The NSF CI Vision and the Office of CyberInfrastructure

Software Engineering for High Performance Computing Applications

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Office of Cyberinfrastructure
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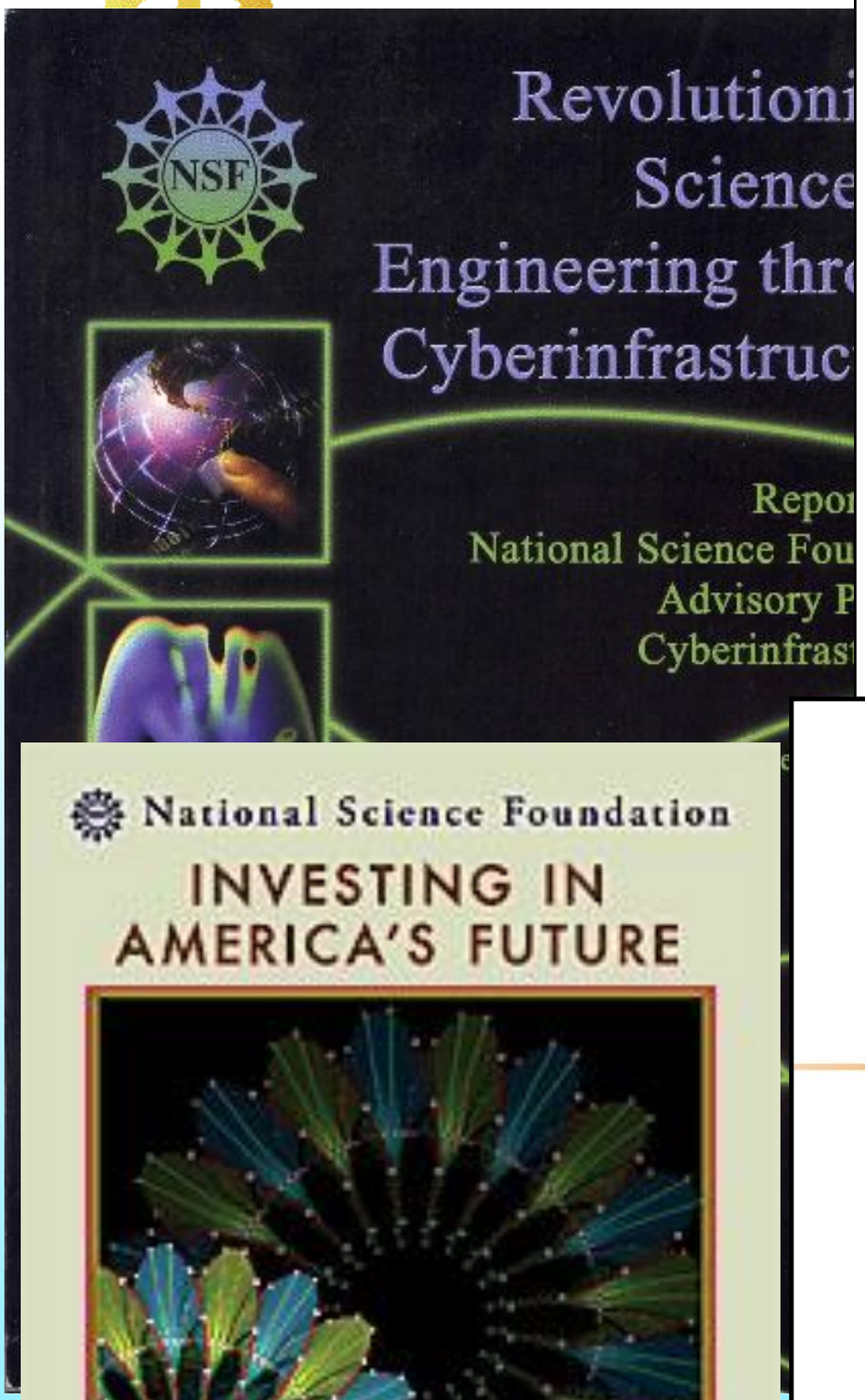
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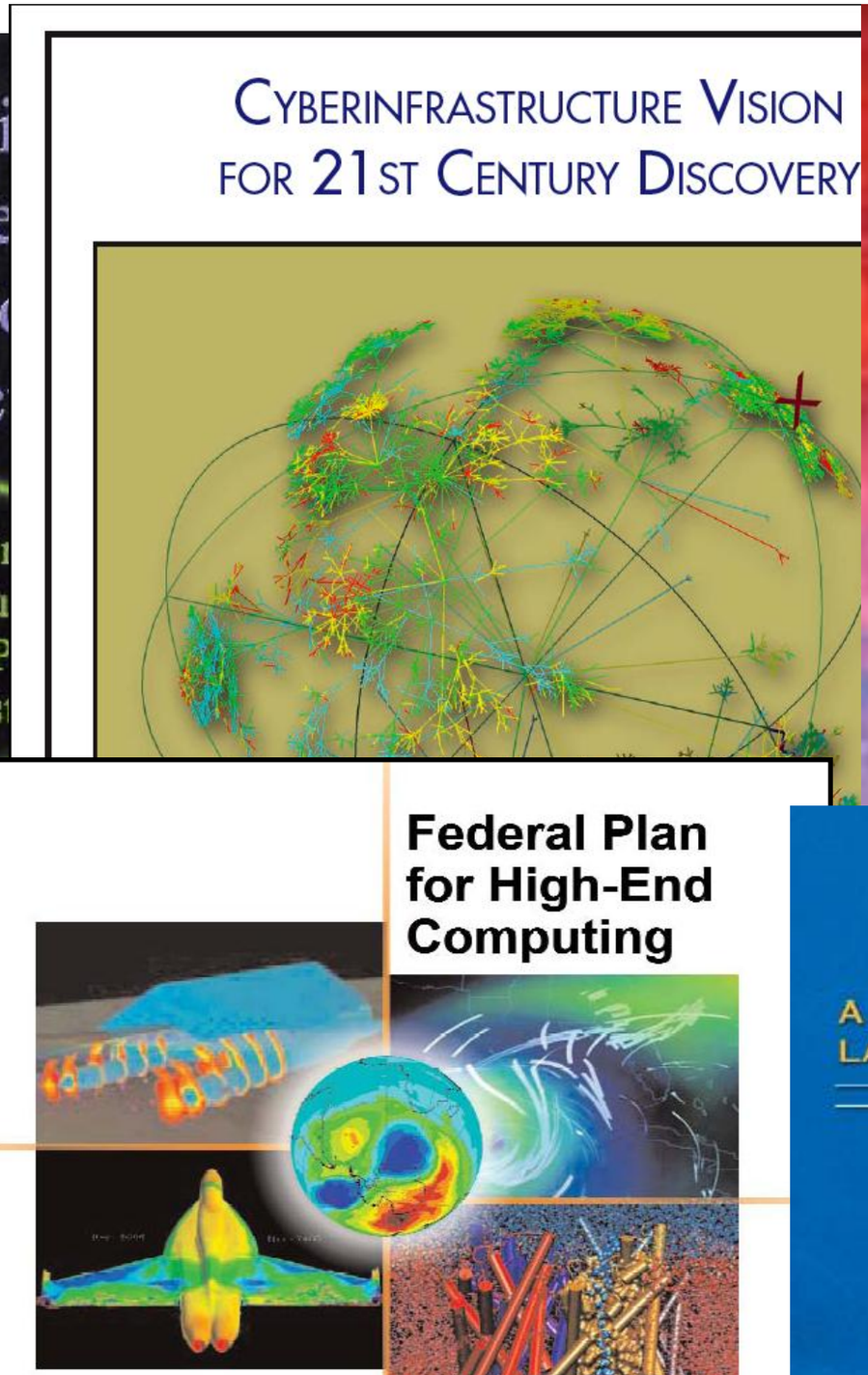
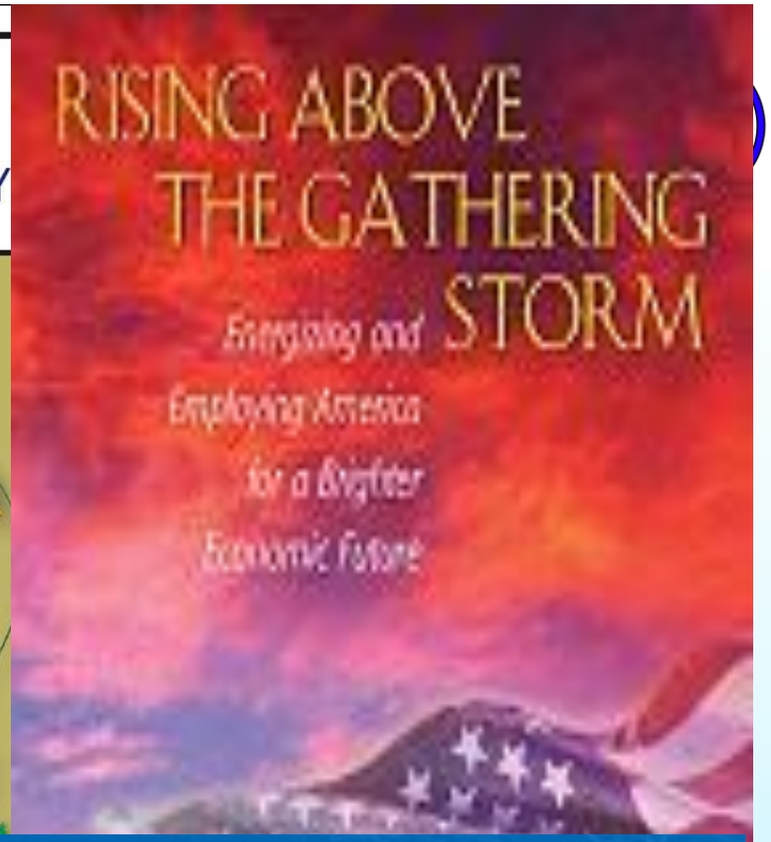
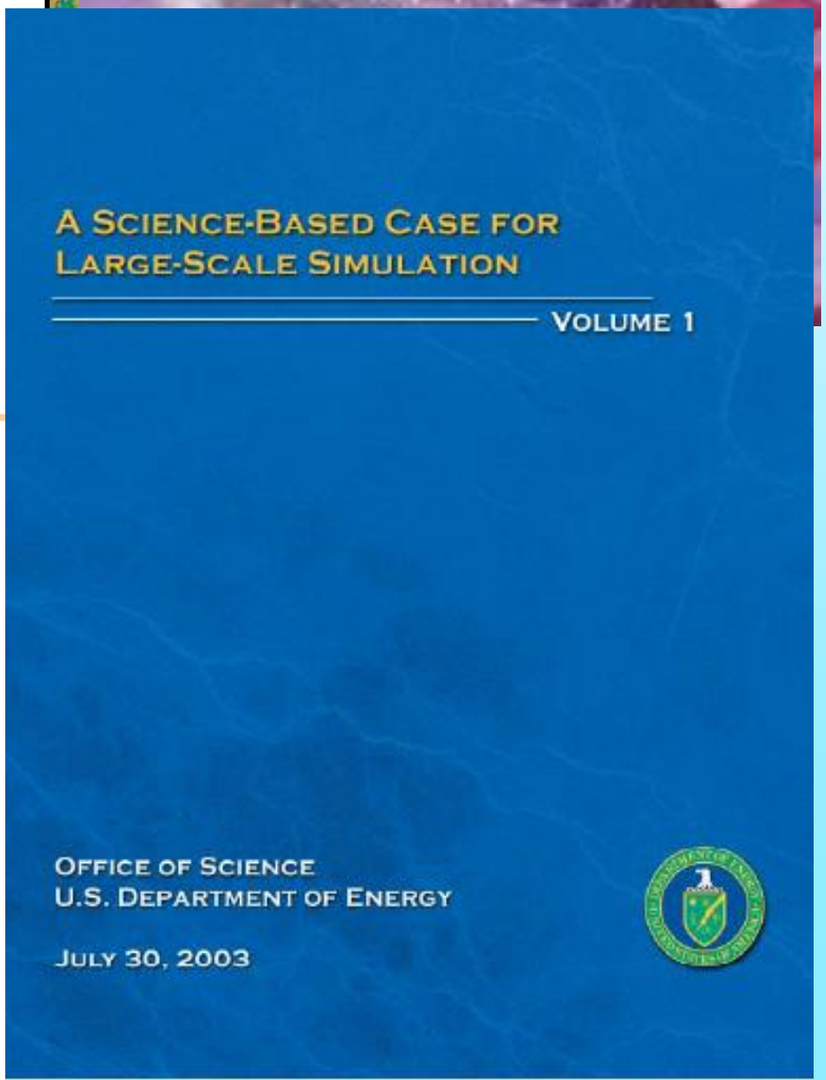

