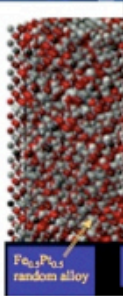
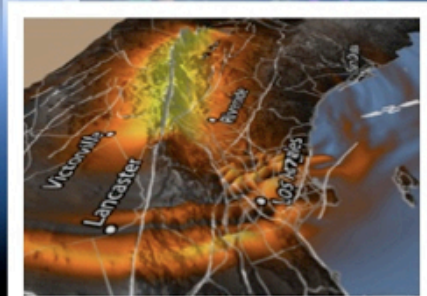
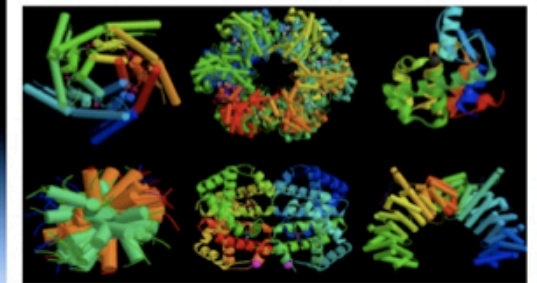
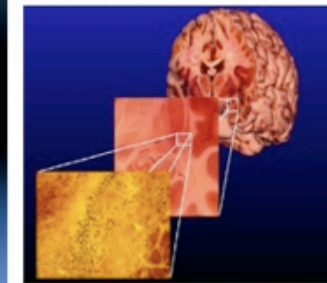


# The International e- Science Movement: Status and Future

Daniel E. Atkins  
W. K. Kellogg Professor of Community  
Informatics  
Professor of EE and Computer Science  
Associate VP for Research Cyberinfrastructure  
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## Three Perspectives

---

- Funders
  - US initiatives: Cyberinfrastructure (CI) enabled science
  - UK initiatives: e-Science
- Researchers
- Universities

*“Matrices of relationships, approaches and sets of goals”*

## Future Focus

---

- Computational Discovery, Computational Thinking for All at Various Service Levels
  - Modeling, Simulation, Prediction, Extracting Knowledge from Data (of all kinds) UK initiatives: e-Science, “Fourth Paradigm”
- ICT/Cyberinfrastructure Rationalization, Multi-Use Cyberinfrastructure. Focus on Efficiency and Mission Effectiveness, Consolidate Demand and Sourcing of Services/
- End-to End Performance: Portfolio of Options, Campus and “Above the Campus”, International
- HPC: High Performance Computing --> High Performance *Collaboration*
- *Managing Data in Difficult Times: policies, strategies, technologies and infrastructure to manage research and teaching data in a fast changing technological and economic environment. Who has the responsibility?*

- e-Science

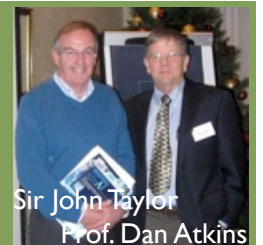
- science increasingly done through distributed global collaborations enabled by the internet
- using very large data collections, terascale computing resources and high performance visualisation

- Grid

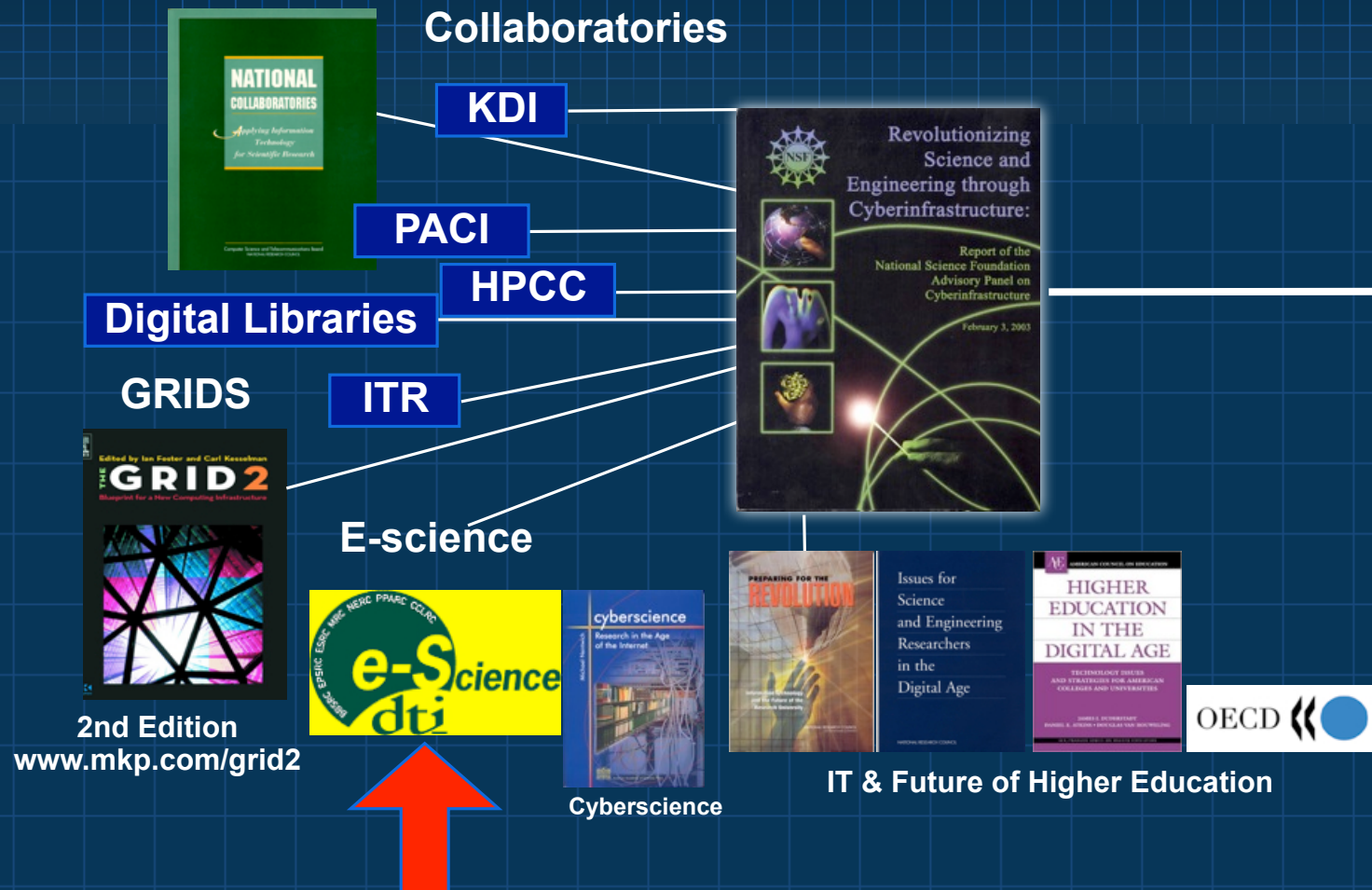
- new generation information utility
- middleware, software and hardware to access, process, communicate and store huge quantities of data
- infrastructure enabler for e-science

