtk is now freely available in source form under the most standard of open source licenses, namely the GNU General Public License (GPL).

Physics

- **The Next Generation Internet – a Computational Data Grid**: Last year, the NSF funded a new collaboration called GriPhyN (for Grid Physics Network). GriPhyN is a collaboration of large experiments: (1) ATLAS and CMS currently being built for the Large Hadron Collider (LHC) at the CERN Laboratory in Geneva Switzerland; (2) the LIGO interferometer developed for the direct detection of gravitational waves; and (3) the Sloan Digital Sky Survey. These experiments, all supported within the

[38] DMS 9973423
[39] DMS 9973308
[40] DMS-9805983
[41] DMS- 9875856

Mathematical and Physical Sciences Directorate, all face a common problem—they produce vast quantities of data - expected to be tens of petabytes per year - and their user community consists of hundreds of scientists throughout the world who to access this data. A computational data grid consisting of a large computer network with high-speed links dynamically assembles the required data, carries out the requested computations, and delivers it to the user in real time. Last year the collaboration developed the toolkit needed for this, and this year it will begin implementation of the grid for the four collaborations mentioned above.

Astronomy

- **Databases.** Much of the research supported by the Division contributes substantially to the creation of scientific databases and tools to use them. Observational projects, in particular the many extensive surveys now underway, routinely create extensive databases that are made available over the web to the astronomical community, and, in many cases, to the public. Examples include the Optical Gravitational Lensing Experiment (OGLE) project led by Bohdan Paczynski of Princeton University,[42] the Galactic Ring Survey (GRS) to map the ^{13}CO emission from a large portion of the plane of the inner Milky Way led by James Jackson of Boston University,[43] and the Virginia Tech Spectral-line Survey led by Simonetti of Virginia Tech,[44] a wide field image survey of the Galaxy's warm ionized interstellar medium.

- **Connectivity.** The astronomical sciences rely heavily on the networking and connectivity of the Internet both for the purposes of research and to make the images and results of astronomical research available to students, teachers, and the public. Remote monitoring and operation of the Gemini telescopes, for example, enable astronomers in Wisconsin to 'eavesdrop' on their observations being taken at Cerro Pachon, in Chile, or at Mauna Kea, Hawaii. These facilities also rely heavily on the web to disseminate the results of their research as well as educational resources to the public.[45]

[42] AST-9820314
[43] AST-9800334 and AST-0098562
[44] AST-9800476 and AST-0098487
[45] http://www.noao.edu/outreach/

Examples of MPS Directorate Performance for FY 2001

Indicator 3. Information and policy analyses that contribute to the effective use of science and engineering resources.

This indicator is not applicable to the activities supported by the Directorate for Mathematical and Physical Sciences.

IV. TABLES

The Tables below provide information on the program assessments and evaluations other than Committee of Visitor and Advisory Committee assessments that were conducted in areas of relevance to activities supported by the Directorate for Mathematical and Physical Sciences.

These reports, studies, and evaluations are frequently used in setting new priorities in a field or in documenting progress in a particular area. Other tables, including the schedule for COV assessments, follow.

Information on obtaining reports produced by the National Research Council or National Academy of Sciences can be found online by searching www.nap.edu or from the National Academy Press, 2101 Constitution Avenue, N.W., Lockbox 285, Washington, D.C. 20055 (1.800.642.6242).

Table 1

Evaluations complet in FY 2000	Scope	Findings	Availability
Challenges for the Chemical Sciences in the 21st Century	Survey of the current status of chemical sciences will evaluate trends and identify key opportunities and challenges.	This study is currently in progress	National Research Council
Physics in a New Era	The report surveys the field of physics broadly, identifies priorities, and formulates recommendations. The overview assesses the state of physics in four broad categories – quantum manipulation and new materials, complex systems, structure and evolution of the universe, and fundamental laws and symmetries – emphasizing the unity of the field and the strong commonality that links the different areas, while highlighting new and emerging ones.	Six high-priority opportunities identified, nine recommendations are made: support of physics by the federal government; physics education; role of basic physics research in national security; increasingly important role of partnerships among universities, industry, and national labs; the stewardship of federal science agencies; and the rapidly changing role of information technology in physics research and education.	National Research Council http://www.nap.edu/catalog/10118.html