CYBERINFRASTRUCTURE VISION
FOR 21ST CENTURY DISCOVERY


RISING ABOVE
THE GATHERING
STORM
Energizing and
Employing America
for a Brighter
Economic Future

National Science Foundation
INVESTING IN
AMERICA'S FUTURE
STRATEGIC PLAN
FY 2006-2011

Federal Plan
for High-End
Computing
Report of the
High-End Computing
Revitalization Task Force
(HECRTF)
MAY 10, 2004
SECOND PRINTING—JULY 2004


A SCIENCE-BASED CASE FOR
LARGE-SCALE SIMULATION
VOLUME 1
OFFICE OF SCIENCE
U.S. DEPARTMENT OF ENERGY
JULY 30, 2003

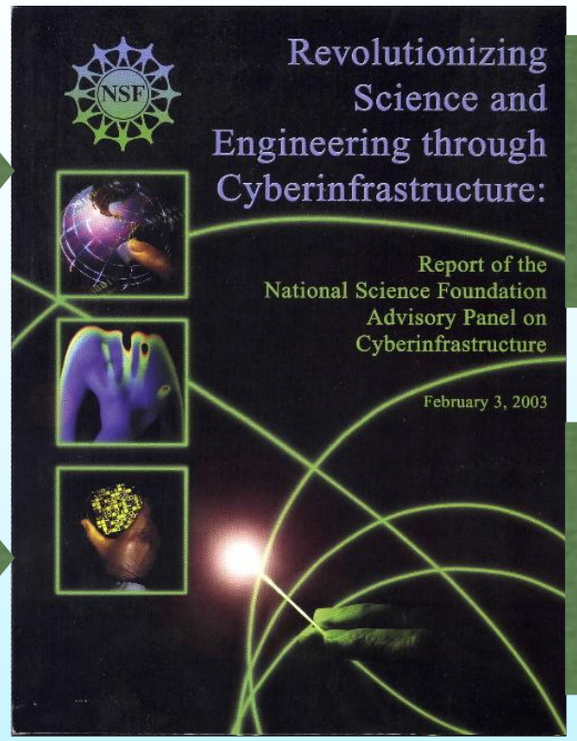
Some Science Drivers

- **Inherent** complexity and multi-scale **nature of todays frontier science challenges.**
- **Requirement for** multi**-disciplinary,** multi**-investigator,** multi**-institutional approach (often multi-national).**
- **High** data intensity **from simulations, digital instruments, sensor nets, observatories.**
- **Increased value of data and demand for data** curation & preservation **of access.**
- **Exploiting infrastructure** sharing **to achieve better stewardship of research funding.**
- **Strategic need for** engaging more students **in high quality, authentic science and engineering education.**

Vision and Activities Based on Broad and Diverse Community Engagement

Advances in components of CI-systems for S&E R&E

Complex, multi-scale, multidisciplinary S&E research challenges



30+ disciplinary workshops on CI vision & impact

NSF internal working groups

CI Council, Directorate/Office CI Activities, OCI, ACCI

NSB & Community Input

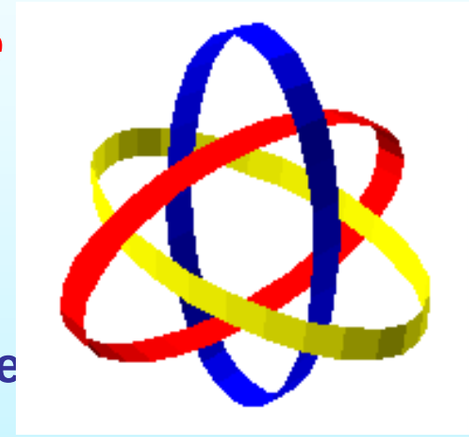
Vision Framework

- High Performance Computing
- Data, Data Analysis & Visualization
- Virtual Organizations
- Learning & Workforce Development

- ***All directorates and offices support cyberinfrastructure.***
- ***Science-driven partnerships between creation, provisioning and use of CI***
- ***Supports integrated research and education and broadened access and participation.***

Mission of OCI

The mission of the OCI is to greatly enhance the ability of the NSF community to create, provision, and use the comprehensive cyberinfrastructure *essential to 21st century advances in science and engineering*. This goal is implicit in many areas of the new NSF Strategic Plan and is being pursued within the context of the evolving *Cyberinfrastructure Vision for 21st Century Discovery*.



OCI will serve the Foundation and the NSF community in its mission through three types of activity:

1. **provisioning of cyberinfrastructure resources together with mechanisms for flexible, secure, coordinated sharing of these resources among collections of individuals, organizations, and institutions;**
2. **partnerships with others in science and engineering-driven, transformative use of CI in research and education; and**
3. **identification and transfer of the results of relevant R&D into the next generation of CI.**

OCI is a cross-cutting enterprise that builds mutually beneficial partnerships will all parts of the NSF, with other Federal agencies, and with the large and growing CI/e-science initiatives in other countries.

Borromean Ring: Symbol of peer-to-peer synergy. The three rings taken together are inseparable, but remove any one ring and the other two fall apart. See www.liv.ac.uk/~spmr02/rings/

OCI is about *Connectedness* between

- Systems
- People
- Organizations

Dualities

cyberinfrastructure ⟷ enables ⟷ research & development

CI is both an object and means for R&D

collaboration ⟷ enables ⟷ CI environments

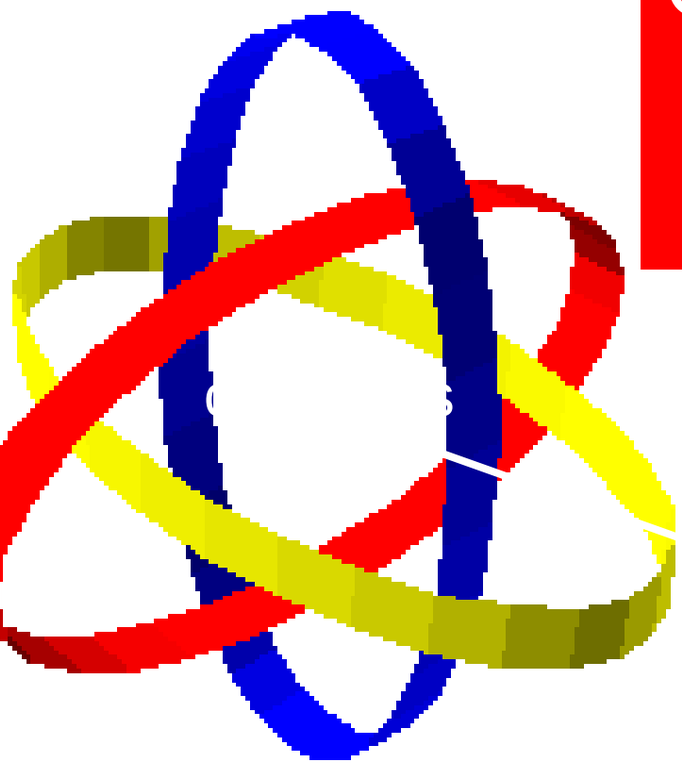
Multi-stakeholder collaboration required to create, provision, and apply CI; CI supports collaborations across time and distance (geographic, disciplinary, institutional)

learning | education ⟷ enables ⟷ CI environments

Learning and workforce development initiatives required to create and use CI; CI enables/enhances learning/education

Achieving the NSF CI Vision requires synergy between 3 types of activities

Transformative Application - to enhance discovery & learning



Provisioning - Creation, deployment and operation of advanced CI

provides shared and connecting CI

Office of Cyberinfrastructure

Borromean Ring: The three rings taken together are inseparable, but remove any one ring and the other two fall apart. See www.liv.ac.uk/~spmr02/rings/

R&D to enhance technical and *social* effectiveness of future CI environments

Strategic Technologies for Cyberinfrastructure

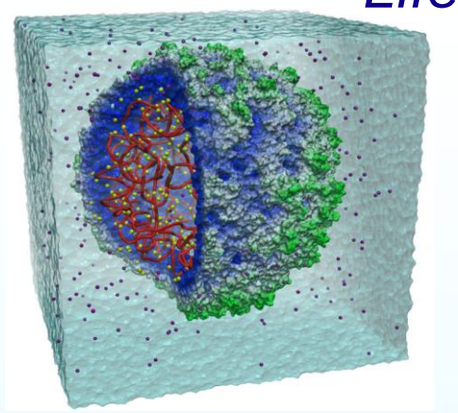
- **PD 06-7231 Standing program Strategic Technologies for CI – Core OCI program**
  - **support work leading to the development and/or demonstration of *innovative* cyberinfrastructure services for science and engineering research and education that fill gaps left by more targeted funding opportunities**
  - **consider highly innovative cyberinfrastructure education, outreach and training proposals that lie outside the scope of targeted solicitations.**
- **Two dates each year**
  - **August 2007**
  - **February 2008**
- **$2M**

"The number and caliber of proposals submitted demonstrate the need for this program." – panelist for STCI.