Definition should likely now be made more agnostic wrt technology

Original UK Definition of e-science by  
Sir John Taylor



# Cyberinfrastructure Genealogy & Movement



# NSF Blue Ribbon Advisory Panel on Cyberinfrastructure

**Daniel E. Atkins, Chair**

University of Michigan

**Kelvin K. Droegemeier**

University of Oklahoma

**Stuart I. Feldman**

IBM

**Hector Garcia-Molina**

Stanford University

**Michael L. Klein**

University of Pennsylvania

**David G. Messerschmitt**

University of California at Berkeley

**Paul Messina**

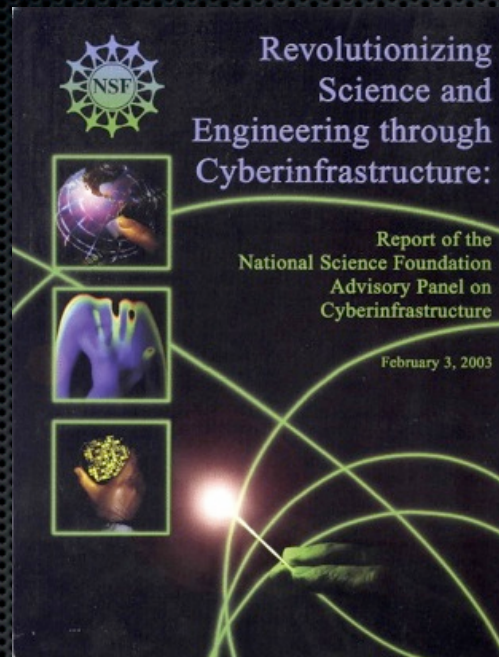
California Institute of Technology

**Jeremiah P. Ostriker**

Princeton University

**Margaret H. Wright**

New York University

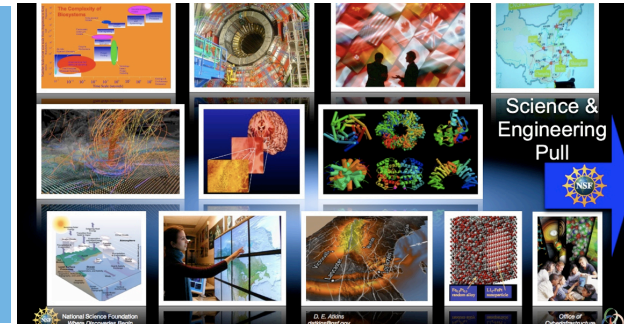


*"a **new age** has dawned in scientific and engineering research, **pushed** by continuing progress in computing, information, and communication technology, and **pulled** by the expanding complexity, scope, and scale of today's challenges. The capacity of this technology has crossed thresholds that 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.**"*

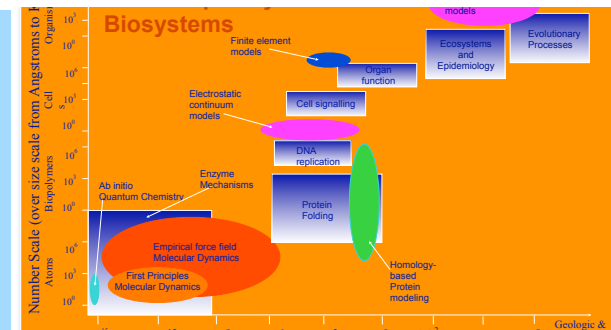


<http://www.nsf.gov/oci>

e-science (research enabled by e-infrastructure/ICT) is increasingly essential for meeting 21st century challenges in scientific discovery and learning



The inherent complexity, multi-scale, and multi-science nature of today's frontier science challenges.



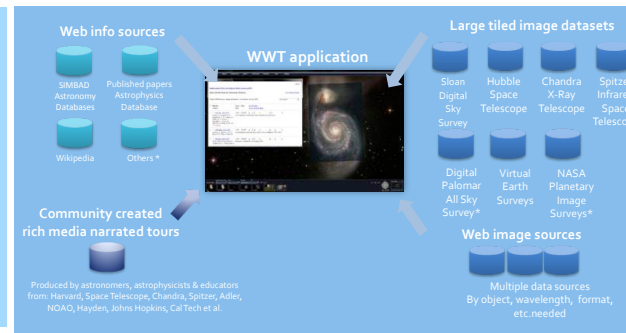
The accompanying requirement for multi-disciplinary, multi-investigator, multi-institutional approach (often international in scope).



The high data intensity and heterogeneity from simulations, digital instruments, sensor nets, and observatories.



The increased scale and value of data and demand for semantic federation, active curation and long-term preservation of access.

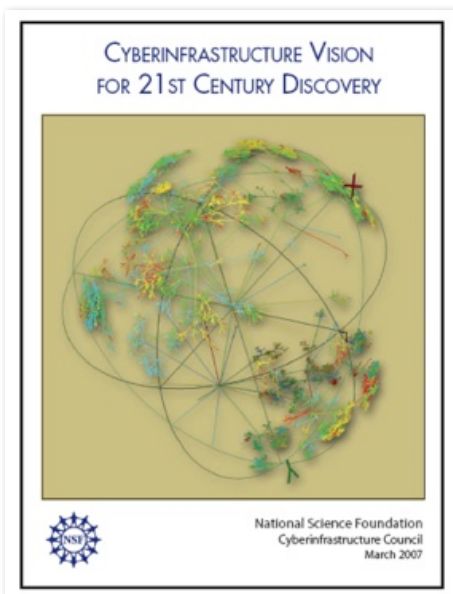


And the need to engage more students in high quality, authentic, passion-building science and engineering education.