Evaluations complet in FY 2000	Scope	Findings	Availability
An Assessment of the Department of Energy's Office of Fusion Energy Sciences Program.	An assessment of the scientific quality of the Office of Fusion Energy Sciences Program	Although this report was generated at the request of the DOE's Office of Science, NSF is often referred to within the document. In particular, the report recommends that NSF play a greater role in extending the reach of fusion science and in sponsoring general plasma science.	National Research Council http://books.nap.edu/catalog/9986.html
Committee on Organization and Management of Research in Astronomy and Astrophysics	To assess the organizational effectiveness of Federal support of astronomical sciences and, specifically, the pros and cons of transferring NSF's astronomy responsibilities to NASA	NSF's astronomy and astrophysics responsibilities should not be transferred to NASA. The Federal government should develop a single integrated strategy for astronomy and astrophysics research that includes supporting facilities both on the ground and in space. An interagency planning board for astronomy and astrophysics should be formed that would receive input from the community through a joint advisory committee of outside experts. Additional recommendations made that address ways to improve the present overall management structure and strengthen NSF's ability to support astronomy	National Research Council The report can be found at http://www.nas.edu/ with the prepublication copy available at http://books.nap.edu/html/integrated_program/comraa.pdf

Evaluations complet in FY 2000	Scope	Findings	Availability
Proceedings of the Workshop on the Present Status and Future Developments of Solid State Chemistry and Materials	Define research opportunities in the field of solid-state chemistry and materials. Identify the most important multidisciplinary areas for involvement by the solid-state chemistry and materials community. Determine novel roles for the Solid State Chemistry and Materials community that will advance educational and training opportunities for future scientists, engineers, and technicians. Develop new approaches that allow for the more effective and efficient conduct of research and educational activities.	Recommendations are listed for various sub-fields in this discipline	Available at the NSF web site http://www.nsf.gov/mps/dmr/ssc.pdf
2001 Workshop on Future Directions in Solid State Chemistry	To articulate the solid state chemistry community's sense of opportunities and directions to be taken in the future, especially in interdisciplinary areas, and to provide a means for informing the solid state chemistry community of programs and opportunities for support in interdisciplinary research at NSF and elsewhere.	To be held in October, 2001	

Evaluations complet in FY 2001	Scope	Findings	Availability
US-Africa Materials Workshop	The workshop explored research opportunities directed towards expanding materials research and education for the purpose of contributing to the development of new technologies as well as promoting collaboration among U.S. and African universities and industries.	Need to establish one or more organizations to ensure the continuation of conversations that began at the workshop. Technical recommendations from a number of working groups are included in the report.	http://iumrs.org/docs/africa.pdf
National Science Foundation Force Transduction in Biology Workshop	The goal of this workshop was to explore recent advances in research on force transduction in biology at all length scales, and to seek possible overlap or synergies between these different areas. An additional goal was to explore the potential interdisciplinary interactions that will lead to significant advances in this area. Also, the workshop was to identify important new directions for research and to make recommendations about potential funding opportunities.	Perhaps the most important conclusion of the workshop was that research in force transduction in biology has important problems that span many length scales and many disciplines. However, the interdisciplinary nature of the research, the quantitative nature of the important problems and the key relationship between the materials properties and the important issues all make this an area that the NSF can play a significant role in fostering progress.	http://hurkle.deas.harvard.edu/nsf/workshop.html

TABLE 2. COMMITTEE OF VISITORS SCHEDULE: FY 2001- FY 2004

FY 2001 COVs	
DIRECTORATE: MATHEMATICAL AND PHYSICAL SCIENCES	
Division	Program/Cluster title
Mathematical Sciences	All Programs
Chemistry	All Programs
FY 2002	
Division	Program/Cluster title
Astronomical Sciences	All Programs
Materials Research	All Programs
FY 2003	
Division	Program/Cluster title
Physics	All Programs
FY 2004	
Division	Program/Cluster title
Mathematical Sciences	All Programs
Chemistry	All Programs

TABLE 3A. COV RESULTS FOR PEOPLE FY 2001

COV Results for Outcome Indicators and Goals by Program/Cluster/Division

Provide program/report titles where available. Insert the COV report rating for each indicator, and for each goal. Examples for ratings include: S (successful); NS (not successful); NR (no rating by COV); DNA (did not apply).

