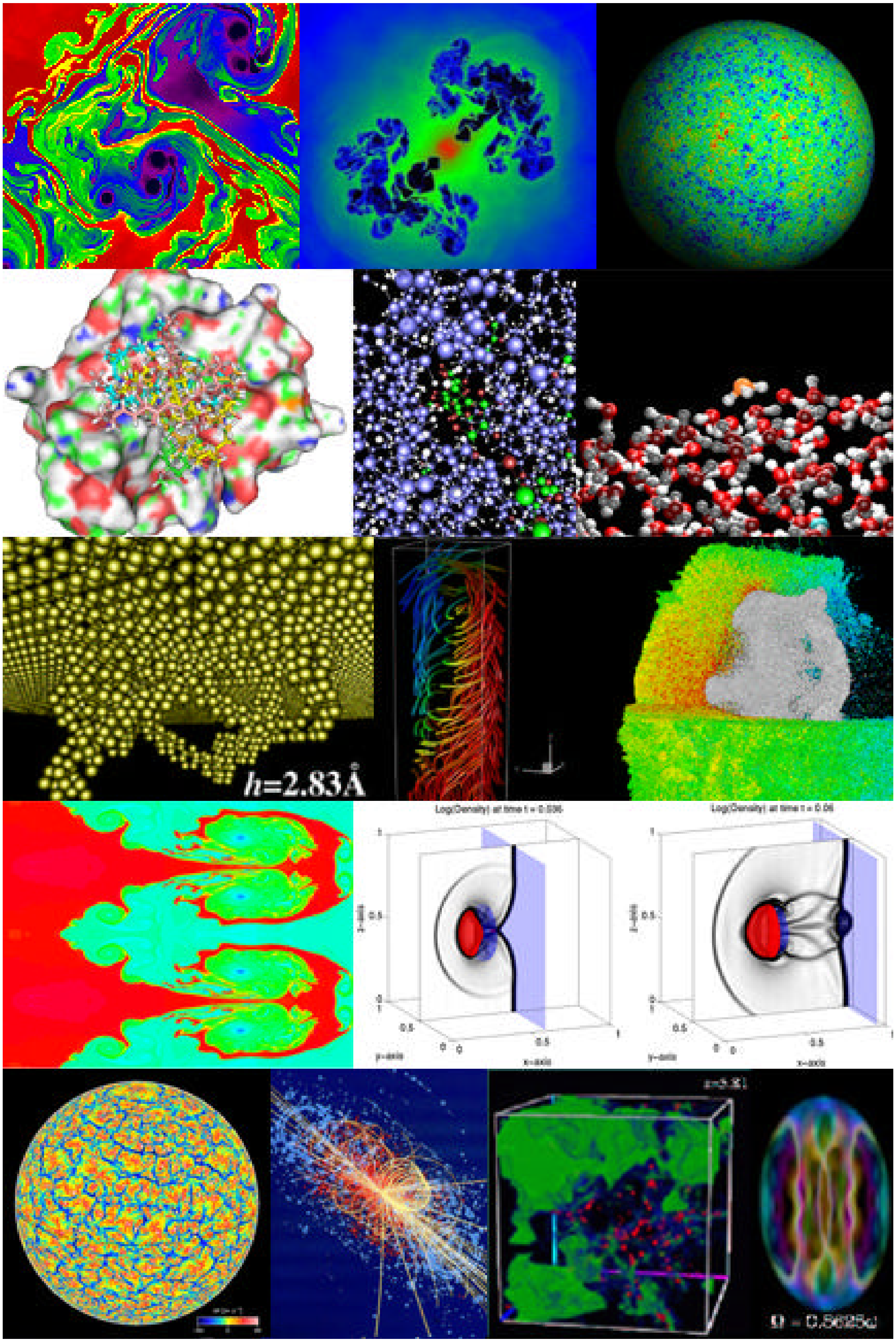
Cyberinfrastructure to enable Cyberscience in the Mathematical and Physical Sciences



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Acknowledgements

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CyberInfrastructure for CyberScience

Vision for NSF CyberInfrastructure

As the recent report to the NSF CI Council, the vision for CyberInfrastructure is stated as "*NSF investments in CyberInfrastructure will enable transformational research, innovation and education in science and engineering, and will engage the full breadth of research communities and institutions.*"

The NSF Mission in Cyberinfrastructure[1] is:

- *To enable a CyberInfrastructure that is driven by science and engineering opportunities, and that is responsive to all research, innovation, and education communities.*
- *To act with inclusiveness so that CyberInfrastructure will be an agent for broadening participation in all areas of science and engineering, and will strengthen the Nation's science and engineering workforce and enhance its global engagement.*
- *To create an integrated and sustainable CyberInfrastructure that is secure, efficient, usable, reliable, dynamically evolving, and ubiquitously available.*
- *To develop CyberInfrastructure as an open system that is engaged and coordinated across sectors, agencies or countries (e.g., public/private, interagency, or national boundaries).*
- *To create a CyberInfrastructure that helps to strengthen the health, competitiveness and security of the Nation*

The Report of the National Science Foundation Advisory Panel on CyberInstrastructure

In February of 2003, the Blue Ribbon Advisory Panel on CyberInfrastructure issued its report entitled, "Revolutionizing Science and Engineering through CyberInfrastructure[2]."
At that time, the panel made the following recommendations to NSF:

- *The Panel.s overarching finding is that a new age has dawned in scientific and engineering research, pushed by continuing progress in computing, information, and communication technology, and pulled by the expanding complexity, scope, and scale of today.s challenges. The capacity of this technology has crossed thresholds that now make possible a comprehensive "cyberinfrastructure" on which to build new types of scientific and engineering knowledge environments and organizations and to pursue research in new ways and with increased efficacy.*

- *Such environments and organizations, enabled by cyberinfrastructure, are increasingly required to address national and global priorities, such as understanding global climate change, protecting our natural environment, applying genomics-proteomics to human health, maintaining national security, mastering the world of nanotechnology, and predicting and protecting against* *natural and human disasters, as well as to address some of our most fundamental intellectual questions such as the formation of the universe and the fundamental character of matter.*

- *The Panel.s overarching recommendation is that the National Science Foundation should establish and lead a large-scale, interagency, and internationally coordinated Advanced Cyberinfrastructure Program (ACP) to create, deploy, and apply cyberinfrastructure in ways that radically empower all scientific and engineering research and allied education. We estimate that sustained new NSF funding of $1 billion per year is needed to achieve critical mass and to leverage the coordinated co-investment from other federal agencies, universities, industry, and international sources necessary to empower a revolution. The cost of not acting quickly or at a subcritical level could be high, both in opportunities lost and in increased fragmentation and balkanization of the research communities.*

- *The emerging vision is to use cyberinfrastructure to build more ubiquitous, comprehensive digital environments that become interactive and functionally complete for research communities in terms of people, data, information, tools, and instruments and that operate at unprecedented levels of computational, storage, and data transfer capacity.*