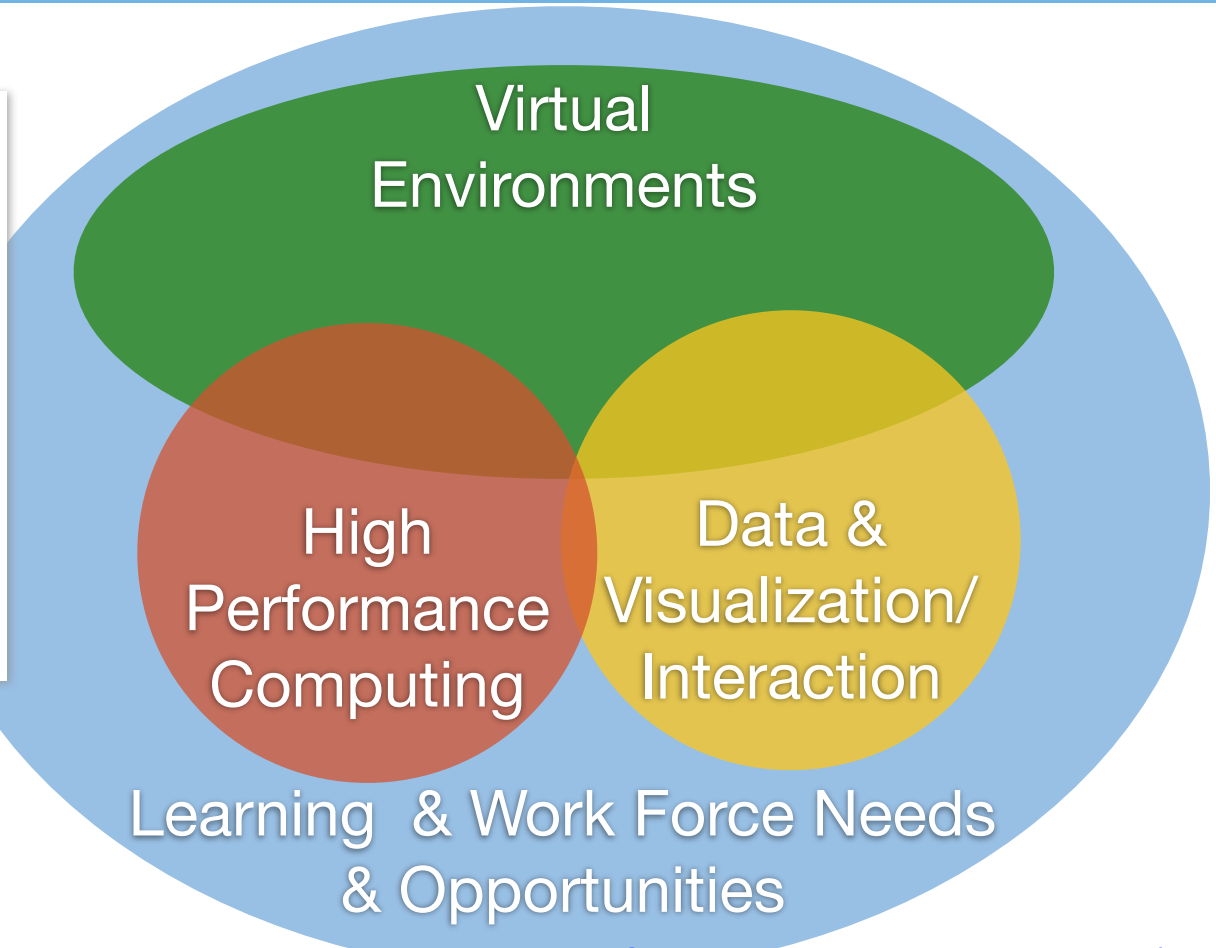




# e-science



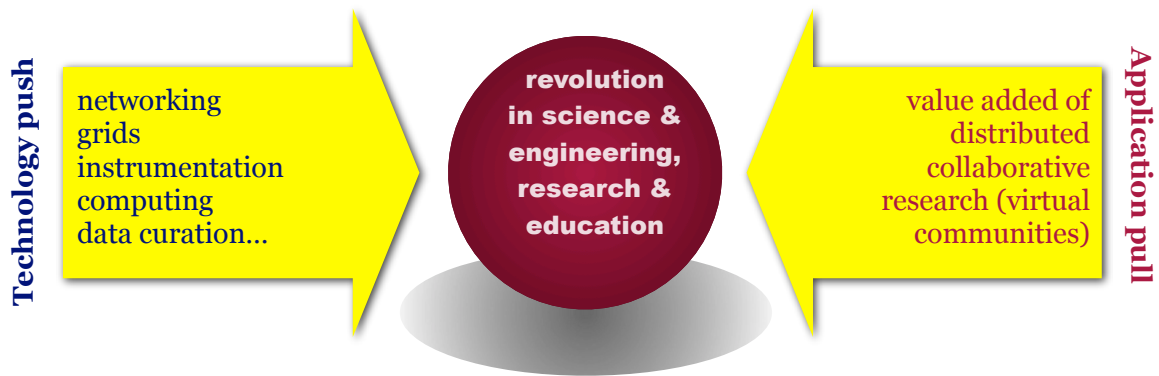
# CI-enabled science



Note: Many other reports on discipline-specific visions of and drivers for e-Science are available at [www.nsf.gov/oci](http://www.nsf.gov/oci)

# a new vision for Science

- **Global challenges with high societal impact**
- **Data deluge... wet-labs versus virtual-labs**
- **Improved scientific process**
- **Cross-disciplinarity**
- **Virtual Research Communities**



## Science Paradigms

- Thousand years ago: science was **empirical**  
*describing natural phenomena*
- Last few hundred years: **theoretical** branch  
*using models, generalizations*
- Last few decades: a **computational** branch  
*simulating complex phenomena*
- Today: **data exploration** (eScience)  
*unify theory, experiment, and simulation*
  - Data captured by instruments or generated by simulator
  - Processed by software
  - Information/knowledge stored in computer
  - Scientist analyzes database/files using data management and statistics

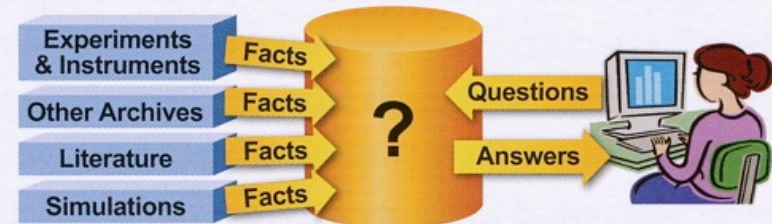


$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{4\pi G\rho}{3} - K\frac{c^2}{a^2}$$



## X-Info

- The evolution of X-Info and Comp-X for each discipline X
- How to codify and represent our knowledge



### The Generic Problems

- Data ingest
- Managing a petabyte
- Common schema
- How to organize it
- How to reorganize it
- How to share it with others
- Query and Vis tools
- Building and executing models
- Integrating data and literature
- Documenting experiments
- Curation and long-term preservation

The Fourth Paradigm:  
Data-Intensive Scientific Discovery



# Opportunities for Research and NIH

by Francis S. Collins, Director

The power of the molecular approach to health and disease has steadily gained momentum over the past several decades and is now poised to catalyze a revolution in medicine. The foundation of success in biomedical research has always been, and no doubt will continue to be, the creative insights of individual investigators. But increasingly those investigators are working in teams, accelerated by interdisciplinary approaches and empowered by open access to tools, databases, and technologies, so a careful balance is needed between investigator-initiated projects and large-scale community resource programs. For both individual and large-scale efforts, it is appropriate to identify areas of particular promise. Here are five such areas that are ripe for major advances that could reap substantial downstream benefits.