People - Development of "a diverse, internationally competitive and globally-engaged workforce of scientists, engineers, and well-prepared citizens."

Indicators	Improved mathematics, science, and technology skills for U.S. students at the K-12 level and for citizens of all ages.	A science and technology and instructional workforce that reflects America's diversity.	Globally engaged science and engineering professionals who are among the best in the world.	A public that is provided access to the benefits of science and engineering research and education.	Overall Rating For Goal by COV
Program/Cluster/Division					
Division of Mathematical Sciences	**S**	**S**	**S**	**S**	**S**
Division of Chemistry	**S**	**S**	**S**	**S**	**S**

TABLE 3B. COV RESULTS FOR IDEAS FY 2001

COV Results for Outcome Indicators and Goals by Program/Cluster/Division

Provide program/report titles where available. Insert the COV report rating for each indicator, and for each goal. Examples for ratings include: S (successful); NS (not successful); NR (no rating by COV); DNA (did not apply).

Ideas -- Enabling "discovery across the frontier of science and engineering, connected to learning, innovation, and service to society."

Indicators	A robust and growing fundamental knowledge base that enhances progress in all science and engineering areas including the science of learning.	Discoveries that advance the frontiers of science, engineering and technology.	Partnerships connecting discovery to innovation, learning, and societal advancement.	Research and education processes that are synergistic.	Overall Rating For Goal by COV
Program/Cluster/Division					
Division of Mathematical Sciences	**S**	**S**	**S**	**S**	**S**
Division of Chemistry	**S**	**S**	**S**	**S**	**S**

TABLE 3C. COV RESULTS FOR TOOLS FY 2001

COV Results for Outcome Indicators and Goals by Program/Cluster/Division

Provide program/report titles where available. Insert the COV report rating for each indicator, and for each goal. Examples for ratings include: S (successful); NS (not successful); NR (no rating by COV); DNA (did not apply).

Tools -- Providing "broadly accessible, state-of-the-art information-bases and shared research and education tools."

Indicators	Shared-use platforms, facilities, instruments, and databases that enable discovery and enhance the productivity and effectiveness of the science and engineering workforce.	Networking and connectivity that take full advantage of the Internet and make science, mathematics, engineering and technology information available to all citizens	Information and policy analyses that contribute to the effective use of science and engineering resources.	Overall Rating For Goal by COV
Program/Cluster/Division				
Division of Mathematical Sciences	**S**	**S**	**S**	**S**
Division of Chemistry	**S**	**S**	**S**	**S**

TABLE 4. DIRECTORATE RESULTS FOR MANAGEMENT GOALS

Management Goals	MPS Directorate Result
	Goal met/not met
M1. Diversity	MET

M1. DIVERSITY. In FY 2001, NSF will show an increase over 1997 in the total number of hires to S&E positions from underrepresented groups.

FY 2001 Results
In FY 1999, 2 of the 14 new hires were female and 3 were from minorities. In FY 2000, 7 of the 21 new hires were female and 4 were from minorities. In FY 2001, 5 of the 18 new hires were female, and 3 were from minorities. This represents a change from 33% to 28% in the number of new female hires in 2001, and a change from 19% to 17% in the number from minorities. While this represents a drop from FY 2000, the differences are due to the statistics of small numbers. We consider our hiring rate of females and minorities to have remained essentially constant from FY 2000 to FY 2001.