CyberInfrastructure in the Mathematical and Physical Sciences

One of the guiding principles within MPS is that the **Cyberscience must be the driver of the CyberInfrastructure[2]**. In April a 2004, a workshop was held to identify the major scientific challenges in MPS and their cyberinfrastructure needs. The conclusions of the workshop were that:

- *Tools for cyberscience should be supported, must be shown to enable accountable science research and sit on the cyberinfrastructure being funded by NSF. The needs of each division will vary across MPS, so guidelines must be developed to allow for these variations. These guidelines must clearly define consistent and reliable policies and programs, and describe science-driven activity, differentiating from that which CISE would naturally fund (or delineate joint projects). [Note that not all cyberscience is large scale. As such, an SBIR-like process could be developed for support of such development, with successful Phase 1 projects leading to further support as Phase 2 projects].*

- *Divisions within the directorate should determine what they are currently spending on cyberscience and share this information with the MPS Directorate and MPSAC.*

- *The MPS budget should be assessed with respect to cyberscience awards, and reallocated with specific verbiage to cyberscience and supplements to proposals with cyberscience tool components. As much as possible, collaborative efforts with CISE should be encouraged as well as interagency collaborations.*

- *Coordination of cyberscience as seen by MPS (and other directorates) and cyberinfrastructure as seen by CISE should be addressed "up front." A cross-cutting office, such as an Office of Shared Cyberscience and Cyberinfrastructure,* *could oversee these efforts, and its location within the Foundation should be evaluated. Such an organization, recently established in CISE as the “Division of Shared Cyberinfrastructure” would serve all NSF Directorates. For the needs of MPS, however, a “Cyber working group” with members from MPS community and representation from the CISE community should be immediately established to begin to develop the detailed guidelines of how MPS operates in this construct based on its enabling science. This group should communicate its findings often to the MPSAC, to the CISEAC and to a larger, overarching NSF-wide team.*

- *The goals of the cyberscience programs should be clearly presented. Metrics and assessment guidelines must be developed to assure accountability and to assess effectiveness of the program*

- *MPS with advice from the MPSAC should develop a means to communicate the opportunities and advances in cyberscience and cyberinfrastructure. One mechanism could be to add an obvious cyberscience component to its web page.*

Computational Facilities

Although the highest end computational facilities are typically supplied through the shared cyberinfrastructure of the supercomputer centers, individual groups often have a need for their own clusters for code development, to run small simulations and for data analysis. Another need is for visualization “caves” so that the complex results generated from computer simulations can be viewed in three dimensional perspectives. Cyberscience researchers in all of the MPS disciplines typically need their own local computational facilities. Within MPS these needs are fulfilled either through divisional instrumentation programs or through the NSF Major Research Instrumentation program.

Modeling and Simulation

As high end computing capabilities have increased, modeling and simulation have become an increasingly important tool for understanding the complex nature of physical processes. In astronomy, for example, since controlled experiments are not possible, this tool can be used to help to understand galaxy formation. In chemistry, materials research and physics where experimental observation is possible, modeling and simulation is used to discern the physical mechanisms of observable processes. Mathematicians and statisticians play an important role in algorithm development in which previously intractable problems, where orders of magnitude in computing capability are needed, solvable.

Linking Resources

Linking resources together is the underlying infrastructure which is the hallmark of modern cyberinfrastructure. It includes networking, distributed operating systems and middleware. The software and networking capabilities will lead to Grid development through such projects as GriPhyN in physics and the iVDGL in astronomical sciences. Currently GRID3 resources link more than 2t sites in the US and Korea for applications in high energy physics, biophysics, astrophysics, and astronomy. This will particularly important as the data from such facilities as the Large Hadron Collider collect massive amounts of data.

Data Resources

One of the important aspects of cyberinfrastructure is the collection, archiving, curation, and preservation of large databases. Petabyte-scale data is expected from facilities such as the Large Hadron Collider. While collecting the data is the first step, the analysis of the data to automatically find rare events of crucial importance. The mathematical sciences are expected to play a significant role in analyzing massive data sets to quantify the physical observations. The astronomical sciences, the mathematical sciences and physicists will continue to play a leading role this aspect of cyberinfrastructure.

CI for Physical Facilities

Connecting physical facilities to the internet has become an important asset of the internet. It allows a research group to view the results of an experiment where one member loads the samples. It has decreased the number of researchers who have to physically go to the facility. Researchers can suggest new experiments as the data is transmitted over the internet, increasing the effectiveness of an experiment with the onsite researchers. This aspect of CI will be of importance to research in astronomy, materials and physics.

Emerging Technology

The best hope of increasing the capabilities of researchers are the advances in computing technology, storage, etc. which will lead to the next generation of cyberinfrastructure. Quantum computing, if it can be achieved in a low cost media, will revolutionize the types of problems which are currently unsolvable in finite times, will lead to a new paradigm in computing. All previous attempts at security through encryption will no longer be possible.

The research which leads to new technology will become an important component of keeping the nation at the forefront of research. Although nascent at the present time, this research is the only hope of reaching beyond the current predictions of Moore's law.

Education and Workforce

Within MPS each division has held workshops on Cyberinfrastructure. In addition a number of centers have been started such as the Center for Theoretical and Computational Biological Physics, the Materials Computation Center's summer school, and the Boulder Summer School in Condensed Matter and Materials Physics.

Organizations, Culture Change and Community Development

The Division of Mathematical Sciences uses the five mathematical institutes to foster cyberinfrastructure education. The Physics Division to plan Grid computing education and outreach. In addition they have sponsored a summer school in grid computing.

International

The Division of Materials Research uses the International Materials Institutes to promote international collaboration in Cyberinfrastructure. The Physics Division is using grid computing to foster international collaboration between scientists in the US and South America. In addition they have held an international cyberscience meeting focused on grid computing.

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2. "Computation as a Tool for Discovery in Physics," October 2002, http://www.nsf.gov/pubs/2002/nsf02176/start.htm

3. *Cyber Chemistry Workshop*; workshop held October 3-5, 2004; http://bioeng.berkeley.edu/faculty/cyber_workshop

4. *Materials Research Cyberscience enabled by Cyberinfrastructure*; workshop held June 17 – 19, 2004; http://www.nsf.gov/mps/dmr/csci.pdf

5. *Multiscale Mathematics Initiative: A Roadmap;* workshops held May 3-5, July 20-22, September 21-23, 2004; www.sc.doe.gov/ascr/mics/amr/Multiscale%20Math%20Workshop%203%20-%20Report%20latest%20edition.pdf

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7. *Planning for Cyberinfrastructure Software;* 2005; workshop held October 5 – 6, 2004; www.nsf.gov/cise/sci/ci_workshop/index.jsp

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9. *Preparing for the Revolution: Information Technology and the Future of the Research University*; NRC Policy and Global Affairs, 2002, 80 pages; http://www.nap.edu/catalog/10545.html