Jan 2010, vol. 326 SCIENCE [www.sciencemag.org](http://www.sciencemag.org)

## POLICYFORUM

RESEARCH AGENDA

### Opportunities for Research and NIH

The promise of fundamental advances in diagnosis, prevention, and treatment of disease has never been greater.

Francis S. Collins

The mission of the National Institutes of Health (NIH) is science in pursuit of fundamental knowledge about the nature and behavior of living systems and the application of that knowledge to extend healthy life and to reduce the burdens of illness and disability. The power of the molecular approach to health and disease has steadily gained momentum over the past several decades and is now poised to catalyze a revolution in medicine. The foundation of success in biomedical research has always been, and no doubt will continue to be, the creative insights of individual investigators. But increasingly those investigators are working in teams, accelerated by interdisciplinary approaches and empowered by open access to tools, databases, and technologies, so a careful balance is needed between investigator-initiated projects and large-scale community resource programs. For both individual and large-scale efforts, it is appropriate to identify areas of particular promise. Here are five such areas that are ripe for major advances that could reap substantial downstream benefits.

#### High-Throughput Technologies

In the past, most biomedical basic science projects required a large amount of time and resources to perform. Now, with the advent of high-throughput technologies, it is possible to screen thousands of compounds and conditions in a matter of days.

#### Regenerative Medicine

Regenerative medicine is a field that seeks to repair or replace damaged tissues and organs. This is a rapidly growing area of research, with many promising therapies in development.

#### Personalized Medicine

Personalized medicine is a field that seeks to tailor medical treatment to the individual patient. This is a rapidly growing area of research, with many promising therapies in development.

#### Complex Data Analysis

Complex data analysis is a field that seeks to extract meaningful information from large, complex datasets. This is a rapidly growing area of research, with many promising techniques in development.

National Institutes of Health, Bethesda, MD 20892, USA.  
E-mail: [collinsf@mail.nih.gov](mailto:collinsf@mail.nih.gov)



...ive information about the genetic underpinnings of 20 major tumor types. This information will likely force a complete revision of diagnostic categories in cancer and will usher in an era where abnormal pathways in specific tumors will be matched with the known targets of existing therapeutics. Another example is the opportunity to understand how interactions between ourselves and the microbes that live on us and in us (the "microbiome") can influence health and disease (2).

...have complained in the past that NIH was slow to translate basic discoveries into therapeutic and treatment advances in the clinic. That criticism may have been warranted. But the pathway from molecular discovery to therapeutic benefit was just not as clear as it is now. Many major factors have contributed to this. The discovery of the fundamental pathways of many diseases has advanced rapidly. The availability of large-scale genomic data, with support from the NIH, has allowed academic investigators supported by the NIH to now have access to resources to perform large-scale assays that can be used to screen thousands of candidates for drug development; (ii) public-private partnerships are being more widely embraced in the drug-development pipeline to enable biotech and pharmaceutical companies to pick up promising compounds that have been effectively "de-risked" by academic investigators and to

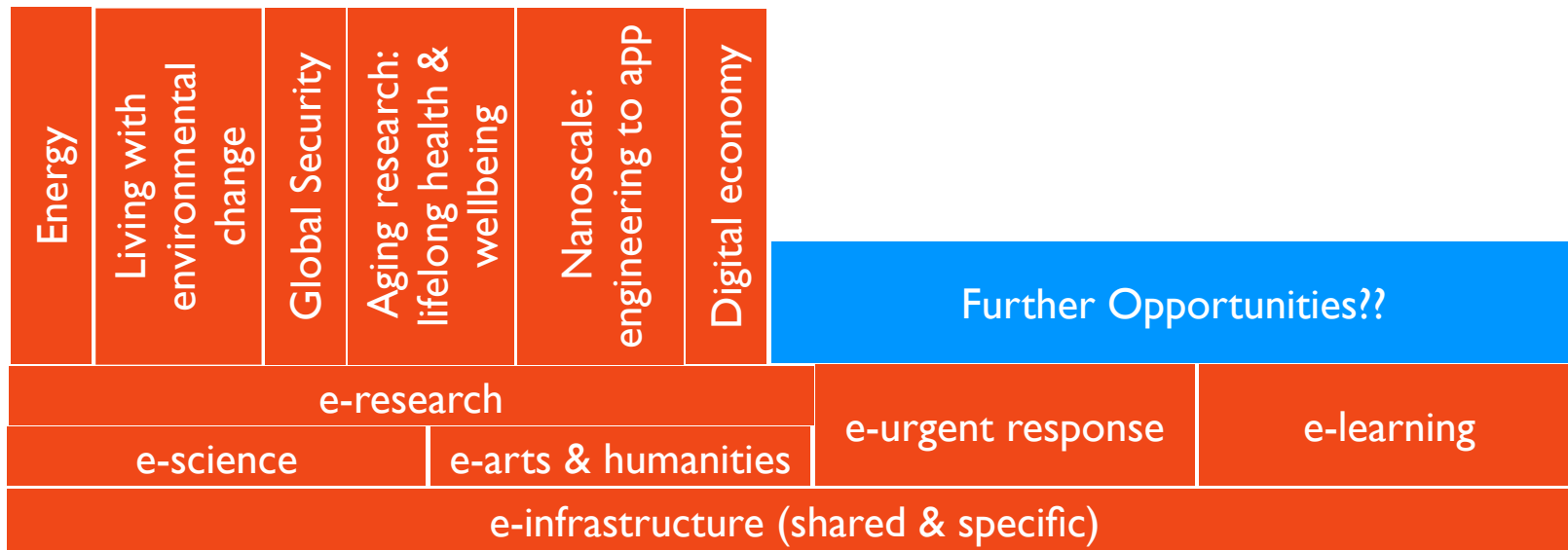
bring them to clinical trials and U.S. Food and Drug Administration (FDA) approval. As one example, the NIH Therapeutics for Rare and Neglected Diseases (TRND) (3) program will allow certain promising compounds to be taken through the preclinical phase by NIH, in an open environment where the world's experts on the disease can be involved. Furthermore, as information about common diseases increases, many are being resolved into distinct molecular subsets, and so the TRND model will be even more widely applicable. The first human protocol (for spinal cord injury) involving human embryonic stem cells (hESCs) was approved by the FDA in 2009, and the opening up of federal support for hESC research will bring many investigators into this field. The capability of transforming human skin fibroblasts and other cells into induced pluripotent stem cells (iPSCs) opens up a powerful strategy for therapeutic replacement of damaged or abnormal tissues without the risk of transplant rejection (4-6). Although much work remains to be done to investigate possible risks, the iPSC approach stands as one of the most breathtaking advances of the last several years, and every effort should be made to pursue the basic and therapeutic implications with maximum speed.