TABLE 5. DIRECTORATE RESULTS FOR INVESTMENT PROCESS GOALS

Investment Process Goals	Directorate Results
	Goal met/not met
I1. Implementation of Merit Review Criteria – Reviewers	See Tables 6 and 7
I2. Implementation of Merit Review Criteria – Program Officers	See Tables 6 and 7
I3. Time to Prepare Proposals	MET
I4. Time to Decision	NOT MET
I5. Award Size	MET
I6. Award Duration	MET
I7. Openness in System	NOT MET

I1. and I2. Implementation of Merit Review Criteria - Reviewers
NSF Performance in implementation of the new merit review criteria is successful when reviewers address the elements of both generic review criteria appropriate to the proposal at hand and when program officers take the information provided into account in their decisions on awards, as judged by external independent experts.

FY 2001 Results
This assessment is provided in the MPS Advisory Committee report for the Division of Mathematical Sciences and the Division of Chemistry.

I3. Customer Service – Time to prepare proposals
95% of program announcements and solicitations will be available to relevant individuals and organizations at least three months prior to proposal deadlines or target dates.

FY 2001 Results
In FY 2001, 100% of the program announcements and solicitation issued by MPS were available at least three months prior to proposal deadlines or target dates.

I4. Customer Service – Time to decision
For 70% of proposals, be able to tell applicants whether their proposals have been declined or recommended for funding within six months of receipt.

FY 2001 Results
In FY 2000, MPS processed 52% of its proposals within six months of receipt. In FY 2001, MPS processed 57% of its proposals within six months of receipt. While this represents an improvement from the previous year, the Directorate is studying the best practices of NSF organizations that have met the NSF goal and will adapt such practices and implement them throughout MPS in FY 2002.

I5. Award Size
NSF will increase the average annualized award size for research projects to $110,000.

FY 2001 Results
In FY 2001, the average annualized award size for MPS was $113, 748.

I6. Award Duration
NSF will increase the average duration of awards for research projects to at least 3.0 years.

FY 2001 Results
In FY 2001, in MPS the average duration of awards for research projects was 3.1 years

I7. Maintaining Openness in the System
The percentage of competitive research grants going to new investigators will be at least 30%,

FY 2001 Results
In FY 2001, MPS had 22% of its competitive research grants going to new investigators.

TABLE 6. COV ASSESSMENT OF THE USE OF THE MERIT REVIEW CRITERIA BY THE DIVISION OF CHEMISTRY PROGRAMS

a. Performance Goal: Implementation of Merit Review Criteria by Reviewers: NSF performance in implementation of the merit review criteria is successful when reviewers address the elements of both generic review criteria. Did reviewers adequately address the elements of both generic review criteria?

b. Performance Goal: Implementation of Merit Review Criteria by Program Officers: NSF performance in implementation of the merit review criteria is successful when program officers address the elements of both generic review criteria. Did program officers adequately address the elements of both generic review criteria?

Organic and Macromolecular Chemistry

- Did reviewers adequately address the intellectual merit criterion in their reviews?

  Yes.

- Did reviewers adequately address the broader impacts criterion in their reviews?

  Reviewer response to the broader impacts was minimal. Approximately 20% of reviewers made any comments in this area.

- Did program officers adequately address the intellectual merit criterion in their decisions?

  Yes.

- Did program officers adequately address the broader impacts criterion in their decisions?

  Program officers make extensive use of the broader impacts criteria, including taking into account the nature of the institution. Occasionally, these broader considerations resulted in approval of proposals that were on the margin of acceptance/declination (e.g. CHE 0078852).

Inorganic, Bioinorganic, and Organometallic Chemistry

- Did reviewers adequately address the intellectual merit criterion in their reviews?

  Yes.

- Did reviewers adequately address the broader impacts criterion in their reviews?

  Not uniformly.

  The interpretation of Criterion 2 differs greatly between reviewers in IBO. In our opinion, however, this confusion is not limited to IBO, but is throughout the Foundation. Exactly what types of information would satisfy Criterion 2 and exactly how much each criterion should be weighted on any individual proposal is unclear. It would be helpful to the reviewing community if the NSF would state clearly that proposals must address both criteria, but that the weighting of the criteria are expected to vary as a function of proposal type, institution, and nature of the research.

- Provide some more examples that illustrate the range of activities that fall under the scope of Criterion 2.

  .