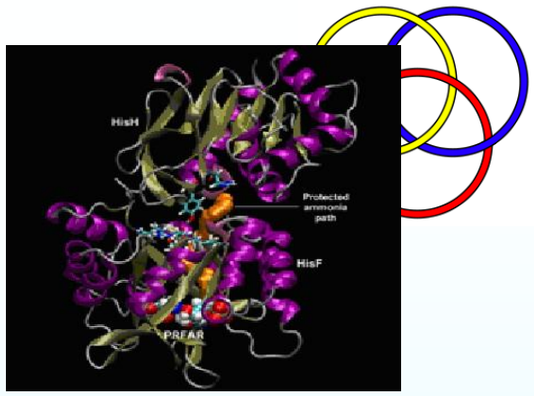
High Performance Computing

increasingly important tool for understanding

Life



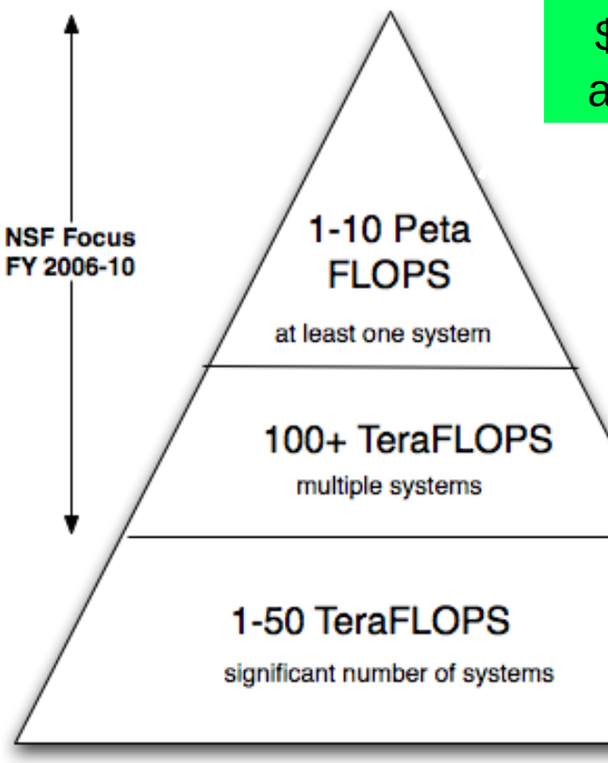
Satellite tobacco mosaic virus, P. Freddolino et al.

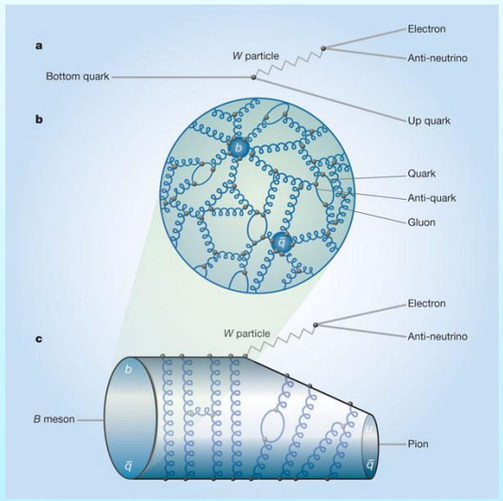


Aldehyde dehydrogenase, T. Wymore and S. Brown

Track 1: One solicitation funded over 4 years: $200M acquisition + additional O&M cost.

Track 2: Four solicitations over 4 years: $30M/yr acquisition + additional O&M cost. First track 1 approved 8-07