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11. *Supplement to the President's Budget for FY 2006*; Report by the Subcommittee on Networking and Information Technology Research and Development (NITRD), February 2005; http://www.nitrd.gov

12. "Quantum Information Science Workshop Proceedings," July 2000, http://www.nsf.gov/pubs/2000/nsf00101/nsf00101.htm

Cyberinfrastructure in Astronomy

The discipline of astronomy has traditionally been heavily involved in what is now called cyberinfrastructure, with the creation of standards for data storage, handling and analysis, with an early understanding of the need for archives and long-term preservation, with involvement in networking for collaboration and remote science (including access to the traditionally hard-to-reach locations of observatories), and with a clear need for computationally intensive simulation, and for high quality, standardized user interfaces. More recently, the explosion in stored digital data has encouraged new studies of techniques and algorithms for data mining, statistical sampling, compression, and interactive visualization, all tools used to assist the science which will flow from this abundance. The use of open-source tools has vastly improved collaboration, as well as involving teachers and students who can be confident their investments of time and money do not tie them to only one or two sources of astronomical information.

Much of the common infrastructure throughout US and world astronomy was, and will be, developed and disseminated with key, if not sole, NSF contributions.

Opportunities for AST in certain critical CI elements

Modeling and simulation

The inability of astronomy easily to conduct controlled experiments, and thus its reliance on purely non-interactive observation, led to an early use of simulation methods as the only way to 'experiment' in most areas of astronomy. Now, as the fourth leg of science (after observation, theory and experiment), astronomical simulation continues to explore otherwise hidden topics and to push the abilities of computer hardware and software.

Traditionally, numerical studies have involved small groups making their own versions of described algorithms, and then enhancing and extending those realizations with no real feedback from, or returned value to, the community. We expect to continue our encouragement for PIs to make code enhancements available: this can be expensive, since there is usually much more effort involved in making a program usable by others than there is in creating it. This may require explicit support, but in the end allowing the rest of the community to benefit from the tools developed during research should be an encouraged goal, if not actually a requirement, of NSF-supported activities.

MPS/AST will continue to push for closer feedback and synergy with observations, to keep simulations grounded in the sky.

Data resources

After some years of investment and effort, bringing data storage and longevity problems to the fore with the creation of an actual data center to implement the vision of the virtual observatory project is a clear top priority and opportunity for MPS/AST. This will be a significant effort, in cooperation with national and international institutions, including support from NASA, to create and operate a repository for all kinds of astronomical data.

This realization of the VO concept is not intended to handle the largest projects. All current and future funded telescope, instrument, and survey projects, are being required to include a data management, release, and access policy. Even for smaller projects, MPS/AST support will increasingly require PIs to include access plans, but also to conform to standards for their data, for the descriptive metadata, and for the user interface. Standards make access and use much easier for the community, while not making those standards compulsory allows for appropriately flexible, case-by-case exceptions, driven by community advice.

Computation facilities

NSF, other agency, and state-supported, supercomputer centers have become an indispensable resource for the conduct of modern astronomy.

Increasingly complex challenges in connecting observational data to the desired science result require more cycles and more collaboration than had previously been imagined. It is not only the simulation theorists discussed above who need major computation: increasingly, data reduction involves sifting vast databases for specific phenomena, and perhaps less noticeably, iterative fitting to disentangle many different sources and reach to the almost-obscured small signal of interest.

Astronomy will need massive CPU power, and both massive and long duration storage, which can best be achieved with a mixture of project-specific and centralized facilities. CI will be critical not only to creating such resources, but to linking them together with each other and with the community to realize their full worth.

International

Astronomy has always had a strong international flavor. The use of far-flung facilities and the need for collaboration with experts across continents will continue, and such interactions will become easier as CI continue to spread. Astronomers expect to continue to be early adopters and willing users of all networking hardware and software, international standards, and remote collaboration tools.

This is just a short list of some of the essential MPS/AST needs for CI, but we confidently expect continued involvement with other identified elements of CI

Astronomy has 'gone digital': photographic techniques have all but vanished and the final image-forming element is now the computer. Theory and simulation have always been computational, and so, increasingly, astronomers meet and science is created across the computer screen. We see that the future holds more and more observational astronomers, especially at smaller or more isolated institutions, doing their research by data mining of archives, and by remote observing with ever more expensive facilities in harder-to-reach locations. CI, in all areas but especially in robust compression, reliable connectivity, archival support, shared software, and the adoption of standards, is absolutely essential to this future of astronomy.

We expect to make continued use of long-standing and respected methods for involving all of US astronomy in the division's major decisions. The obvious benefits of CI must be contrasted with all research support in the competition for funding, and value judgments and cost trade-offs will be made in full partnership with the community.

Cyberinfrastructure in Chemisty

Background

The Division of Chemistry has recognized the transformational potential of cyber-based tools. As articulated in the January 2003 Atkins report (http://www.nsf.gov/publications/pub_summ.jsp?ods_key=cise051203), the April 2004 Mathematical and Physical Sciences Directorate workshop report on cyberscience (http://www.nsf.gov/attachments/100811/public/CyberscienceFinal4.pdf), and the October 2004 Division of Chemistry workshop report on cyber-enabled chemistry (http://bioeng.berkeley.edu/faculty/cyber_workshop/), cyberinfrastructure can enable the chemistry enterprise to address scientific problems of unprecedented complexity, leverage resources by facilitating the sharing of instrumentation, data, and expertise, and broaden participation by creating a national and international community that permits investigators to collaborate with anyone, anywhere, anytime on projects of mutual interest in basic research and education. The most recent Committee of Visitors report urges the Division of Chemistry "…to energize the community to take part in the nascent NSF programs in cyber-technology" (http://www.nsf.gov/od/oia/activities/cov/mps/2004/CHEcov.pdf). A description of the Division's cyber-enabled chemistry efforts and some nuggets of current awards that utilize cyberinfrastructure may be found on the Division's new webpage devoted to cyber, http://www.nsf.gov/chem/cyber.

Opportunities

The emerging national cyberinfrastructure is enabling new chemical research and education activities through grid computing, community databases, remote instrumentation, electronic support for geographically dispersed collaborations, and other web-accessible services. A team of researchers in a virtual laboratory can now assemble distributed expertise and resources to target chemical research and educational priorities. Cyberinfrastructure advances in areas such as scientific portals, workflow management, computational modeling, and data visualization will clearly impact the day-to-day practice of chemistry in the near future. Certain characteristics of the chemistry research community – specifically, the broad range of its computational techniques and data types and its large number of independent data producers – pose unique challenges. Close interaction between practicing chemists and information technology developers, iterative approaches to software development and deployment, and mechanisms to share best practices will all be critical in advancing a cyber-enabled chemistry community using limited resources. The Divisions of Chemistry and of Shared Cyberinfrastructure have shared this vision with the chemical sciences community via a guest editorial in the March 14, 2005 issue of the American Chemical Society's weekly trade journal, *Chemical and Engineering News*, http://pubs.acs.org/cen/editor/83/8311edit.html.