  Note for example:

  Award number CHE-9816356 – Simonis
  Dr. Simonis' demonstrated record of productivity and excellent management of resources (human and physical infrastructure) was an important factor in the decision to award funding for this proposal. Dr. Simonis' work on the electronic and molecular structure of paramagnetic iron porphyrins probed by NMR spectroscopy was cited in the Division's FY2000 annual report. Particularly noteworthy was the strong educational impact of this work in mentoring undergraduate and graduate students from an under-represented group in an inner city institution.

  Award number CHE-9501992 – Cummins
  An important factor in awarding a CAREER grant to Dr. Cummins was the scientific component of his proposal. The education elements of his proposal received mixed reviews, nevertheless Cummins' enthusiasm for teaching was noted.

Proposal No. CHE-9904798 – Barry
This proposal was highly rated on Criterion #1. This was the most important factor in the decision to award funding.

- Did program officers adequately address the intellectual merit criterion in their decisions?

  Yes.

- Did program officers adequately address the broader impacts criterion in their decisions?

  Yes, but with some difficulty since reviewers were not applying the criterion uniformly.

Analytical and Surface Chemistry and Advanced Materials Chemistry

- Did reviewers adequately address the intellectual merit criterion in their reviews?

  The main text of all the reviewers' comments that the COV panel read critiqued the intellectual merit of the proposal. However, the quality of the reviews varied; about half of the review read by the COV were substantive, the other half less so. For each proposal, there were enough substantive reviews to address the intellectual merit of the proposed research.

- Did reviewers adequately address the broader impacts criterion in their reviews?

  Only ~20% of the reviewers mentioned the broader impacts (except for the case of the CAREER awards). This panel suggests a separate text box on Fastlane for this part of review. The reviewers who addressed Criterion No. 2 did so primarily in terms of the impact of the proposed activity to enhancing the infrastructure and moving the boundaries of our scientific/technological understanding. The CAREER proposals cut across the two programs and clearly young faculty members who are starting their academic careers more carefully delineated educational plans, which would impact the participation of underrepresented groups or the impact of the work to society. The reviewers for the CAREER proposals clearly and carefully assessed the proposals according to the educational impact and those proposals awarded showed a clear description of their broader impact.

- Did program officers adequately address the intellectual merit criterion in their decisions?

  Yes. The program officers clearly paid attention to this intellectual merit criterion; in comparing the novelty, risk, and disciplinary impact of the proposals, the average scores of AMP were significantly higher (2.80, 2.27, 2.93) for funded proposals compared to unfunded proposals (1.83, 1.44, 1.47). Similar data were found for ASC: 2.56, 2.40, 2.72 for funded compared to 1.65, 1.56, 1.76 for unfunded. The program officers take into consideration the substantiveness of the reviews received and exercise excellent judgement.

- Did program officers adequately address the broader impacts criterion in their decisions?

  The program officers do carefully address the broader impacts criterion in their decisions. There were two examples in the jackets the panel read (CHE-9978556, CHE-9728644) in which program officers made awards on the strength of Criterion 2. There was another example (CHE-9984563) in which the program officer and review panel did not fund an otherwise meritorious CAREER proposal because of its superficial educational plan.

Physical Chemistry

- Did reviewers adequately address the intellectual merit criterion in their reviews?

  Yes. Most of the reviewers provided insightful and carefully thought out reviews. The committee was impressed with the quality and care of the reviews.

- Did reviewers adequately address the broader impacts criterion in their reviews?

  Reviewers typically discussed scientific impacts in some detail. Often broader societal and educational impacts were not addressed in as great detail. Typically, one or more of the reviewers in each jacket did provide some useful comment. In contrast with Criterion 1, which was well understood and evenly applied, Criterion 2 was interpreted very differently from reviewer to reviewer. In some cases, the reviewers identified proposal sections that addressed Criterion 2 and discussed their merits. In others, no comment was made. Even within our committee, opinions varied significantly on how this criterion should be addressed in a particular proposal. The committee believes that the scientific community is still in a learning phase and recommends that the NSF continue to educate the research community as how best to address this criterion.

- Did program officers adequately address the intellectual merit criterion in their decisions?

  Yes. Very thorough documentation was provided concerning intellectual merit.