...Benefiting Health Care Reform. U.S. expenditures on health care now represent 17% of our Gross Domestic Product, are continuing to grow, and are excessive as a percentage of per capita gross income com-



# e-Infrastructure and e-Science as a Platform for Meeting Grand Challenges

## Grand Challenge Research Initiatives



# UK e-infrastructure for Science and Innovation

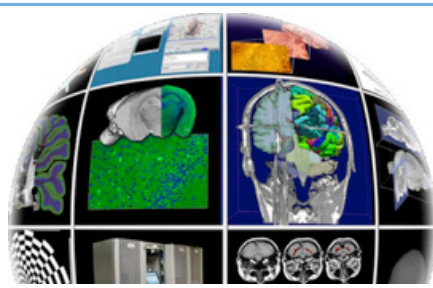
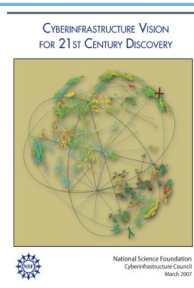
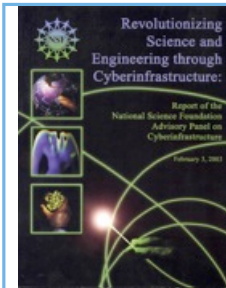
*sets out the requirements for a national e-infrastructure to help ensure the UK maintains and indeed enhances its global standing in science and innovation in an increasingly competitive world.*

## Executive Summary

The growth of the UK's knowledge-based economy depends significantly upon the continued support of the research community and in particular its activities to engage with industry and to apply its world-leading innovations to commercial use. A national e-infrastructure for research provides a vital foundation for the UK's science base, supporting not only rapidly advancing technological developments, but also the increasing possibilities for knowledge transfer and the creation of wealth.

<http://www.nesc.ac.uk/documents/OSI/index.html>

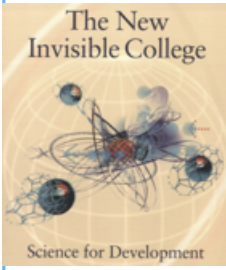




e-Science



e-Humanities & Arts



e-Learning

e-Development

The Research University in the Digital Age



(left to right)

**Anders Ynnerman**

Linköping University, Sweden

**Paul Tackley**

ETH Zürich, Switzerland

**Albert Heck**

Utrecht University, Netherlands

**Dieter Heermann**

U. of Heidelberg, Germany

**Ian Foster**

ANL & U. of Chicago, USA

**Mark Ellisman**

U. of California, San Diego, USA

**Wolfgang von Rueden**

CERN, Switzerland

**Christine Borgman**

U. of California, Los Angeles, USA

**Daniel Atkins**

University of Michigan, USA

**Alexander Szalay**

Johns Hopkins University, USA

**Julia Lane**

US National Science Foundation

**Nathan Bindoff**

University of Tasmania, Australia

**Stuart Feldman**

Google, USA

**Han Wensink**

ARGOSS, The Netherlands

**Jayanth Paraki**

Omega Associates, India

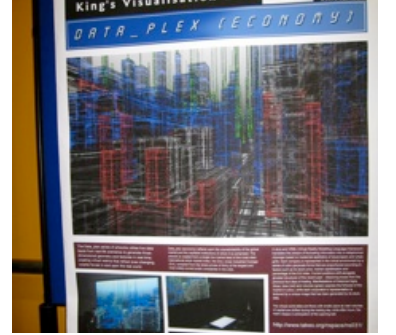
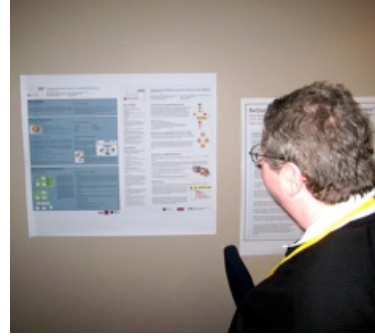
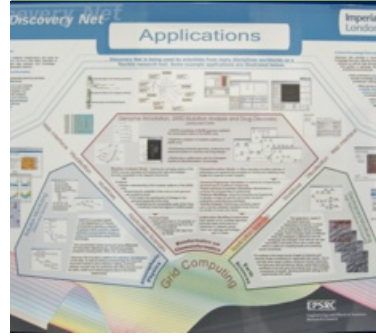
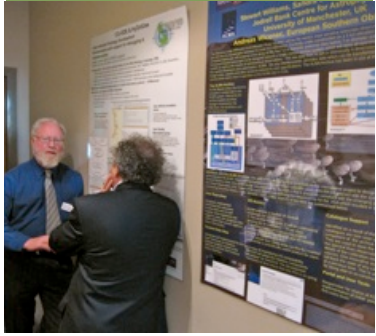
**Luciano Milanesi**

National Research Council, Italy



International Panel for 2009 Review of  
the RCUK e-Science Program





**Disciplinary research**  
 The research projects have generated a large number of high-impact journal articles related to the application areas of the projects. These articles do not necessarily emphasise scientific technology aspects of projects, but focus on advancing the state of scholarship in application domains rather than to advance science per se. Rarely do these articles explicitly refer to how influential the distance program had been on their work that could not have been accomplished, research partnerships that would not have been formed without a KCLC. The panel was presented with a large number of examples of work that could not have been accomplished, research partnerships that would not have been formed without a KCLC. The panel was presented with a large number of examples of work that could not have been accomplished, research partnerships that would not have been formed without a KCLC.

**Information technology as a**  
 We also saw much growth in the use of information technology in research. These and the differential impact reflects the absence of the need to deliver applications that meet the user's expectations. The panel was presented with a large number of examples of work that could not have been accomplished, research partnerships that would not have been formed without a KCLC.

**Interdisciplinary and collaborative research**  
 Perhaps the largest – and in the long term most important academic impact of the program found in the interdisciplinary (i.e. new social academic networks) and collaborative research. The panel was presented with a large number of examples of work that could not have been accomplished, research partnerships that would not have been formed without a KCLC.