Existing Programs

The Division of Chemistry has updated, and will continue to update, its instrumentation and multi-investigator programs (see http://www.nsf.gov/chem for a complete listing) to encourage projects that contribute to the development of cyber-enabled chemistry. However, the Division recognizes that its core, traditional source of bold, transformative ideas – individual investigators – has much to contribute to this important effort. Therefore, unsolicited research proposals to the Division that include innovative uses of cyber-based tools that can impact chemistry broadly have been strongly encouraged through an April 2005 Dear Colleague letter, NSF 05-024, http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf05024. As is standard practice, these proposals will be submitted to disciplinary programs (Analytical & Surface Chemistry; Inorganic, Bioinorganic & Organometallic Chemistry; Organic & Macromolecular Chemistry; Physical and Theoretical Chemistry). Support for both the research and the cyberinfrastructure innovation can be requested in the budget.

New Programs

In addition, the Division of Chemistry has issued a newly expanded version of its "Chemistry Research and Instrumentation Facilities" solicitation, NSF 05-555, (http://www.nsf.gov/publications/pub_summ.jsp?ods_key=NSF05555) to specifically call for innovative proposals that address the growing importance of cyber-enabled chemistry in the research endeavor. The first proposals in this competition arrived in May 2005, and the Division anticipates making four million dollars' worth of awards. Under this program, investigators may seek funding to establish and support centers for the development of cyber-enabled chemical research. Important components of these awards, to be assessed through additional criteria in the review process, will be the investigators' plans for dissemination of software and for education of potential users, as well as the breadth of the chemical sciences community that is impacted.

Future Plans

Future activities of the Division of Chemistry include assistance with the planning of a cyber-enabled chemistry symposium at one of the two 2006 national American Chemical Society meetings. The two co-chairs of the Division's October 2004 workshop are organizing this symposium. As well, discussions are underway between the Division and the co-chairs for a follow-on meeting of the workshop steering committee in the fall of 2005. The Division's cyber-enabled chemistry plans have also been presented at several venues: the March 2005 FICR meeting of federal agencies who fund chemical research; the May 2005 NCSA strategic planning retreat; and with funding agency counterparts in Europe and Asia, who have been invited to partner with the Division as our plans develop over the coming year.

The Division of Chemistry anticipates that, like the ITR initiative, this is likely to be a five-year effort, by which time cyber will be fully mainstreamed into the Division's portfolio and into the activities of the national chemistry community.

Cyberinfrastructure in Materials Research

As defined by the Cyberinfrastructure Initial Implementation Working Group in **NSF and Cyberinfrastructure**, *CyberInfrastructure is the coordinated aggregate of software, hardware and other technologies, as well as human expertise, required to support discovery and advance understanding in science and engineering. The challenge of CyberInfrastructure is to integrate relevant and often disparate resources to provide a useful, usable, and enabling framework for research, innovation and education characterized by broad access and "end-to-end" coordination.* There are a circle of opportunities for DMR in the area of Cyberinfrastructure (CI) DMR recognizes that a thoughtful CI driven by the needs of science at the frontiers and deliberately implemented, has the potential to revolutionize how the science of materials research is done by forging closer collaborations that have no borders, by engaging the computational frontiers enabling the prediction of new materials and the understanding of new phenomena, and by educating and training the next generation of condensed matter and materials scientists to empower them to advance the frontiers of knowledge. The science of materials research naturally closes the circle of CI opportunities; DMR engages the fundamental and scientific and technical challenges that lay the foundations for the technologies that will become the next generation of CI. Because of the interdisciplinary nature of materials research, flexibility and diversity are key ingredients to realize the potential that CI holds for materials science, condensed matter physics, and solid state chemistry.

Opportunities for DMR in key critical CI elements

Emerging Technology

Materials research paves the way to discover and invent new ways to control and manipulate nature to advance materials and device technologies. Materials research holds the promise for developing dramatically improved materials for CI components leading to faster, cheaper, and better devices to manipulate electron charge and spin, and light down to the level of a single photon. The seemingly counterintuitive quantum mechanics is needed to describe, understand, and predict the properties of these materials, the operation of the devices made from them, and the new condensed matter phenomena that will be discovered. New physical realizations of computing based on the preparation and manipulation of quantum mechanical states may enable logic operations, new methods for information transfer, and a new frontier for parallel computing.

CI for Physical Facilities

CI provides an opportunity to create and deploy standardized data gathering, visualization, and advanced data analysis tools for major materials research facilities, including the National High Magnetic Field Laboratory, CHERNS, the Spallation Neutron Source, and the advanced light source. CI will enable the global sharing of data and will enable collaborations for data analysis and interpretation. Direct comparisons of data from Facilities with theory enhanced by computation may also guide the direction of experiments in real time. For example computations using standard shared electronic structure codes may speed the determination of crystal structures and Fermi surface geometries from diffraction and dHVA data.

Modeling and Simulation

Through modeling and simulation, we have the potential to predict properties of materials before they are synthesized as well as to predict and understand new condensed matter phenomena. While great advances have been made in simulating the properties of materials starting from constituent atoms, the reverse process remains a holy grail of the materials research community: How does one design a material starting with constituent atoms, that will possess a desired macroscopic property? The solution of this problem requires both conceptual advance and advances in computational capabilities (through algorithmic development and code development efforts integrated with research that lead to mature codes that can be shared by the research community) of materials research along many avenues. At the same time, simulation also holds the key to understanding challenging problems, such as: Can transitions from one electronic state of matter to another at absolute zero of temperature lead to unusual electronic states at finite temperature? Are there new mechanisms that enable electrons to become superconducting at high temperatures? Inspired simulation will accelerate the theoretical prediction and eventual discovery of new states of matter. It may in fact be critical to the realization of such discoveries. CI can enable the creation of standard simulation codes with benchmarked accuracy and support their distribution across the materials research community. Because of the inherent intellectual diversity of this community, the best strategies will stimulates new ideas, support their implementation, and advance the best algorithms and codes into mature shared software for the entire community. This activity involves support at various levels from the individual investigator to groups and centers that can effectively maintain and distribute advanced software.

Computation Facilities

There is a need to support the acquisition of capacity high performance computing, best associated with Centers and Facilities. The need for computing to determine the consequences of increasingly complex theories and understand their relationship with experiment continues to grow, particularly as new materials and new phenomena are discovered. Computation will be needed to meaningfully compare theory and experiment. Computational facilities are the natural distributors and repositories of shared software. Through linkages with diverse efforts from individual investigators to research groups across the global community, they should play a key role in developing mature user friendly codes and their maintenance. Facilities should be encouraged to linkages that are diverse and of broad scope to include minority serving institutions, institutions in EPSCoR states, and international partners.