- Did program officers adequately address the broader impacts criterion in their decisions?

  Program officers addressed broader impacts more completely despite uneven responses of the reviewers. For example, we saw a declination that was significantly based on the lack of student or postdoctoral support, which speaks to educational benefit (CHE-9810145).

Chemical Instrumentation, Centers and Facilities, and Education

- Did reviewers adequately address the intellectual merit criterion in their reviews?

  There was no problem noted here.

- Did reviewers adequately address the broader impacts criterion in their reviews?

  The Chemistry Division needs to be sure that all reviewers know to make a statement on the broader impacts criterion. While it was felt that reviewers in this particular set of programs did a better job of dealing with Criterion 2 than reviewers generally did in other programs of the Chemistry Division, there was still unevenness in this regard, especially within the instrumentation program. We estimated that approximately 75% of the reviewers dealt in some way with Criterion 2, although some quite superficially.

  In FastLane, if a reviewer must make an entry on criterion #2 to get the review accepted, then it will be addressed. That change will get reviewers, and therefore PI's, to think harder about the impact.

  Broader impacts must take into account the locale and local conditions, like in the RSEC proposals from New Orleans (CHE-9974846) or in New Mexico (CHE-9974883). A site visit might have helped in the review of those proposals, the second of which was funded while the first was not.

- Did program officers adequately address the intellectual merit criterion in their decisions?

  Intellectual merit criterion was addressed adequately by program officers.

- Did program officers adequately address the broader impacts criterion in their decisions?

  Program officers adequately discussed the criterion of broader impacts. In fact, within certain programs such as POWRE and REU, the broader impacts tend to have a particularly strong influence on the funding decision, as they should.

TABLE 7. COV ASSESSMENT OF THE USE OF THE MERIT REVIEW CRITERIA BY THE DIVISION OF MATHEMATICAL SCIENCES

- Performance Goal: Implementation of Merit Review Criteria by Reviewers: NSF performance in implementation of the merit review criteria is successful when reviewers address the elements of both generic review criteria. Did reviewers adequately address the elements of both generic review criteria?

  Successful/Unsuccessful

  The reviewers always addressed adequately the intellectual merit criterion in their reviews. For disciplinary proposals, on the broader impact criterion, most reviewers' comments, if present at all, are limited to impacts on science and technology and training of graduate students and postdocs. These comments are more common in Computational Math. The broader impacts criterion was not usually addressed by reviewers unless issues relevant to that criterion (e.g. the presence of minority students) were raised by the proposer. In Applied Mathematics and in the various cooperative and interdisciplinary programs we looked at, impact on other sciences and applications was a major factor; impact on students was still rarely addressed by reviewers.

  Reviewers rarely comment on diversity, infrastructure and dissemination. We suspect that most reviewers focus on the scientific aspects of a disciplinary proposal and tend not to read the reviewing instructions. Also, these criteria are relatively new and most reviewers may not be familiar with them. For infrastructure proposals (Institutes, VIGRE), both criteria seem to be used properly.

- Performance Goal: Implementation of Merit Review Criteria by Program Officers: NSF performance in implementation of the merit review criteria is successful when program officers address the elements of both generic review criteria. Did program officers adequately address the elements of both generic review criteria?

  Successful/Unsuccessful

  Program officers always addressed adequately the intellectual merit criterion in their decisions. Program officers were inconsistent in addressing the broader impacts criterion in their decisions. The documentation was inconsistent in showing that the broader impact was considered (again, individual grants). We know from personal experience on panels that these issues have been discussed without being documented in the jacket, but cannot verify that this always happens from the jackets alone. If program officers regularly address these issues in their feedback on both successful and unsuccessful proposals, it would help generate new ideas in the mathematical community.