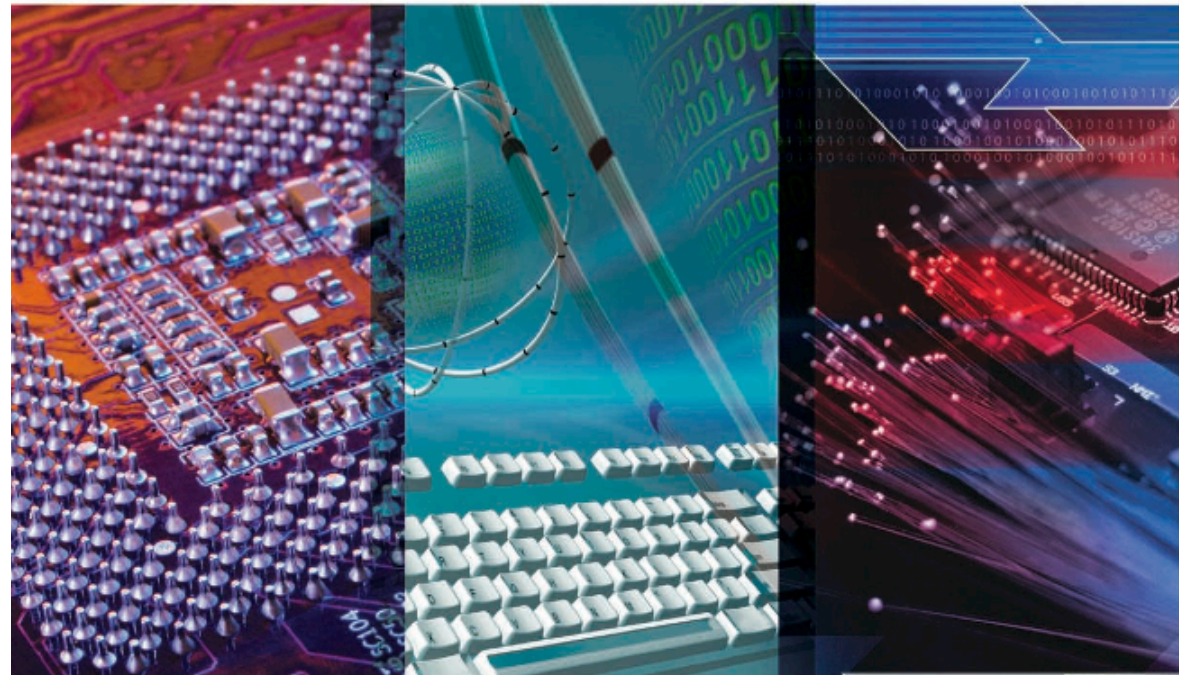
The panel noted that the formation of these new multidisciplinary (i.e. new social academic networks) and collaborative research. The panel was presented with a large number of examples of work that could not have been accomplished, research partnerships that would not have been formed without a KCLC.

Available at

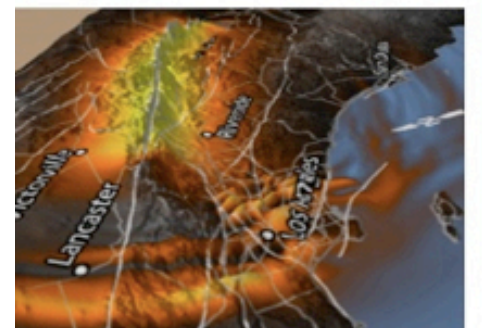
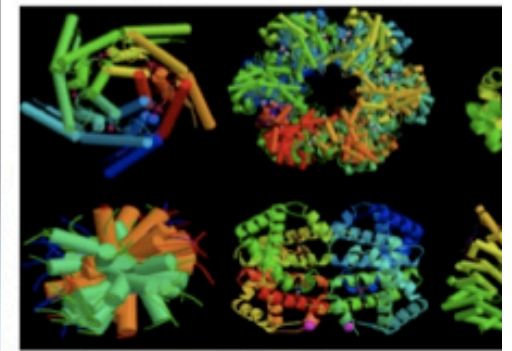
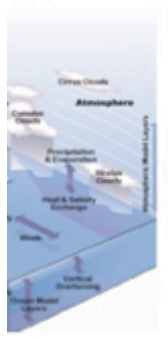
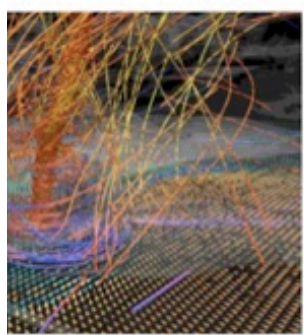
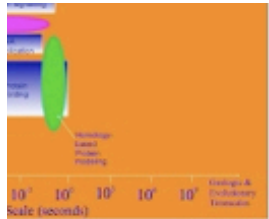
- <http://www.epsrc.ac.uk/SiteCollectionDocuments/Publications/reports/RCUKe-ScienceReviewReport.pdf>

## RCUK Review of e-Science 2009

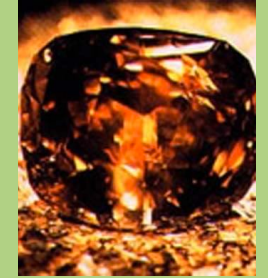
**BUILDING A UK FOUNDATION FOR THE TRANSFORMATIVE  
ENHANCEMENT OF RESEARCH AND INNOVATION**



# Findings and Recommendations



The UK has created a “jewel” -- a pioneering, vital activity of enormous strategic importance to the pursuit of scientific knowledge and the support of allied learning.



Golden Jubilee  
Diamond

- ▶ The UK e-Science Programme is in a **world-leading** position.
- ▶ Investments are already empowering **significant contributions** in the UK and beyond.
- ▶ The UK **must decide** whether to create the necessary combination of financial, organisational, and policy commitments to capitalise on their prior investments,.
- ▶ e-Science is an organic, emergent process requiring ongoing, **coordinated investment** from multiple funders and **coordinated action** by multiple research and infrastructure communities. It is both an **enabler of** research and an **object of** research,
- ▶ The UK should continue to **nurture a robust infrastructure** that couples and balances research, application development, and training processes.
- ▶ None of this is easy, but done well could achieve **enormous reward**.

# SIGNIFICANT FINDINGS: STRENGTHS (I)

- ▶ Produced competent people for both academia and industry.
- ▶ Created and enriched *interdisciplinary* collaborations (faculty & students) that are increasingly important for progress at the frontiers of scientific discovery.
- ▶ Created interdisciplinary e-science doctoral training programs.
- ▶ Stimulated industry up-take of e-science.
- ▶ Situated the UK reputation in e-science among the top nations.
- ▶ Accelerated the penetration of e-science capability in UK and Europe.
- ▶ Contributed significantly to establishing standards and tools for national and european consortial networked science projects.

## SIGNIFICANT FINDINGS: STRENGTHS (2)

- ▶ Stimulated university leaders to establish e-science buildings and organizations on campus.
- ▶ Promoted recognition of digital data as an asset and the need for greater attention to its stewardship.
  - ▶ But still lacking adequate repository capacity and the trained human capacity that is needed.
- ▶ Supported directly and indirectly scientific international collaborations.
  - ▶ But very little (any?) participation by developing countries.
- ▶ Enabled science not otherwise possible.
- ▶ Initiated a national framework for sharing large-scale resources that will be increasingly important to both large and small scale research and education.

## SIGNIFICANT FINDINGS: STRENGTHS (3)

- ▶ Supported important work in the humanities and social sciences.
- ▶ Promoted increasing standardization for data interoperability and aggregation.
- ▶ Promoted interdisciplinary work and provided mechanisms to link projects to projects on an on going way. (All-hands Meetings; community building activities)
- ▶ Leveraged investments from other sources (regional, industrial, international)
- ▶ Stimulated local/regional economies.
- ▶ Accelerated the productivity of researchers and science processes.
- ▶ Accomplished some knowledge/technology transfer but there could be more.