Education and Workforce

The opportunities for the materials research community in this area are twofold. First, CI offers unprecedented access to knowledge, education, and training that can crush geographical, economical, and sociological barriers. Individual grants have contributed to a materials research educational cyberinfrastructure; the possibility exists to harvest these seeds to create a coherent educational tool, while pushing development to the next level. Second, education is required to effectively use the developed and developing materials research and broader CI to advance the scientific frontiers effectively. Support from the individual investigator to the Center and Facility level is required to achieve these goals.

International

CI is a natural tool to enhance collaboration – it is the next best thing to being in the room. As such, it can enable and help sustain collaborations involving investigators across the world. Where sensible and mutually beneficial, opportunities to coordinate research projects involving CI creation and utilization of CI with partners in other nations should be pursued. Facilities, centers, and large groups should be encouraged to include international partners where appropriate for doing the science.

Crosscutting strategy

The ultimate success of CI hinges on its use and effectiveness. Implementations of CI should be integrated into all solicitations where it can play a sensible role. Flexible and dynamic “science focused networks” (SFN) that involve participation from institutions, individual PIs, facilities, centers, etc., provide a natural mechanism to achieve the goal of science driving the development of CI that is needed. The creation of new networks and enhancing existing networks should be encouraged to focus the talents of the community on challenging problems and to harvest ripe opportunities. Science Focused Networks – like “soft-matter net, light source-net, etc.” would exist at various levels and intersect and feed into each other. The science thrusts inside a center would likely couple to different networks at different times. SFN’s may at once keep members of the community abreast of developments in fast moving fields while avoiding needless duplication of effort.

Cyberinfrastructure in the Mathematical Sciences

It's Not Just About the Hardware, Systems Software, and Middleware:
The Cyberscientific Case for Mathematical Soft Cyberinfrastructure

The core of the DMS view of cyberinfrastructure is this: **To solve the scientific problems of the age, a mathematical infrastructure of models, algorithms, and software is crucial.** Computational science, complementing and fostering communication between theoretical and experimental science, has become a vital "third mode" that opens previously unattainable insights and advances. In "focusing on the science and engineering frontier" (Bement, *NSF's Cyberinfrastructure Vision for 21st Century Discovery,* NSB Meeting, 5/26/05), fulfillment of the potential of this ongoing scientific revolution demands development of this mathematical infrastructure, which could be called a mathematical *soft cyberinfrastructure.*

Computational science

Scientific progress in which computation is fundamental can take many forms, but a typical, simple paradigm incorporates the following interdependent elements:

1. *Domain application and mathematical model* – the expression of the scientific problem in mathematical terms, frequently including a system of differential equations, with a recent trend toward discrete structures in many cases.
2. *Mathematical algorithms and software* – procedures and implementations that obtain analytical or approximate solutions of the mathematical model.
3. *Hardware and middleware* – computers to execute the software implementations, and software modules and tools that assist in building application-specific codes.

The case to be made here is that among these elements, **"cyberinfrastructure" includes more than 3.; it also includes much of 2. and some modeling aspects of 1.** In many settings, these latter elements need the expertise of mathematicians who deeply understand the principles underlying the applications and who can connect the models to the appropriate mathematical structures.

Scientific drivers

Cyberinfrastructure is driven by ***cyberscience:*** *science that cannot be done without the advanced capability of cyberinfrastructure* (so defined in the report of the MPS Cyberscience Workshop, April 2004, page 1). DMS has identified the following scientific drivers that it sees as central to the advances of the next ten years:

A. Modeling of complex systems, particularly ones with multiple space and time scales.
B. Incorporation and quantification of uncertainty in physical and biological systems.
C. Identification of patterns and low-dimensional structures in massive data sets.

Soft cyberinfrastructure for the scientific drivers

Central to the drivers are 1. and 2. above:

A. The executive summary of a recent DOE Office of Science report, *Multiscale Mathematics Initiative: A Roadmap,* December 2004, identifies the scientific need: "[M]athematical modeling and computational simulation have reached the point where simulation of most physical processes over relatively narrow ranges of scales has become an essential tool for both scientific discovery and engineering design. Further growth, however, is significantly limited by the absence of a *mathematical framework and software infrastructure* [italics added] to integrate heterogeneous models and data over the wide range of scales that characterize most physical phenomena. Fundamentally new mathematics and considerable development of computational methods and software will be required to address the challenges of multiscale simulation." This prescription includes the modeling part of 1. and all of 2.

B. Peter Bickel, in NSF 0120, *Opportunities for the Mathematical Sciences,* October 2001, writes: "Computer models … are sometimes deterministic (the atmosphere), sometimes stochastic (parts of the immune system), and sometimes both (transportation) … Validation of these models is largely not performed, or is an art. These problems pose important joint challenges to applied mathematics, numerical analysis, computer science, and statistics … How does one allocate resources between replication of experiments, constructing better algorithms, and building in improvements to basic theory in refining the scale of the models? To make these compromises intelligently involves studying the interaction of statistical uncertainties coming from the data, with numerical error, with model uncertainty, with computational speed, all in the light of what the model is going to be used for. *The theory of this type of combination of error analyses still has to be developed* [italics added] and should be done in an interdisciplinary fashion. These questions are becoming more and more central as experimentation in many areas, if not impossible, is ruinously expensive, analytic approximations are largely impossible, and computing is ever cheaper." Again, the need is for a mathematical cyberinfrastructure to cover the modeling part of 1. and all of 2.

C. The report of the MPS Theory Workshop, October 2004, page 12, notes: "The nature of experimental data is changing rapidly. Astronomers, particle physicists, meteorologists, and geneticists are all blessed and cursed with data-gathering techniques that can put terabytes of data on record in short periods. These data have features that confound traditional statistical methodology: signals may be tiny compared to noise, features to be identified may be rare and unknown in shape, … and the data sampled in a single instant may have enormous apparent dimension. Ongoing work by statistical scientists addresses problems of pattern discovery and description, dimension reduction, and compression by applying methods of topology, computer science, and approximation theory." Again, this depends on modeling in 1. and on all of 2.

Modeling and simulation in general

The CIIWG report, *NSF and Cyberinfrastructure (CI),* April 2005, Section 3, page 7, focuses on applied research and technology development, as opposed to basic research funded through regular disciplinary and interdisciplinary programs. For basic research on mathematical structures and algorithms, regular DMS program funds are the expected source. **Software implementation of these structures and algorithms should be seen as CI: it is appropriate for the reasons outlined above, and it lacks a home in the existing funding structure.** DMS focuses on mathematical advances, not on complex production codes that can be shared by many applications; CISE has limited interest in mathematical software; codes supported by other divisions and directorates tend to be application-specific. **This gap should be of concern throughout the research divisions of NSF.**

Software development support

"Balanced hardware-software investments" (Bement, 5/26/05) should include a software portfolio that is balanced between middleware and implementations of mathematical models and algorithms. CIIWG Section 3.2, pages 8-9, advocates support for meta-modeling approaches to complex phenomena, multiscale platforms with wide applicability, and advanced numerical models. It suggests **emulation of the DOE SciDAC (Scientific Discovery through Advanced Computing) program** to support teams of basic researchers, computational mathematical scientists, and computer scientists in areas not covered by SciDAC. This would **"complement the HPC investments of partners"** (Bement, 5/26/05), bringing basic structures to implementation in a non-mission-oriented way. Key components of this recommendation are dissemination of algorithmic developments across research communities to uncover unifying principles, and exchange and sharing of codes. The report of the MPS Cyberscience Workshop, pages 14-15, recommends an SBIR-like funding mechanism and long-term investments where warranted, noting the long start-up cost and time involved.