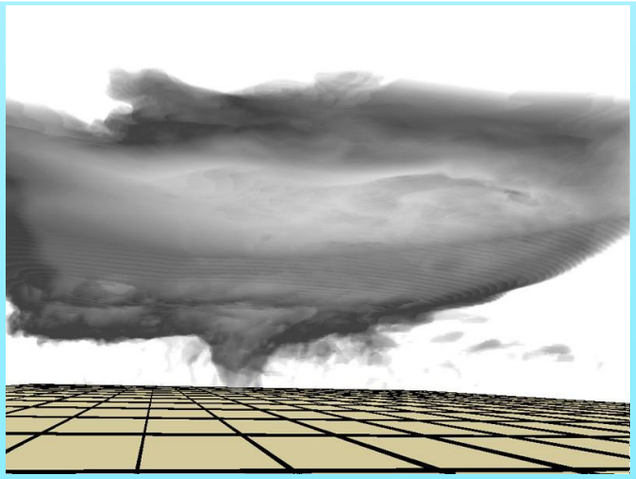


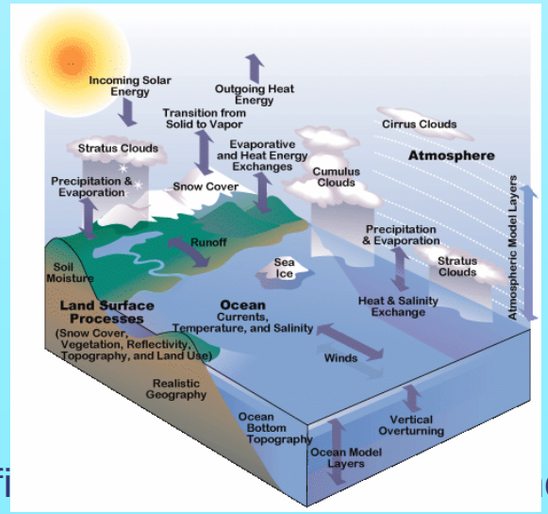
I. Shipsey

Matter

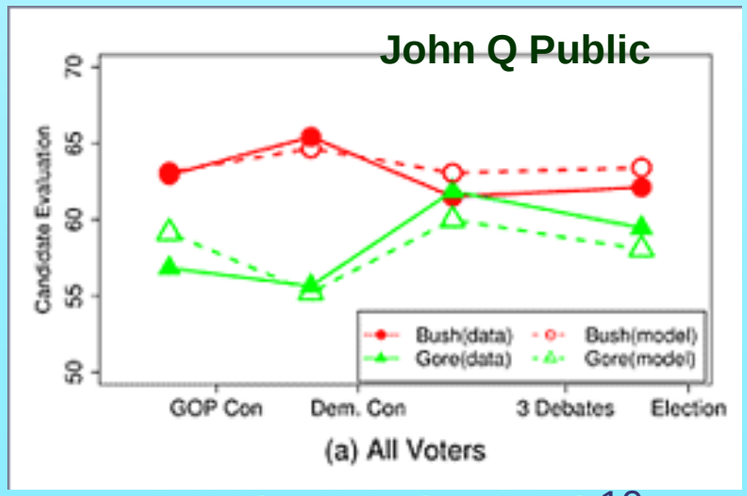
Society

The Environment



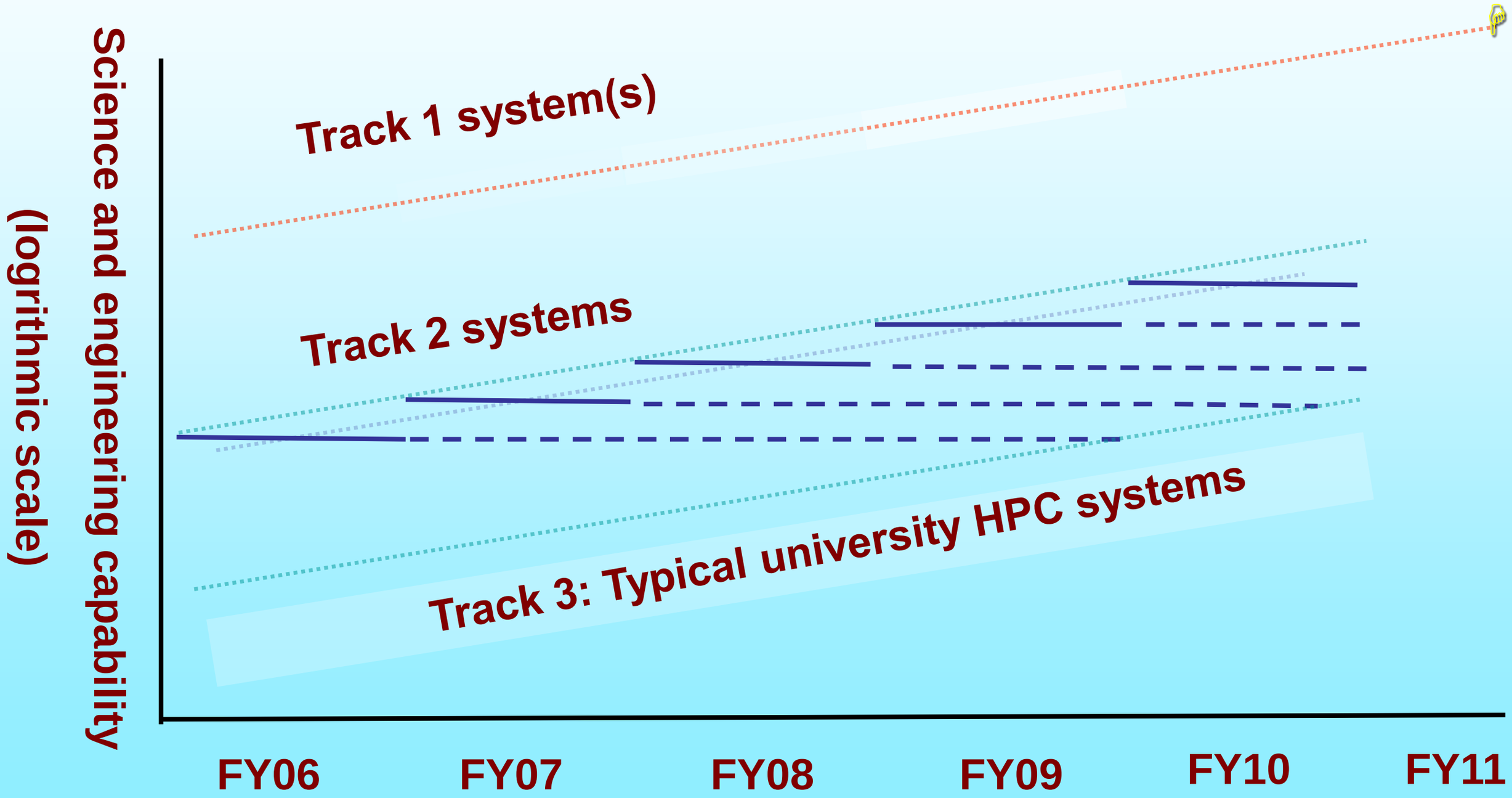


John Q Public



S.-Y. Kim, M. Lodge, C. Taber

NSF HPC Acquisition Strategy



Track 2 Acquisitions

- Individual systems - provide capabilities beyond those typically obtainable with university or state funds
- Collectively, as part of TeraGrid - provide a diverse HPC portfolio to meet the HPC needs of the academic research community
- Annual competition: roughly $30M/year for acquisition costs
- O&M costs via a TeraGrid RP award
- Primary selection criterion: Impact on science and engineering research

Track 2 Benchmarks

- HPCC CHALLENGE
- SPIOBENCH

- WRF (weather framework)
- OOCORE (Out of core solver)
- GAMES (ab initio chemistry package)
- MILC (particle physics lattice QCD code)
- PARATEC (Parallel total energy code)
- HOMME (tools to create a high-performance scalable global atmospheric model)

Thanks to HPCMOD and DOE Office of Science

TACC Track-2 Ranger System Configuration

- **Compute power - 529 Teraflops aggregate peak**
  - 3,936 Sun four-socket, quad-core nodes
  - 15,744 AMD Opteron "Barcelona" processors
    - Quad-core, four flops/cycle (dual pipelines)
- **Memory**
  - 2 GB/core, 32 GB/node, 125 TB total
  - 132 GB/s aggregate bandwidth
- **Disk subsystem**
  - 72 Sun x4500 "Thumper" I/O servers, 24TB each
  - 1.7 Petabyte total storage
- **Infiniband interconnect**
  - Full non-blocking 7-stage Clos fabric
  - Low latency (~2 μsec), high-bandwidth (~950 MB/s)
- **System Power: 3 MW**
  - 90 racks, 4,000 sq. ft.

Courtesy of TACC

TACC Track-2 Impact in NSF TeraGrid

- 470M CPU hours to TeraGrid per year
  - more than double current total capacity of all TG HPC systems
  - 1.8 Billion CPU hours over operational life
- 529 Teraflops peak
  - 2x total performance of all TeraGrid HPC systems
  - 8x top TeraGrid HPC system in performance, memory, disk
- Balanced, general-purpose capability system
  - More than 60,000 cores available
  - Unprecedented scaling opportunities for computational science and research
- Production for early capability users Dec 1, 2007

Courtesy of TACC

Track 1 Acquisition (FY07-10)

Examples of research problems:

- **The origin and nature of intermittency in turbulence**
- **The interaction of radiative, dynamic and nuclear physics in stars**
- **The dynamics of the Earth's coupled carbon, nitrogen and hydrologic cycles**
- **Heterogeneous catalysis on semiconductor and metal surfaces**
- **The properties and instabilities of burning plasmas and investigation of magnetic confinement techniques**
- **The formation of planetary nebulae**
- **The interaction of attosecond laser pulse trains with polyatomic molecules**
- **The mechanisms of reactions involving large bio-molecules and bio-molecular assemblages**
- **The structure of large viruses**
- **The interactions between clouds, weather and the Earth's climate**

Track 1 Acquisition (FY07-10)

- A system that will permit revolutionary science and engineering research
- Capable of delivering large numbers of cycles and large amounts of memory to individual problems
- Capable of sustaining at least 10^{15} arithmetic ops/second on a range of interesting problems
- Have a very large amount of memory and a very capable I/O system
- An architecture that facilitates scaling of codes
- Robust system software with fault tolerance and fault prediction features
- Robust program development tools that simplify code development
- A single physical system in a single location

Other Federal Government HPC Activities in (near) Petascale

- DARPA High Productivity Computing Systems
  - Sustainable petascale systems
  - PRODUCTIVITY
  - In Phase 3: IBM, Cray
- DOD HPC Modernization Office
- DOE Office of Science
  - ORNL, NERSC, ANL
- DOE National Nuclear Administration Agency
  - Capacity/capability computing systems
  - LLNL, LANL, Sandia

ACCELERATING DISCOVERY IN SCIENCE AND ENGINEERING THROUGH PETASCALE SIMULATIONS AND ANALYSIS

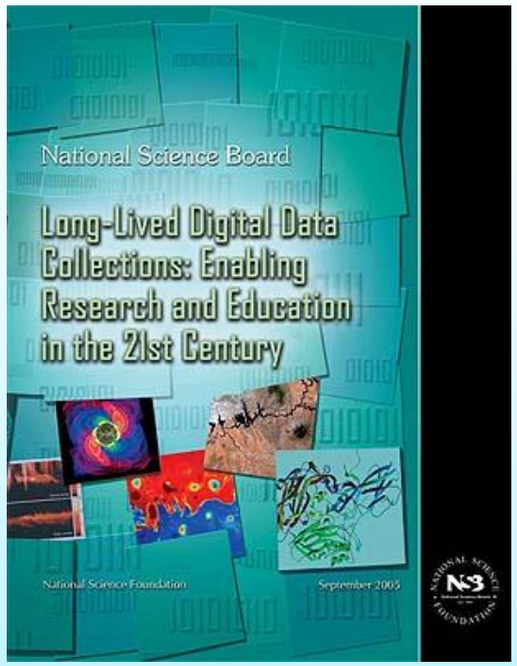
- **NSF 07-559: PetaApps**
  - **Several NSF Directorates participating**
- **develop the future simulation, optimization and analysis tools that can use petascale computing to advance the frontiers of scientific and engineering research**
- **beyond the current state-of-the-art.**
  - **emphasis is on implementation and exploitation of forefront techniques.**
- **research problem that *requires* or can exploit petascale computing capabilities**
- **$21.5M (11 – 22 awards)**
- **July 2007**

High-End Computing University Research Activity

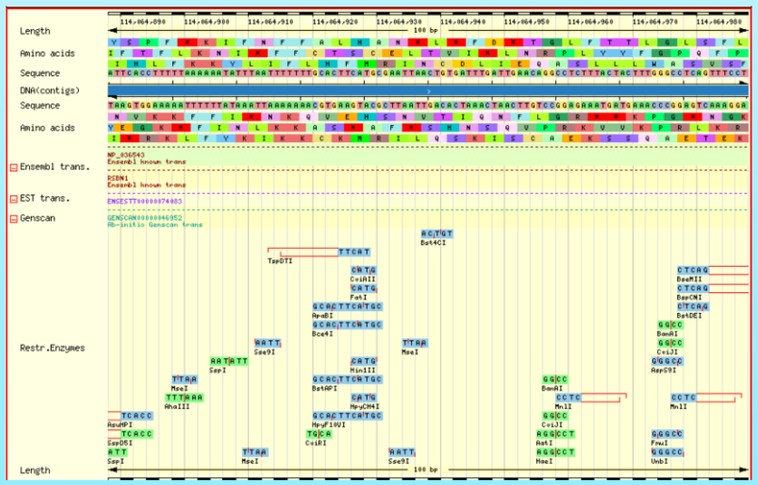
- HECURA FY 2006 Budget 14.5M
- **NSF/DARPA/DOE/EPSCoR activity**
  - Input/Output capabilities
  - File Systems
  - Storage Systems
- **62 proposals submitted in February 2006**
- **Nineteen projects were awarded**.

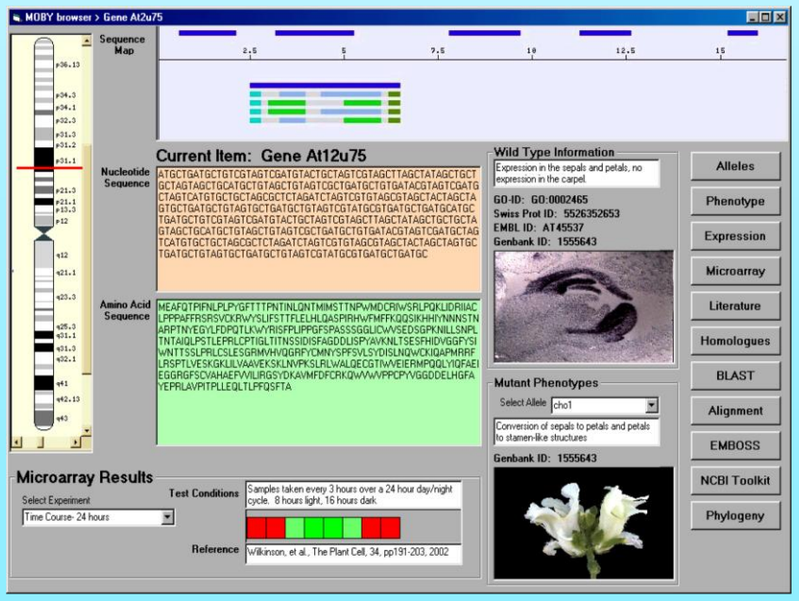
- FY 2008 Budget 8M (Planned)
- **NSF activity will be focused on**
  - HEC Programming Models
  - HEC Languages
  - HEC Compilers