# SIGNIFICANT FINDINGS: WEAKNESS (I)

- ▶ Too early and rapid reduction of core funding and high level leadership, resulting in
  - ▶ Sense of abandonment by some researchers and career shift away from e-science
  - ▶ Failure to reap the benefits of prior investments.
    - ▶ The time constants for real transformative impact and significant competitive advantage is decades.
  - ▶ Reduced momentum of an important movement in which UK established a global leadership role
  - ▶ Perception that RCs don't appreciate the strategic importance of e-science and the special handling that it still needs



# SIGNIFICANT FINDINGS: WEAKNESS (2)

- ▶ Lack of models for sustaining/maintaining software, platform/infrastructure operations, and data resources
  - ▶ e-infrastructure providers are being forced to compete for research funding (rather than targeted infrastructure/facilities funding) every two years
- ▶ Missed opportunities to transfer successful software tools/systems and best practices to other fields. Lack of regularized processes and organizations to do so.

# SIGNIFICANT FINDINGS: WEAKNESS (3)

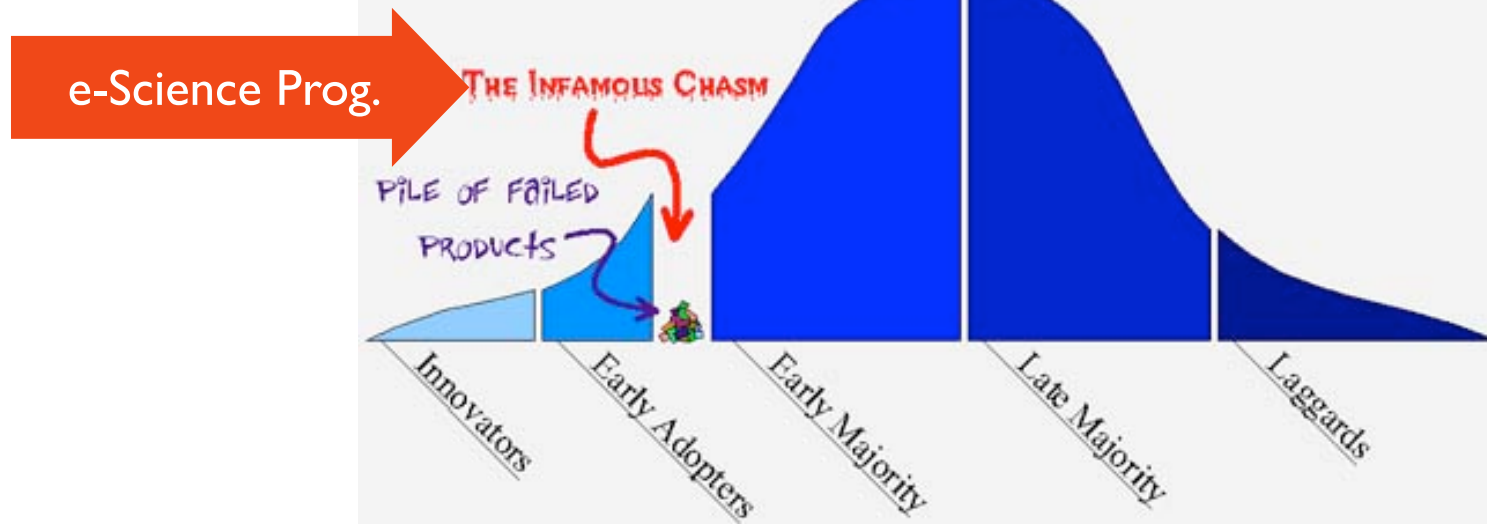
- ▶ Lack of adequate structure, leadership, and resources to promote constructive interplay and achieving balance (1) between shared/generic and specific e-infrastructure and (2) between e-science core and disciplinary research.
  - ▶ This situation raises barriers to interdisciplinary work; to developing and exploiting common infrastructure, middleware, tools, systems; and to interoperability between disciplines, projects, platforms and shared use of resource
- ▶ Overly focused on computational "grid" platforms
  - ▶ Good fit to physics but not necessarily all other domains. But there are variations in what "grid" means. (computational, data, all types of resources)
- ▶ Knowledge transfer (KT) potential higher than was actually achieved. Need more systematic and staffed KT processes.

# SIGNIFICANT FINDINGS: WEAKNESS (4)

- ▶ Shortage of women participants (as judged by data in evidence document and gender balance during review)
- ▶ Gaps in the e-science program conceptualization.
  - ▶ sensor networks
  - ▶ usability, human-computer-interaction
  - ▶ understanding of social/behaviors barriers to technology mediate science collaboration and ways to design systems and processes to reduce barriers

# Crossing the Chasm – Modified

Geoffrey Moore's *Revised* Technology Adoption Life Cycle



## Recent novel examples of government, industry, academia partnerships on e-Science research

<http://www.networkworld.com/community/node/27219>

[http://www.nsf.gov/news/news\\_summ.jsp?cntn\\_id=116336&org=NSF&from=news](http://www.nsf.gov/news/news_summ.jsp?cntn_id=116336&org=NSF&from=news)

<http://www.nytimes.com/2010/02/05/science/05cloud.html>

### Google, IBM and NSF offer up \$5M for large-scale computing research

By [Layer 8](#) on Thu, 04/24/08 - 12:36pm.

[Share](#) [Tweet This](#) [Email this page](#) [Comment](#) [Print](#)

[Newsletter Sign-Up](#)

The [National Science Foundation](#) in cooperation with [Google and IBM](#) today said it was [seeking proposals](#) for the group's Cluster Exploratory ([CluE](#)) initiative to explore innovative research ideas in data-intensive computing.

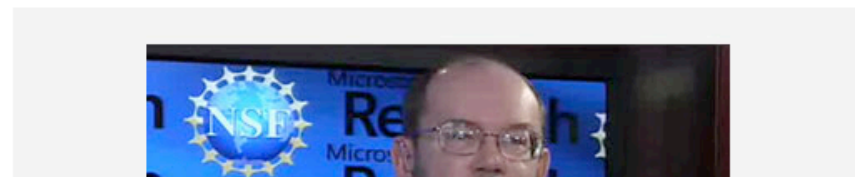
The NSF said it expects to award up to \$5 million spread between



**Press Release 10-023**

### Microsoft and NSF Enable Research in the Cloud

**Agreement will offer free access to new computational and collaborative services to accelerate scientific discovery for research communities.**



### U.S. Scientists Given Access to Cloud Computing

By JOHN MARKOFF  
Published: February 4, 2010

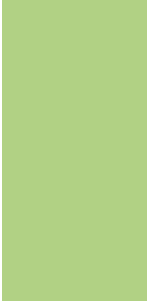
The [National Science Foundation](#) and the [Microsoft Corporation](#) have agreed to offer American scientific researchers free access to the company's new cloud computing service.