Partnerships

DMS has used its former ITR funds to expand interagency activities, including the NSF/NIH/NASA/DOE program on Multiscale Modeling of Biomedical, Biological, and Behavioral Systems (MSM-BBB). CIIWG Section 3.1, pages 7-8, discusses partnerships with DOE and NASA for availability of compute resources; **science-driven intellectual partnerships such as MSM-BBB and an emulation of SciDAC should be the soft cyberinfrastructure complement to this.**

Education and workforce

CIIWG Section 7, page 29, notes that emulation of SciDAC as above would match the emergence of academic programs in **Computational Science and Engineering (CS&E). This will be the core of training in the "third mode" of science,** developing the fundamental skills needed to formulate mathematical models, choose and/or design appropriate algorithms, implement them in mathematical software, and evaluate the scientific implications of the results.

Cyberinfrastructure in Physics

The Physics Division supports experimental and theoretical research in elementary particle physics, nuclear physics, particle and nuclear astrophysics, gravitational physics, atomic, molecular, and optical physics, plasma physics, biological physics, and at the interfaces among these fields and research in other MPS divisions and other NSF directorates. These research efforts range from individual research awards supporting summer salary to support for large facilities costing hundreds of millions of dollars. Almost all these activities require some cyberinfrastructure support for desktop computers, internet access, and computer interfaces to experimental equipment. There are, however, several areas of research at the frontiers of computational physics that are heavily reliant on state-of-the-art cyberinfrastructure and are also contributing to the next generation of cyberinfrastructure.

Computer simulation

Computer simulation bridges the gap between the limits of formal theory and experiment. It allows the exploration of physical systems beyond the limits of experiment and provides a way to predict the behavior of complex, nonlinear systems to difficult for mathematical analysis. Examples include simulations of the strong interaction (quantum chromodynamics) that are just now approaching the ability to predict the properties of elementary particles and nuclei, development of techniques to enable the simulation of realistic astrophysical systems that are expected to be sources of gravitational waves, the use of computer simulation to explore novel behavior observed in Bose-Einstein condensates and laser interaction with matter, and modeling of complex biological systems. Computer simulations are also used to model complex physics experiments to predict or control their performance expected backgrounds to the desired signals. Infrastructure required for computer simulation includes algorithm development (often engaged in by supported PI's), computer hardware including clusters of moderate size for code development and supercomputers for production runs, and tools for visualization and data analysis.

Data analysis

The Physics Division supports a number of large facilities either producing or expected to produce huge amounts of data. The need to analyze the petabyte-scale data expected from the Large Hadron Collider (LHC) motivated the development of the Grid, a paradigm to enable any scientist to call upon huge computational resources in a seamless and transparent way. The LHC scientists (and computer scientists) have contributed to Grid development and use through their leadership of the large ITR projects GriPhyN and iVDGL. The operating GRID3 allows computer resources from more than 25 sites in the US and Korea to be used for 7 scientific applications in high energy physics, biophysics, astrophysics, and astronomy. As one of the partners in the iVDGL (with LHC and the Sloan Digital Sky Survey), the LIGO Scientific Collaboration (LSC) is already using Grid tools and protocols to analyze its data. The Grid effort is pointed toward infrastructure development with the potential for broad application in data-intensive scientific research. In a parallel effort, the LSC is approaching analysis of its terabyte-scale data with distributed computing, in collaboration with the computer scientists who developed SETI@home. Einstein@home has extended the SETI@home interface to enable an all sky search for gravitational waves from neutron stars. This paradigm is an alternative to Grid for computationally intensive data analysis. Many other experiments in elementary particle physics and nuclear physics require significant computer infrastructure to analyze large data sets, simulate backgrounds, and maintain effective communications in international collaborations.

Revolutionary computing

Although computer hardware has made great leaps in the past decades, eventually hardware development using semiconductors will run into physical limits that will prevent further performance increases. To overcome these obstacles, a number of schemes to use quantum effects in atomic or molecular scale systems as computers are being pursued. Both theoretical and experimental research is supported. Examples include programs to create actual qubit processors by using lasers to control atoms and theoretical studies of quantum information processing. Revolutionary computing is expected to be an essential component of future cyberinfrastructure.

Experimental control

An underappreciated form of cyberinfrastructure is exemplified by the beyond-the-state-of-the-art instrumentation at Physics Division large facilities. Computer control is essential for such instruments, is highly complex, and must be developed by the participating scientists.

Reports

"Computation as a Tool for Discovery in Physics," October 2002, http://www.nsf.gov/pubs/2002/nsf02176/start.htm
"Quantum Information Science Workshop Proceedings," July 2000, http://www.nsf.gov/pubs/2000/nsf00101/nsf00101.htm
"Physics of the Universe," February 2004, http://www.ostp.gov/html/physicsoftheuniverse2.pdf
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MPS Investment by CI Element

Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
Computation Facilities	$ 2.49	$ 4.59	$ 6.63	Major computing capabilities at national centers; MRSEC facilities; cluster hardware supported under CRIF, MRI, IMR, ITR and core programs (e.g., MT), and EMSI and CRC; Computer clusters for data analysis for gravitational waves (LIGO) and elementary particle physics (D0, ATLAS).	See comments from Divisional tables.
Modeling and Simulation	$ 5.31	$ 9.63	$ 13.91	Numerical algorithm development, computational sciences; Institute for Theory of Advanced Materials for Information Technology; Quantum Mechanical Modeling; Computational Tools for Materials research; ITR (shared software); Materials Computation Center [software archive + research thrusts]; IMI: Materials Informatics and Combinatorial Materials Science. Computational and mathematical framework for annotation of large image databases; computational toolbox for multiscale surface processes; computer algebra system and software to manipulate large data sets in theoretical mathematics; symbolic software for analytical evaluation of integrals; high-resolution simulations of magnetohydro-dynamic turbulence; computational tools, utilizing grid-computing, to assist natural resource managers in assessing the impacts of alternative management plans; simulators and large-scale optimization techniques for modeling and data-driven decision-making in subsurface environments. Gravitational wave source simulation, lattice gauge theory simulations of elementary particles and their interactions, simulations to calculate the electronic structure of atoms and molecules, computational biological physics; algorithm development for gravitational wave data analysis.	See comments from Divisional tables.