Data, Data Analysis & Visualization

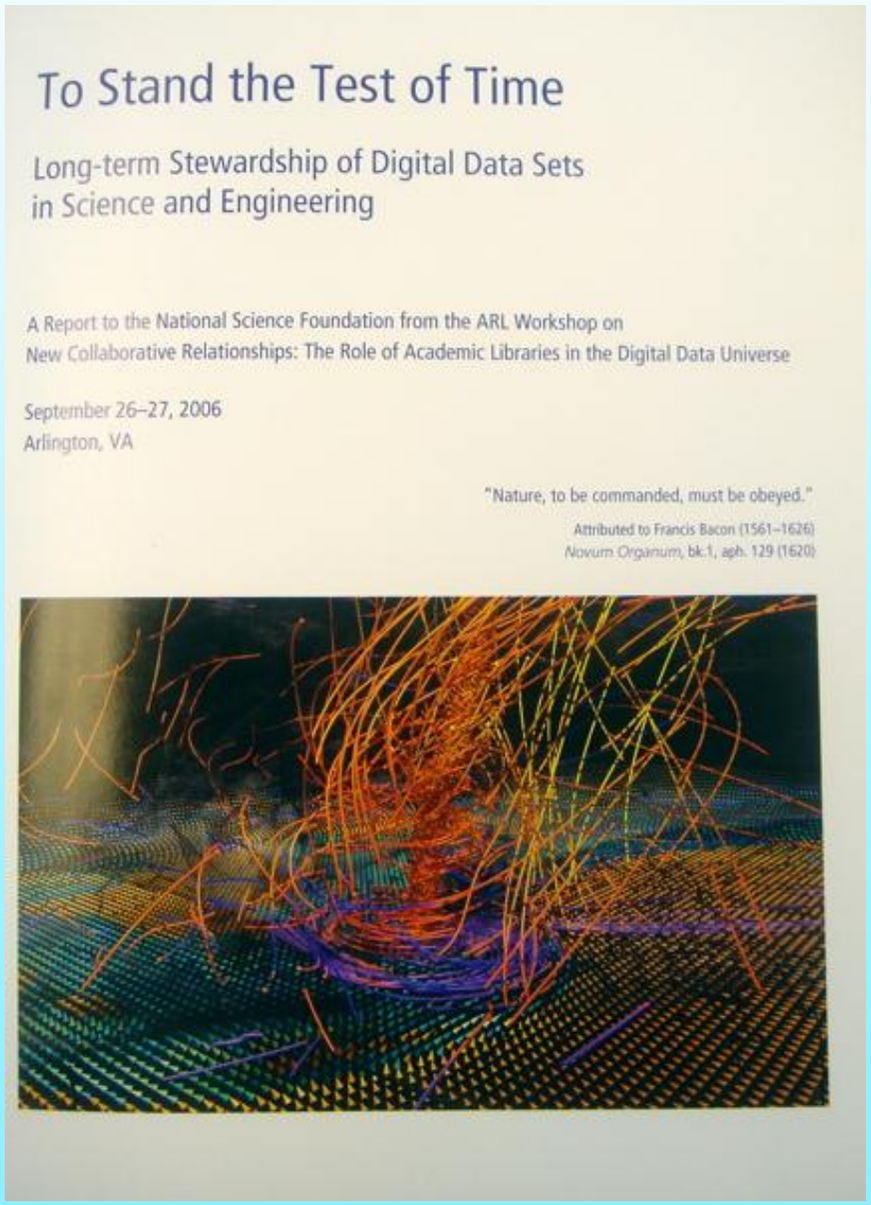


- **Challenges: increased scale, heterogeneity, and re-use value of digital scientific information and data. Inadequate digital preservation strategy of long-lived data.**
- **Taking initial steps to catalyze the development of a federated, global system of science and engineering data collections that is open, extensible, evolvable, (and appropriately curated and long-lived.)**
- **Complemented by a new generation of tools and services to facilitate data mining, integration, analysis, visualization essential to transforming data into knowledge.**
- **NSF Leadership for OSTP/Interagency Working Group on Digital Data**





New Report: *To Stand the Test of Time*


To Stand the Test of Time

Long-term Stewardship of Digital Data Sets in Science and Engineering

A Report to the National Science Foundation from the ARL Workshop on New Collaborative Relationships: The Role of Academic Libraries in the Digital Data Universe

September 26–27, 2006
Arlington, VA

"Nature, to be commanded, must be obeyed."

Attributed to Francis Bacon (1561–1626)
Novum Organum, bk.1, aph. 129 (1620)

Available online at http://www.arl.org/info/events/digdatarpt.pdf

Community Based Data Interoperability Networks

- NSF 07-565 “INTEROP”
  - Several NSF Directorates participating
- Support community efforts to provide for broad interoperability through the development of mechanisms such as robust data and metadata conventions, ontologies, and taxonomies
- Each project shall have two goals:
  - Develop community consensus (e.g. workshops, task groups, community websites, etc.)
  - Turn consensus into technical standards with implementation tools (e.g. ontologies, taxonomies, software tools, web resources, etc.)
- Approximately 10 $250K/yr. awards (3-5 yrs.)
- August 2007

Virtual Organizations

NVO

LEAD

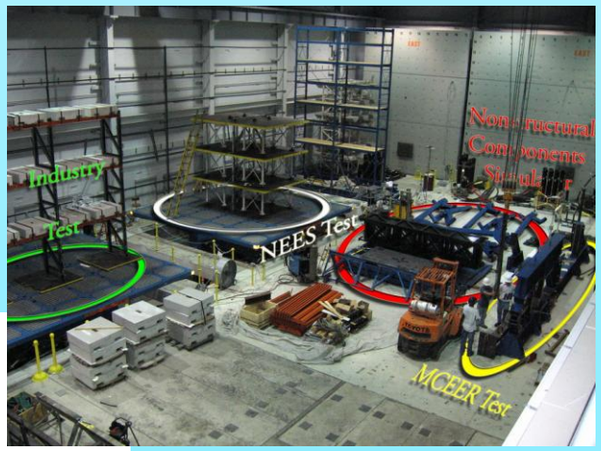
iVDgL

- To catalyze the development, implementation and evolution of a national cyberinfrastructure that integrates both physical and cyberinfrastructure assets and services.
- To promote and support the establishment of world-class VOs that are secure, efficient, reliable, accessible, usable, pervasive, persistent and interoperable, and that are able to exploit the full range of research and education tools available at any given time
- To support the development of common cyberinfrastructure resources, services, and tools that enable the effective, efficient creation and operation of end-to-end cyberinfrastructure systems for and across all science and engineering fields, nationally and internationally.

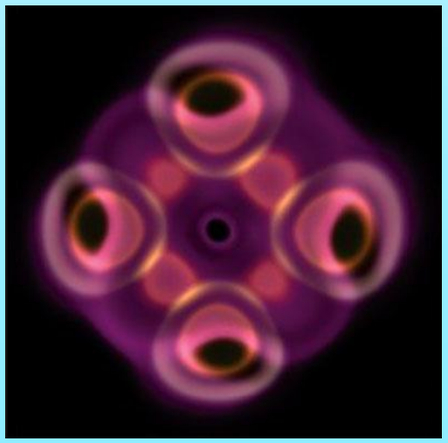
TeraGrid

Open Science Grid

Enabling Grids for E-sciencE

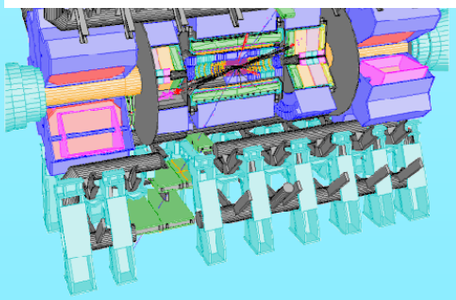


NEES



NanoHub

CMS



ATLAS

Virtual Organizations offer additional modes of interaction between People, Information, and Facilities

Time

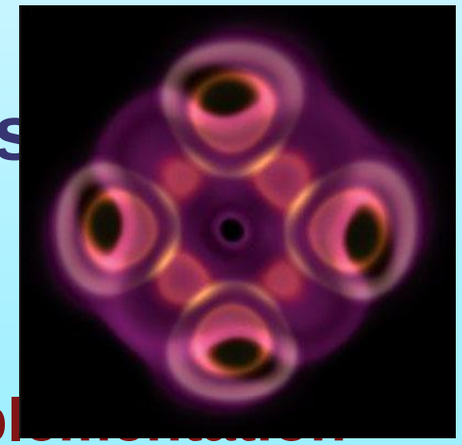
Geographic Place	Same (synchronous)	Different (asynchronous)
Same	**ST-SP** **P**: Physical mtgs **I**: Print-on-paper books, journals **F**: Physical labs, studios, shops	**DT-SP** **P**: Shared notebook **I**: Library reserves **F**: Time-shared physical labs, ...
Different	**ST-DP** **P**: AV conference **I**: Web search **F**: Online instruments	**DT-DP** **P**: Email **I**: Knowbots **F**: Autonomous observatories

P: people, **I**: information, **F**: facilities, instruments

Engineering Virtual Organizations (EVO)

NSF 07-558

- Primary purpose of this solicitation is to promote the use of Virtual Organizations (VOs) in ENG communities
  - flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources
- Early ENG experience with gateways has been very positive
  - nanoHUB.org for nanotechnology researchers
  - NEES for earthquake engineering researchers
- EVO will provide seed grants to ENG communities
  - Defining **user needs** for **shared community resources**
  - Formulating **organizing principles** and VO structure
  - Building a prototype and developing a **plan for full-scale implementation**
- Program size: 10-15 awards, $100-200K
- Letter of Intent: May 31, 2007; Full Proposal: July 3, 2007