TABLE 1. ANNUAL PERFORMANCE GOALS FOR NSF'S STRATEGIC OUTCOMES [5,6,7]

Strategic Outcome	FY 2001 Annual Performance Goals	FY 2001 Areas of Emphasis
	NSF is successful when, in the aggregate, results reported in the period demonstrate significant achievement in one or more of the following indicators:	
People -- Development of "a diverse, internationally competitive and globally-engaged workforce of scientists, engineers, and well-prepared citizens."	❖ Improved mathematics, science, and technology skills for U.S. students at the K-12 level and for citizens of all ages, so that they can be competitive in a technological society. ❖ A science and technology and instructional workforce that reflects America's diversity. ❖ Globally engaged science and engineering professionals who are among the best in the world. ❖ A public that is provided access to the benefits of science and engineering research and education.	◆ K-12 systemic activities ◆ Enhancing Instructional Workforce - Centers for Learning and Teaching - Graduate Teaching Fellows in K-12 Education ◆ Broadening Participation - Tribal Colleges - Partnerships for Innovation ◆ Addressing near-term workforce needs - Advanced Technological Education
Ideas -- Enabling "discovery across the frontier of science and engineering, connected to learning, innovation, and service to society."	❖ A robust and growing fundamental knowledge base that enhances progress in all science and engineering areas including the science of learning. ❖ Discoveries that advance the frontiers of science, engineering and technology. ❖ Partnerships connecting discovery to innovation, learning, and societal advancement. ❖ Research and education processes that are synergistic.	◆ Appropriate balance of high risk, multidisciplinary or innovative research across all NSF programs. Investments in three initiatives: ◆ Information Technology Research ◆ Nanoscale Science and Engineering ◆ Biocomplexity in the Environment Investments in non-initiative fundamental research: ◆ Mathematical Sciences Research ◆ Functional Genomics ◆ Cognitive Neuroscience
Tools -- Providing "broadly accessible, state-of-the-art information-bases and shared research and education tools."	❖ Shared-use platforms, facilities, instruments, and databases that enable discovery and enhance the productivity and effectiveness of the science and engineering workforce. ❖ Networking and connectivity that take full advantage of the Internet and make science, mathematics, engineering and technology information available to all citizens ❖ Information and policy analyses that contribute to the effective use of science and engineering resources.	Investments in Major Research Equipment Continue investments in: ◆ Terascale Computing System ◆ Major Research Instrumentation ◆ S&E information/reports/databases ◆ New types of scientific databases & tools for using them

[5] These strategic outcomes are stated in the alternative format provided for by GPRA legislation. How performance will be assessed and how the areas of emphasis will be addressed can be found in Section III.

[6] Elements in italics are highlighted in the FY 2001 federal performance plan.

[7] Additional Information on these strategic outcomes can be found in Section III.

ANNUAL PERFORMANCE GOALS FOR NSF'S MANAGEMENT [8]

Performance Areas	FY 2001 Annual Performance Goal
NSF Business Practices	
Electronic Proposal Submission	95 percent of full proposals will be received electronically through FastLane, improving upon the FY 1998 result of 17.5 percent, the FY 1999 achievement of 44 percent and the FY 2000 result of 81 percent.
Electronic Proposal Processing	NSF will conduct ten pilot paperless projects that manage the competitive review process in an electronic environment. (New goal)
Video-Conference/Long Distance Communications	By the end of FY 2001, NSF will increase usage of a broad-range of video-conferencing/long distance communications technology by 100 percent over the FY 1999 level. (New goal)
NSF Staff	
Diversity	NSF will show an increase over 1997 in the total number of hires to S&E positions from underrepresented groups. FY 1997 baseline: 16 females and 15 members of underrepresented minority groups were hired. FY 2000 result: 35 females and 19 members of underrepresented minority groups were hired.
Work Environment	NSF will establish various baselines that will enable management to better assess the quality of worklife and work environment within the Foundation. (New goal)

ANNUAL PERFORMANCE GOALS FOR NSF'S INVESTMENT PROCESS [9,10]