MPS Investment by CI Element

Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
Linking Resources	$ 2.38	$ 4.71	$ 7.05	Virtual Observatory connectivity; ITR projects (e.g., web-based grid-computing environment for chemistry, materials, and engineering research); NIH/NSF collaborative project to develop a protein structure cyber environment; Computational Tools for Multicomponent Materials Design; Multiscale Simulations of Nanosystems; Grid middleware for simulators and data-driven decision-making in subsurface environments; Grid computing middleware.	See comments from Divisional tables.
Data Resources	$ 1.18	$ 1.89	$ 2.63	National observatories: development of standards and maintenance of archives; Databases are supported in ASC and EMSI programs; IMI: Materials Informatics and Combinatorial Materials Science; Computational Tools for Multicomponent Materials Design; Computational and mathematical framework for annotation of large image databases; computer algebra system and software to manipulate large data sets in theoretical mathematics.	See comments from Divisional tables.
CI for Physical Facilities	$ 2.64	$ 4.28	$ 5.71	Remote observing and operations; software tools for analyzing data obtained at National facilities; sensors and instrumentation and remote experiment support	See comments from Divisional tables.
CI Systems Design	$ -	$ -	$ -		See comments from Divisional tables.
Emerging Technology	$ 5.94	$ 10.17	$ 14.07	ITR and ASC investments in revolutionary computing; “Quantum computing” ITR grants and MT core; revolutionary computing; application of Grid computing tools to elementary particle experiments.	See comments from Divisional tables.

MPS Investment by CI Element

Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
Education and Workforce	$ 0.15	$ 0.24	$ 0.33	Dissemination and training; URC, CRC and URC planning grants, DCF, and NUE; CSWUG [Workshop for under represented groups.]; education activities of Center for Theoretical and Computational Biological Physics; Materials Computation Center summer school activity; Boulder Summer School Condensed Matter and Materials Physics; mathematical institutes that establish community connections, with some activities related to CyberInfrastructure education; conferences to stimulate diverse scholarly communities; education and outreach as a part of Grid computing projects; summer school in grid computing.	See comments from Divisional tables..
Organizations, Culture Change and Community Development	$ 0.22	$ 0.38	$ 0.54	See comments from Divisional tables.	See comments from Divisional tables.
Inside NSF	$ -	$ -	$ -		See comments from Divisional tables.
Partnering (agencies, industry, university)	$ -	$ -	$ -		See comments from Divisional tables.
International	$ 0.80	$ 1.52	$ 2.22	International VO Alliance; international collaboration on databases and algorithms; IMI: Materials Informatics and Combinatorial Materials Science; CyberInfrastructure equipment to enable Grid computing between US and South America; educating international partners in relevant experiments in Grid computing; presentation of Grid computing at international cyberscience meeting.	See comments from Divisional tables.
Totals	$ 21.10	$ 37.40	$ 53.10		

AST Investment by CI Element

Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
Computation Facilities	$ 0.55	$ 0.89	$ 1.24	Major computing capabilities at national centers	individual investigator, group, and departmental compute servers
Modeling and Simulation	$ 1.20	$ 1.96	$ 2.72	Numerical algorithm development in many fields of astrophysical simulation (e.g., supernovae, accretion&jets, galaxy dynamics of stars and gas).	research use of “static” simulation methods, not involving algorithm development and enhancement.
Linking Resources	$ 0.73	$ 1.20	$ 1.66	Work under the Virtual Observatory umbrella; work supported by national observatories for connectivity to and between mountain-tops in both North and South America.	hard to estimate, but significant, informal contributions
Data Resources	$ 0.86	$ 1.40	$ 1.94	National observatories:development of standards and maintenance of archives	maintenance of data sets by individual investigators
CI for Physical Facilities	$ 0.17	$ 0.28	$ 0.39	Remote observing and operations	
CI Systems Design	$ -	$ -	$ -		
Emerging Technology	$ 0.38	$ 0.61	$ 0.86	Limited investments: we try to adopt and adapt rather than invent	
Education and Workforce	$ 0.04	$ 0.06	$ 0.09	Dissemination and training, both on-line (interaction, web sites) and via meetings	the “usual” training of students and postdocs, increasingly involving CI
Organizations, Culture Change and Community Development	$ -	$ -	$ -		
Inside NSF	$ -	$ -	$ -		
Partnering (agencies, industry, university)	$ -	$ -	$ -		
International	$ -	$ -	$ -		
Totals	$ 3.92	$ 6.40	$ 8.90		

CHE Investment by CI Element

Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
Computation Facilities	$ 0.61	$ 1.39	$ 2.17	Hardware is supported under CRIF, MRI, and core programs, as well as EMSI and CRC.	Hardware supported under individual investigator and group grants
Modeling and Simulation	$ 1.13	$ 2.59	$ 4.03	CHE support includes computational chemistry, broadly defined, in its core programs. Much of this research, while not currently making "fullest use of cyberinfrastructure capabilities," certainly contributes through, e.g., algorithm development that will impact cyber environments.	Theoretical and Computational Chemistry Program, e.g., as well as other modeling and simulation efforts in core programs
Linking Resources	$ 0.40	$ 0.93	$ 1.44	A majority of CHE ITR activities can be placed in this category. However, some of this investment covers hardware and education. Other examples include an NIH/NSF collaborative project to develop a protein structure cyber environment, and an ITR grant to develop a web-based grid-computing environment for chemistry, materials, and engineering research.	Many CHE facilities and other larger-scale grants contain middleware and other cyber infrastructure in their operations.
Data Resources	$ 0.06	$ 0.13	$ 0.21	Databases are supported in ASC and EMSI programs.	Databases in individual investigator awards
CI for Physical Facilities	$ -	$ -	$ -		
CI Systems Design	$ -	$ -	$ -		
Emerging Technology	$ 0.06	$ 0.15	$ 0.23	ITR and ASC investments in revolutionary computing.	Related individual investigator and NANO awards
Education and Workforce	$ -	$ -	$ -		Training of students and postdocs, increasingly involving CI
Organizations, Culture Change and Community Development	$ 0.09	$ 0.20	$ 0.32	Annualized FY04 investments include URC , CRC and URC planning grants, DCF, and NUE.	Related workshops
Inside NSF	$ -	$ -	$ -		
Partnering (agencies, industry, university)	$ -	$ -	$ -		
International	$ -	$ -	$ -		
Totals	$ 2.35	$ 5.40	$ 8.40		