NanoHub

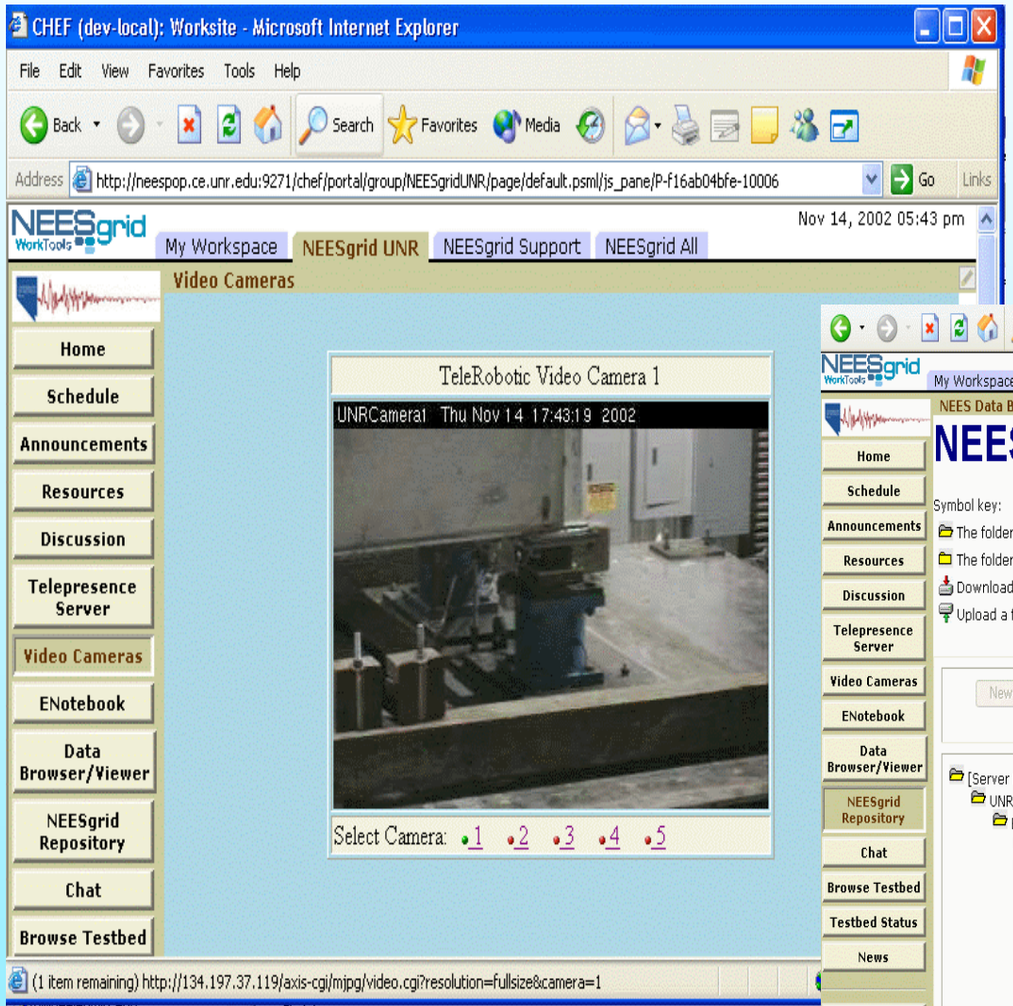
ENG, OISE

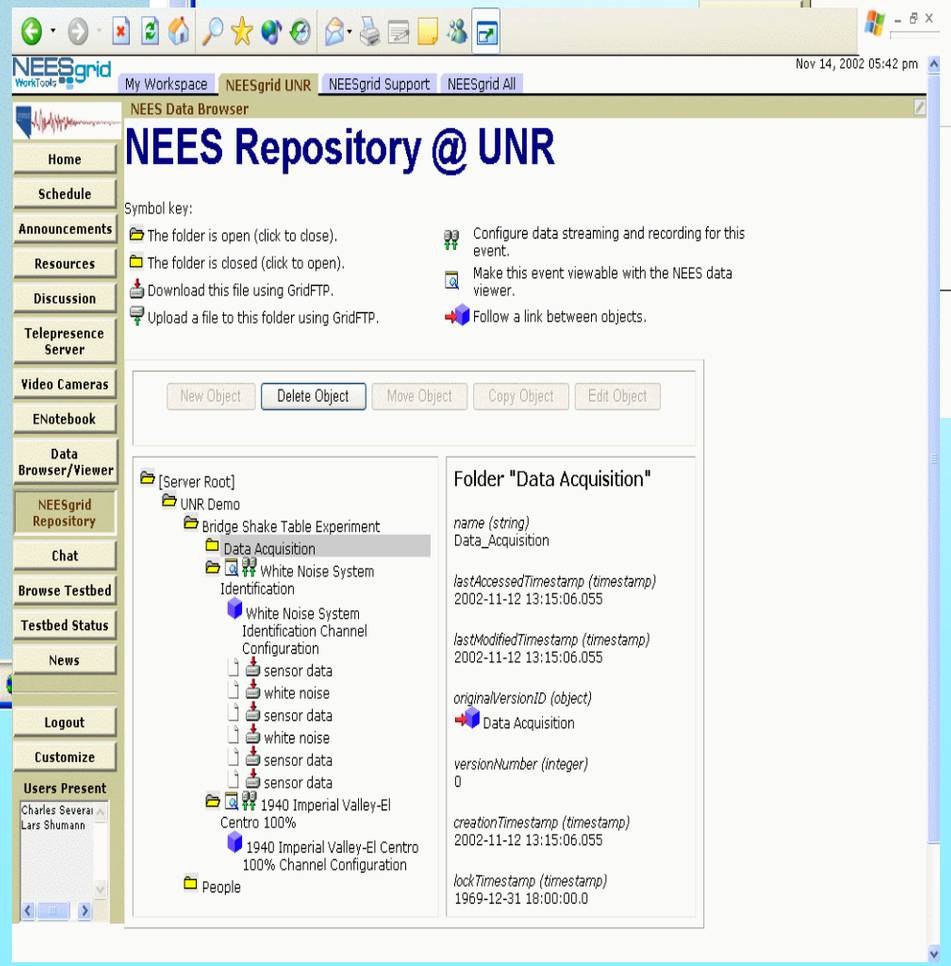
Let's look at a few real example Grid Science Gateways

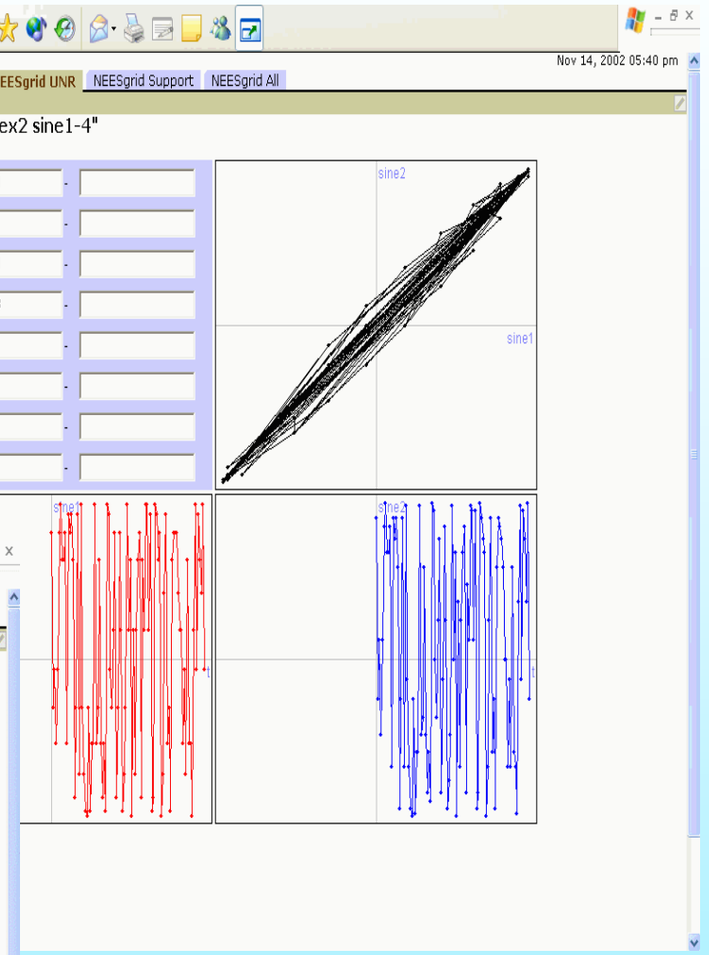
These example slides courtesy of D. Gannon

NEESGrid

Real-time access to earthquake
Shake table experiments at remote sites.