Performance Area	FY 2001 Annual Performance Goal
Proposal and Award Processes	
Use of Merit Review	*At least 85 percent of basic and applied research funds will be allocated to projects which undergo merit review. (Revised goal)*
Implementation of Merit Review Criteria - Reviewers [11]	NSF performance in implementation of the merit review criteria is successful when reviewers address the elements of both generic review criteria. (Revised goal)
Implementation of Merit Review Criteria - Program Officers [11]	NSF performance in implementation of the merit review criteria is successful when program officers address the elements of both generic review criteria when making their award decisions. (Revised goal)
Customer Service - Time to Prepare Proposals	Maintain the FY 2000 goal that 95 percent of program announcements will be available to relevant individuals and organizations at least three months prior to the proposal deadline or target date. FY 1998 baseline: 66%. FY 1999 goal: 95%. FY 1999 result: 75%. FY 2000 result: 89%.
Customer Service - Time to Decision	For 70 percent of proposals, be able to tell applicants whether their proposals have been declined or recommended for funding within six months of receipt, improving upon the FY 1997 baseline of 61%. FY 1998 result: 59%. FYs 1999 and 2000 goal: 70%. FY 1999 result: 58%. FY 2000 result: 54%.
Award Size	NSF will increase the average annualized award size for research projects to $110,000. (New goal) FY 1998 baseline: $90,000. FY 1999 data: $94,000. FY 2000 data: $105,800.
Award Duration	NSF will increase the average duration of awards for research projects to at least 3.0 years. FY 1999 goal: 2.8 years. FY 1999 result: 2.8 years. FY 2000 goal: N/A. FY 2000 data: 2.8 years.
Maintaining Openness in the System	NSF will award 30 percent of its research grants to new investigators. FY 1997 baseline: 27%. FY 1998 data: 27%. FYs 1999 and 2000 goal: 30%. FY 1999 result: 27%. FY 2000 result: 28%.
Broadening Participation	
Reviewer Pool	NSF will begin to request voluntary demographic data electronically from all reviewers to determine participation levels of members of underrepresented groups in the NSF reviewer pool. (New goal)

[8] In FY 2001, NSF continues to emphasize the area of managing information technologies. For details, see Section V.

[9] Additional information on performance goals in this section can be found in Section IV.

[10] Performance goals in italics are highlighted in the FY 2001 federal performance plan and apply to science, space, and technology agencies.

ANNUAL PERFORMANCE GOALS FOR NSF'S INVESTMENT PROCESS [12,13] (continued)

Performance Area	FY 2001 Annual Performance Goal
Facilities Oversight	
Construction and Upgrade of Facilities	*For 90 percent of facilities, keep construction and upgrades within annual expenditure plan, not to exceed 110 percent of estimates. (Revised goal)*
	Ninety percent of facilities will meet all annual schedule milestones by the end of the reporting period. (Revised goal)
	Maintain FY 2000 goal: For all construction and upgrade projects initiated after 1996, keep total cost within 110 percent of estimates made at the initiation of construction. FY 1999 result: No projects completed in FY 1999. FY 2000 result: No projects completed in FY 2000.
Operations and Management of Facilities	*For 90 percent of facilities, keep operating time lost due to unscheduled downtime to less than 10 percent of the total scheduled operating time. (Revised goal)*

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COV Assessment of the Use of the Merit Review Criteria by Division of Chemistry Programs

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- Did reviewers adequately address the intellectual merit criterion in their reviews?

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COV Assessment of the Use of the Merit Review Criteria by Division of Mathematical Sciences Programs

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  The reviewers always addressed adequately the intellectual merit criterion in their reviews. For disciplinary proposals, on the broader impact criterion, most reviewers' comments, if present at all, are limited to impacts on science and technology and training of graduate students and postdocs. These comments are more common in Computational Math. The broader impacts criterion was not usually addressed by reviewers unless issues relevant to that criterion (e.g. the presence of minority students) were raised by the proposer. In Applied Mathematics and in the various cooperative and interdisciplinary programs we looked at, impact on other sciences and applications was a major factor; impact on students was still rarely addressed by reviewers.

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  Program officers always addressed adequately the intellectual merit criterion in their decisions. Program officers were inconsistent in addressing the broader impacts criterion in their decisions. The documentation was inconsistent in showing that the broader impact was considered (again, individual grants). We know from personal experience on panels that these issues have been discussed without being documented in the jacket, but cannot verify that this always happens from the jackets alone. If program officers regularly address these issues in their feedback on both successful and unsuccessful proposals, it would help generate new ideas in the mathematical community.