DMR investment by CI Element					
Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
Computation Facilities	$ 1.03	$ 1.67	$ 2.23	Instrumentation program, National facilities, MRSEC shared computational infrastructure, MT program and ITR support for compute clusters.	Compute clusters and computers provided through the NSE competition
Modeling and Simulation	$ 1.30	$ 2.11	$ 2.81	M&S activities supported by MT program, MRSEC's, ITR awards, and International Materials Institutes	Production runs using existing codes supported through individual investigator awards, group awards and centers
Linking Resources	$ 0.05	$ 0.08	$ 0.11	Supported through ITR medium grants aiming to use GRID computing to calculate materials properties.	Preliminary connectivity of DMR centers and national facilities
Data Resources	$ 0.10	$ 0.16	$ 0.22	Part of COSMIC International Materials Institute activities and ITR medium awards involving database creation and enhancement	Maintenance of data sets by individual investigators, groups, centers and facilities
CI for Physical Facilities	$ 2.47	$ 4.00	$ 5.32	Software tools at National Facilities for data analysis. Facilities and centers sensor and remote instrumentation support.	
CI Systems Design	$ -	$ -	$ -		
Emerging Technology	$ 4.56	$ 7.39	$ 9.85	Estimate includes "revolutionary computing" related ITR awards and estimates from core programs across DMR.	Does not include contributing research supported by other solicitations, e.g. NSE, and core research related to revolutionary computing.
Education and Workforce	$ 0.11	$ 0.18	$ 0.24	Includes education activities supported through ITR medium awards, e.g., MCC, and Boulder Summer School on Condensed Matter and Materials Physics summer schools that are CI related.	The training of students at all levels and postdoc's through compute-intensive awards (primarily MT)
Organizations, Culture Change and Community Development	$ -	$ -	$ -		
Partnering (agencies, industry, university)	$ -	$ -	$ -		
International	$ 0.38	$ 0.62	$ 0.82	CI related activities supported under International Materials Institutes, notably COSMIC, and other DMR initiatives focused on promoting international collaboration.	Does not include extensive international computational collaborations embedded in core awards (primarily MT)
Totals	$ 10.00	$ 16.20	$ 21.60		

DMS investment by CI Element

Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
Computation Facilities	$ -	$ -	$ -		Scientific Computing Research Equipment for the Mathematical Sciences (SCREMS) program: provides hardware for departments and research groups; occasional larger investments handled through MRI
Modeling and Simulation	$ 0.73	$ 0.93	$ 1.19	Computational and mathematical framework for annotation of large image databases; computational toolbox for investigation of multiscale surface processes that are central to nanotechnology; computer algebra system and software to manipulate large data sets in theoretical mathematics; symbolic software for analytical evaluation of integrals; high-resolution simulations of magnetohydrodynamic turbulence; computational tools, utilizing grid-computing, to assist natural resource managers in assessing the impacts of alternative management plans; simulators and large-scale optimization techniques for modeling and data-driven decision-making in subsurface environments.	Computational Mathematics program: supports research in algorithms, numerical and symbolic methods, and mathematical research in all science areas where computation plays a central and essential role. Awards range from single-investigator projects that develop and analyze innovative computational methods to interdisciplinary team projects that not only create new mathematical and computational techniques but use them to model, study, and solve important application problems. Major driving scientific themes include data sets and pattern discovery, complex multiscale systems, and stochasticity and uncertainty. Highly interdisciplinary; co-funds with most NSF research divisions and other agencies. Other programs using funds formerly allocated to ITR: Multiscale Modeling of Biomedical, Biological, and Behavioral Systems (MSM-BBB, with CISE, ENG, NIH, NASA, DOE); Analysis, Modeling, and Computation for Stochastic Systems.
Linking Resources	$ 0.09	$ 0.12	$ 0.15	Grid middleware for simulators and data-driven decision-making in subsurface environments.	
Data Resources	$ 0.16	$ 0.20	$ 0.26	Computational and mathematical framework for annotation of large image databases; computer algebra system and software to manipulate large data sets in theoretical mathematics;	Mathematical and statistical projects in data representation, manipulation, and analysis
CI for Physical Facilities	$ -	$ -	$ -		
CI Systems Design	$ -	$ -	$ -		
Emerging Technology	$ -	$ -	$ -		

DMS investment by CI Element

Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
Education and Workforce	$ -	$ -	$ -		Education and interdisciplinary training in computational science and engineering, mathematical software development
Organizations, Culture Change and Community Development	$ 0.12	$ 0.16	$ 0.20	Five mathematical institutes that establish community connections, with some activities related to cyberinfrastructure education; conferences to stimulate diverse scholarly communities;	
Inside NSF	$ -	$ -	$ -		
Partnering (agencies, industry, university)	$ -	$ -	$ -		Interagency activity on Multiscale Modeling of Biomedical, Biological, and Behavioral Systems (MSM-BBB, with CISE, ENG, NIH, NASA, DOE)
International	$ -	$ -	$ -		
Totals	$ 1.10	$ 1.40	$ 1.80		

PHY investment by CI Element

Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
Computation Facilities	$ 0.30	$ 0.64	$ 0.99	Computer clusters for data analysis for gravitational waves (LIGO) and for elementary particle physics (D0, ATLAS).	Many theory awards include support for computers or small computer clusters. Computer clusters obtained as part of large facility operations (e.g. LIGO) are not broken out (those for collaboration members are broken out).
Modeling and Simulation	$ 0.95	$ 2.04	$ 3.16	Gravitational wave source simulation, lattice gauge theory simulations of elementary particles and their interactions, simulations to calculate the electronic structure of atoms and molecules, computational biological physics; algorithm development for gravitational wave data analysis.	Algorithm development as part of individual investigator grants for projects with a computational physics component. Modeling and simulation to characterize (usually large) instruments such as LIGO, ATLAS in order to understand data as part of individual investigator or facility operations awards.
Linking Resources	$ 1.11	$ 2.38	$ 3.69	Grid computing middleware	
Data Resources	$ -	$ -	$ -		
CI for Physical Facilities	$ -	$ -	$ -		Last mile linkage of LIGO laboratory sites to high speed networks is part of facility operations and not broken out.
CI Systems Design	$ -	$ -	$ -		
Emerging Technology	$ 0.94	$ 2.02	$ 3.13	Revolutionary computing; application of Grid computing tools to elementary particle experiments.	
Education and Workforce	$ -	$ -	$ -		.
Organizations, Culture Change and Community Development	$ 0.01	$ 0.02	$ 0.02	Meeting to plan Grid computing projects' education and outreach; summer school in grid computing.	
Inside NSF	$ -	$ -	$ -		
Partnering (agencies, industry, university)	$ -	$ -	$ -		

PHY Investment by CI Element

Cluster or Element	FY04 Actual	FY05 Plan	FY06 (request)	Text describing content of the CI cross-cut portfolio	Text describing content of investments not included in the CI cross-cut
International	$ 0.42	$ 0.90	$ 1.40	Cyberinfrastructure equipment to enable Grid computing between US and South America; educating international partners in relevant experiments in Grid computing; presentation of Grid computing at international cyberscience meeting.	Einstein@home is an international effort to use individual desktop computers in LIGO data analysis.
Totals	$ 3.73	$ 8.00	$ 12.40		