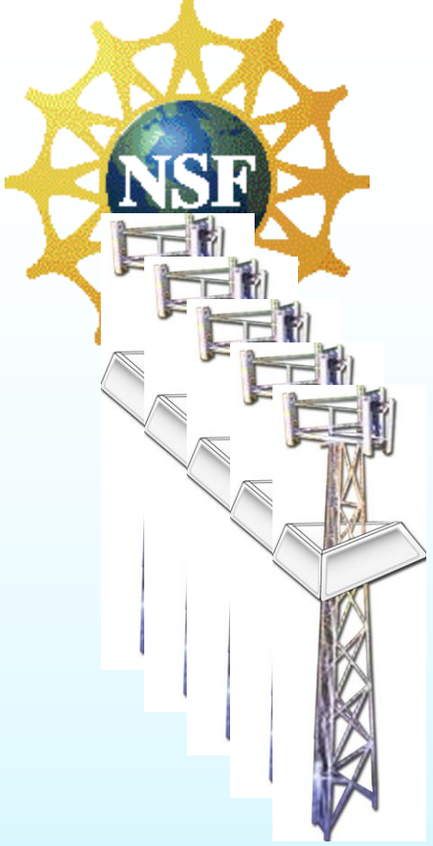


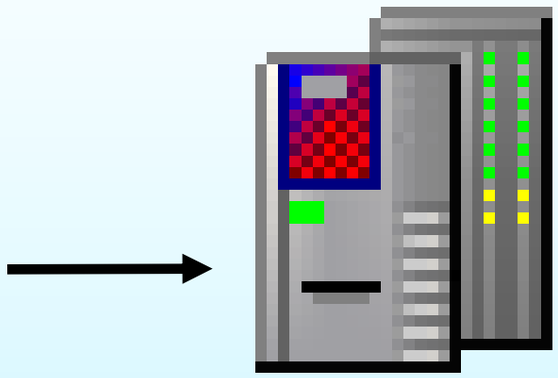


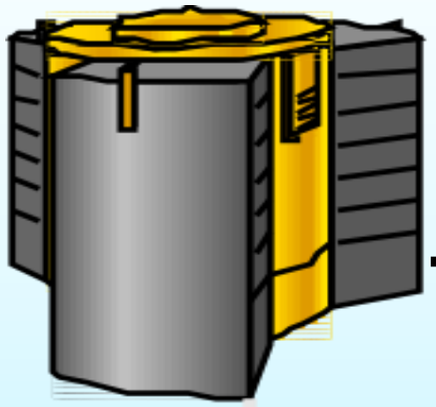
NEESgrid

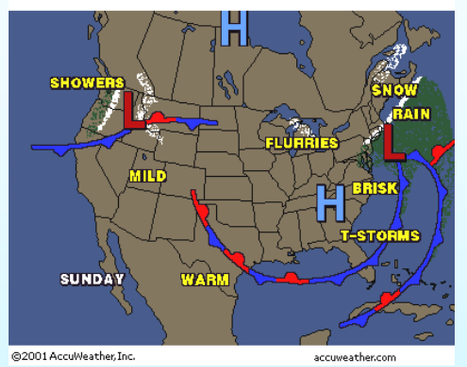
BIRN – Biomedical Information

The LEAD Vision: Adaptive Cyberinfrastructure









- DYNAMIC OBSERVATIONS

Analysis/Assimilation

Quality Control
Retrieval of Unobserved Quantities
Creation of Gridded Fields

Prediction/Detection

PCs to Teraflop Systems

Product Generation, Display, Dissemination

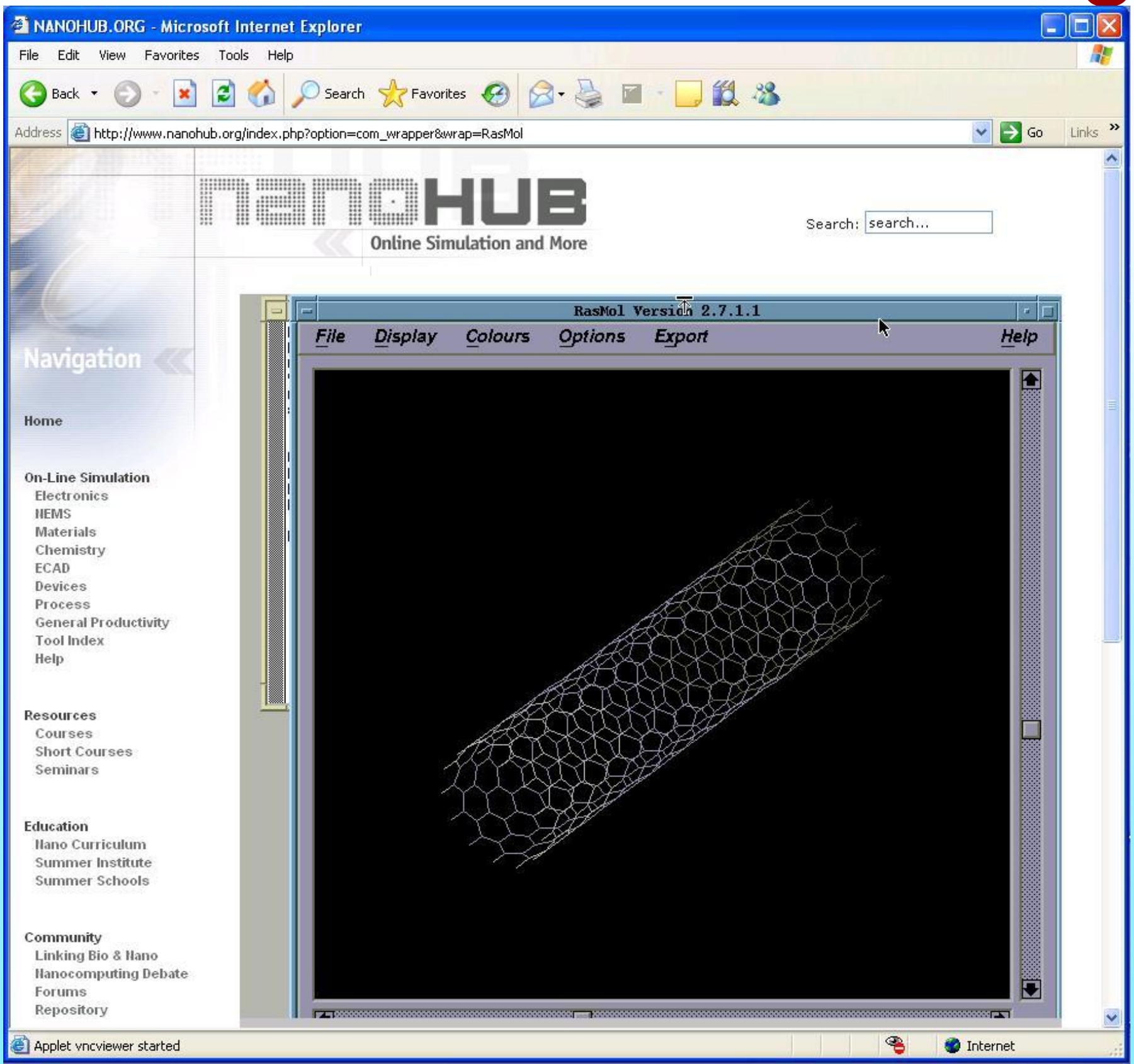
Models and Algorithms Driving Sensors

End Users

NWS
Private Companies
Students

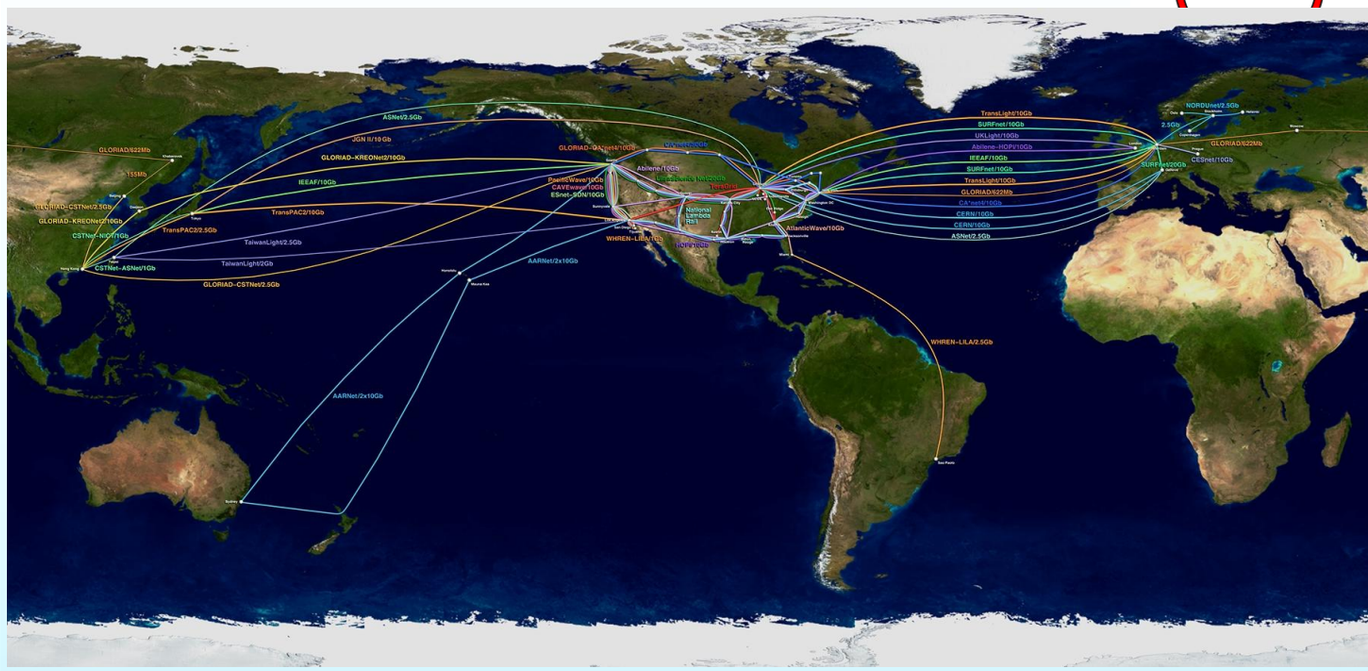
The CS challenge: Build cyberinfrastructure services that provide adaptability, scalability, availability, useability, and real-time response.

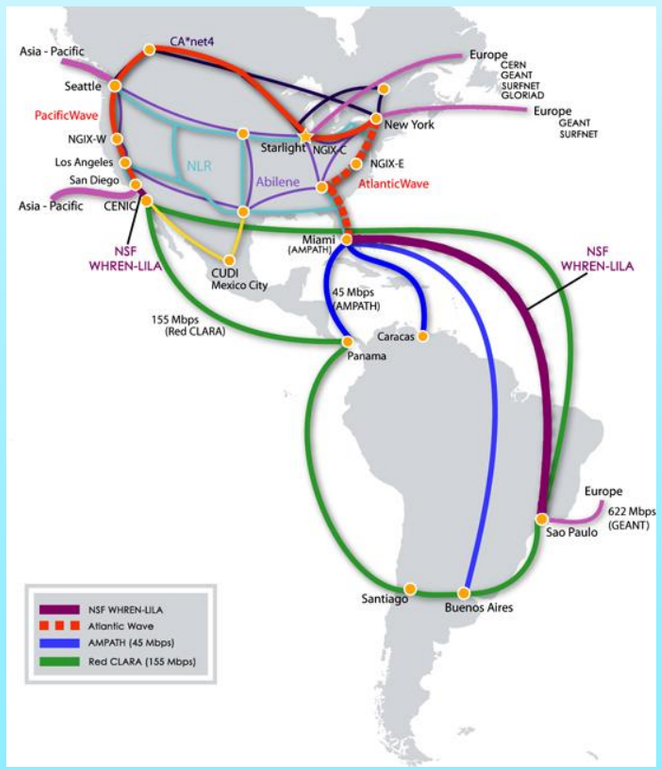
Nanohub - nanotechnology

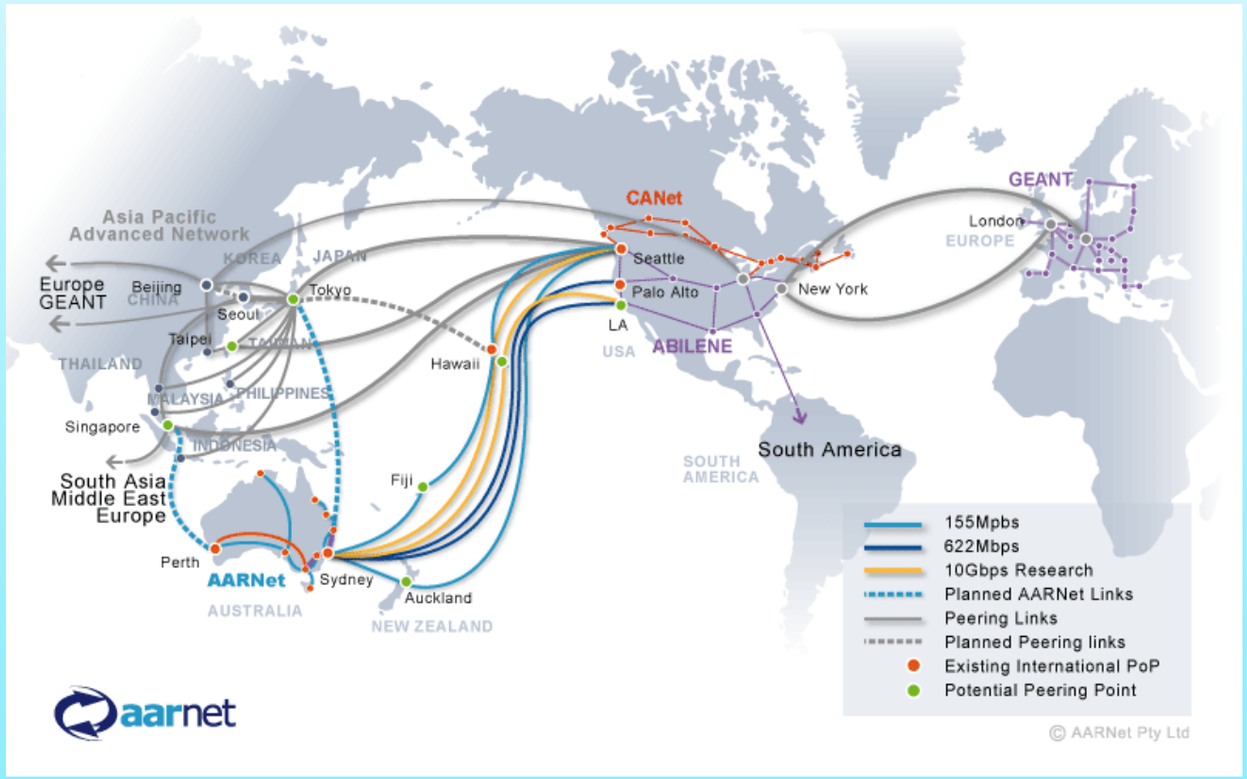


May 2007

VO-substrate: International R&E Networking







Cyber-enabled Discovery and Innovation

NSF Priority Area (FY 2008 – 2012)

Cyber-enabled Discovery and Innovation (CDI) will broaden the Nation's capability for innovation by developing a new generation of computationally based discovery concepts and tools to deal with complex, data-rich, and interacting systems.

- **Conduct of science and engineering has been revolutionized by**
  - **the infusion of computational science and simulation in the traditional experimentation-observation-analysis-theory loop, and**
  - **by eliminating the geographic constraints for collaboration and experimentation.**
- **Primary CDI Themes**
  - **Knowledge Extraction**
  - **Complex Interactions**
  - **Computational Experimentation**
  - **Virtual Environments**
  - **Educating Researchers and Students**

    Computational Discovery
- **Be on the look-out during FY08**

Courtesy of Deshmukh/OCI

Learning & Workforce Development

- Learning **supported by** CI. (cyber-enabled learning).
- Workforce development **to create and use** CI for S&E research and education.
- **Broadened participation**: Exploit the new opportunities that cyberinfrastructure brings for … people who, because of physical capabilities, location, or history, have been excluded from the frontiers of scientific and engineering research and education.

- Explore CI support for **integrated research and education**.
- Effective, Transferable, Sustainable, Scalable

BIOINFORMATICS CI INSTITUTE

EPIC

MARIACHI

CyberBridges

CI-TEAM

- **The CI-TEAM program supports projects that position the national science and engineering community to engage in integrated research and education activities that promote, leverage, and optimize cyberinfrastructure technologies, tools, and services. CI-TEAM awards will:**
  - **Prepare current and future generations of scientists, engineers, and educators to use, support, deploy, develop and design cyber-augmented research and learning environments, both formal and informal;**
  - **Establish collaborative teams representing the expertise of at least one disciplinary domain with that of computer/information sciences and education or social sciences in order to inform CI-TEAM activities from an appropriately interdisciplinary knowledge base; and,**
  - **Expand participation in cyberinfrastructure activities of diverse groups of people and organizations, with particular emphasis on partnerships with traditionally underserved groups, communities, and institutions as bother creators and users of CI.**

CI-TEAM FY07-8

Refined CI-TEAM Solicitation

- Reflects CI VISION statement
- Encourages INTEGRATION of research and education
- Emphasizes BROADENED PARTICIPATION of underrepresented populations, institutions, and fields
- Requires EVALUATION of project process and outcomes
- FY07/08 program funds ~ $10M for two types of awards:
  - Demonstration Projects ≤ $250,000
  - Implementation Projects ≤ $1,000,000

Grantees & Aspiring Grantees Workshop

- July 9-11, 2007 in Washington, DC
- 130-150 grantees, aspiring grantees and cyberlearning community builders F2F; ∞ by Webcast
- Where has CI-TEAM been and where should cyberlearning and discovery go?

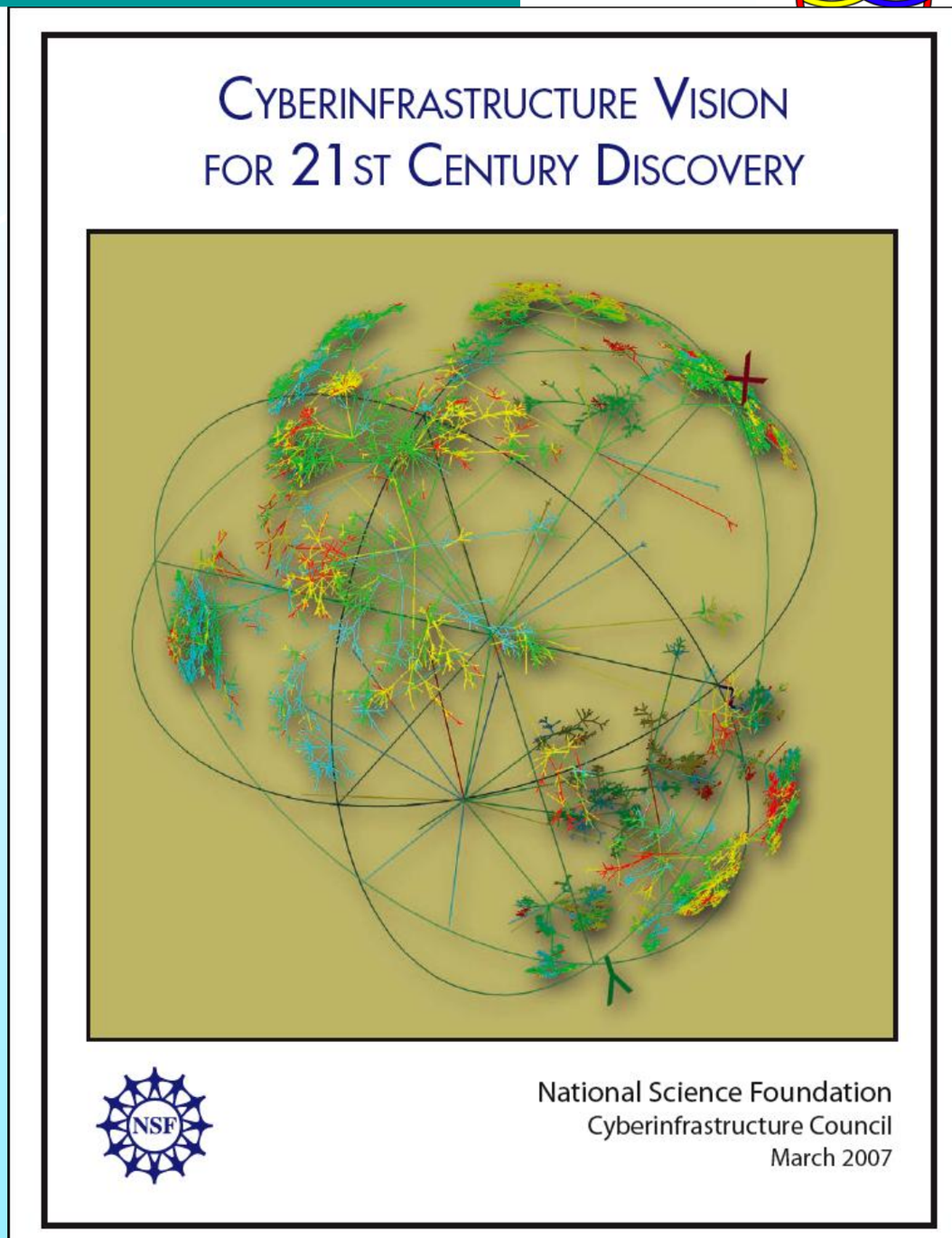
Proposals due August 27, 2007
Diana Rhoten drhoten@nsf.gov

Courtesy of D. Rhoten/OCI

Software Development for CyberInfrastructure

- NSF 07-503 (closed)
- Develop, deploy and sustain a set of reusable and expandable software components and systems that benefit a broad set of science and engineering applications
  - software activities for enhancing scientific productivity and for facilitating research and education collaborations through sharing of data, instruments, and computing and storage resources. The program requires open source software development
- Three focus areas: HPC, Middleware, Digital Data
- Pending funding will be re-issued in 2008

www.nsf.gov/oci/



Solicitations Posted Here

Seeking more program officers.

http://www.nsf.gov/pubs/2007/nsf0728/index.jsp

CyberInfrastructure: The Tide that Raises All Boats