**RSS Feed**

A goal of the three-year project is to give scientists the computing power to

- SIGN IN TO RECOMMEND
- TWITTER
- E-MAIL
- SEND TO PHONE
- PRINT

Creating a  
Transformative  
e-Science  
Programme is  
a Complex  
Balancing Act



# A Research Cyberinfrastructure Strategy for the CIC: Advice to the Provosts from the Chief Information Officers

CIC = Committee for  
Inter Institutional  
Committee [www.cic.net](http://www.cic.net)  
University of Chicago  
University of Illinois  
Indiana University  
University of Iowa  
University of Michigan  
University of Nebraska  
Michigan State  
University  
University of Minnesota  
Northwestern University  
Ohio State University  
Pennsylvania State  
University  
Purdue University  
University of Wisconsin-  
Madison



CIC = Committee for Inter Institutional Committee  
[www.cic.net](http://www.cic.net)

D. E. Atkins • [atkins@umich.edu](mailto:atkins@umich.edu)

RECENT REPORT

## Recommendations

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- Our goal should be to enable scholarship at the cutting edge of every discipline, while getting as much value as possible from every dollar spent on cyberinfrastructure.
- The CIC campuses are very richly endowed with cyberinfrastructure resources but can be even more effective by adopting good practices that support greater coordination at every level:
  - Plan.
  - Share (at the highest level possible).
  - Design funding models that promote scholarship and stewardship.
  - Rely on user governance.
  - Conduct cyberinfrastructure impact analysis.
- Over the long run, these practices should help our institutions produce **more scholarship (learning and research) per dollar invested.**



## We should all currently be investing in:

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- Preparing for **federated identity management** and other enabling technologies for virtual organizations.
- Maintaining **state-of-the-art** communication **networks**.
- Providing institutional **stewardship of research data**.
- **Consolidating** computing resources while **maintaining diverse** architectures.
- Expanding cyberinfrastructure **support to all** disciplines.
- Exploring **cloud computing** to manage longterm financial commitments.

# Cornell NSF Workshop on Sustainable HPC



- [https://mw1.osc.edu/src/index.php/Main\\_Page](https://mw1.osc.edu/src/index.php/Main_Page)

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[page](#) [discussion](#) [view source](#) [history](#)

## Main Page

### Sustainable Research Computing Centers

[Join the Sustainable Research Computing Centers LinkedIn Group](#)

**NSF Workshop on Sustainable Funding and Business Models for High Performance Computing**  
Contribute to the report writing discussions by creating a wiki account and adding content.

### Schedule

May 8, 2010 - May 22, 2010:

1. Contribute your workshop take-aways and findings via the SRCC-L Listserv or the [Sustainable Research Computing Centers LinkedIn group](#)
2. Review the breakout discussion findings (found below) and add your input to the report outline on the [discussion tab](#) of this wiki
3. Help develop the report outline on the [discussion tab](#) of this wiki

### NSF Workshop on Sustainable Funding and Business Models for High Performance Computing

#### Presentations & Breakout Reports

[Cornell CAC Sustainability Model - Dave Lifka](#)

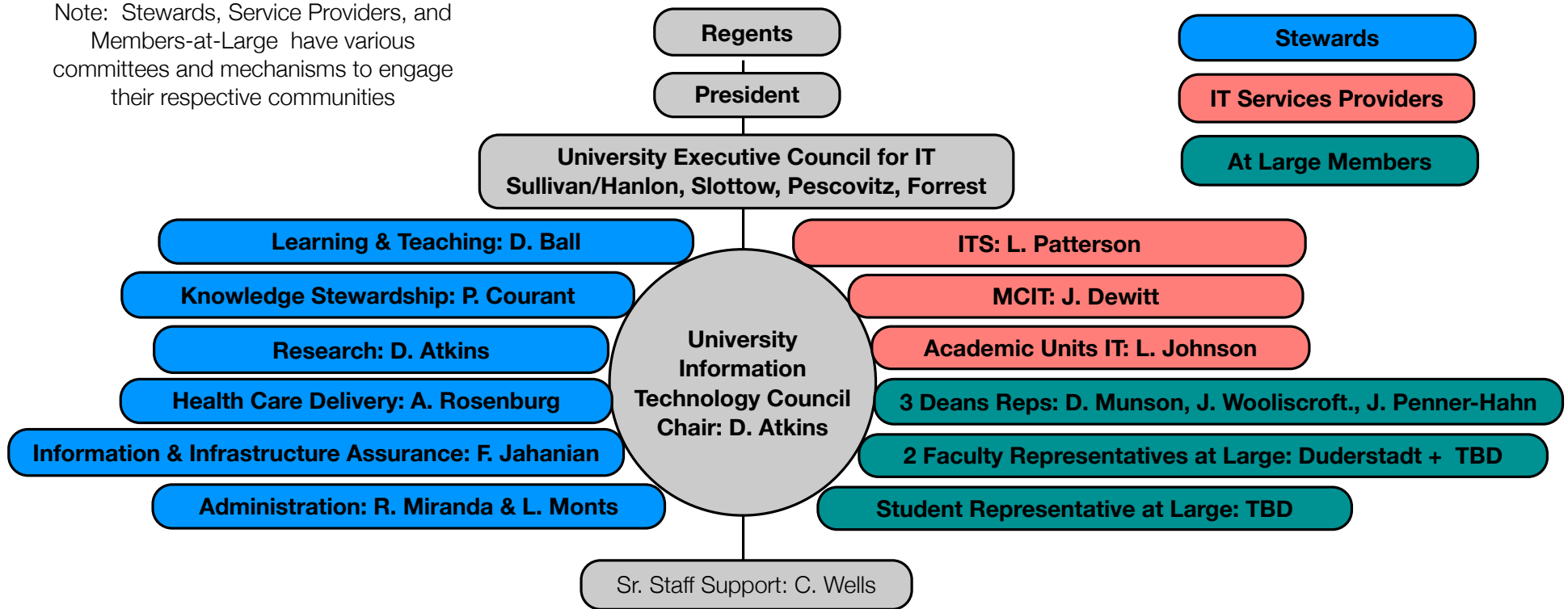
[Bridging Campuses to National Cyberinfrastructure – Overview of OCI Sustainable Center](#)

[Penn State Sustainability Model - Vijay Agarwala](#)

[Organizational Models, Staffing & Succession Planning](#)

# New University of Michigan IT Visioning, Planning, and Governance Model

Note: Stewards, Service Providers, and Members-at-Large have various committees and mechanisms to engage their respective communities



## **Mission Statement: UM Office of Research Cyberinfrastructure (ORCI)**

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*To create and nurture a modern, fiscally responsible, and sustainable cyberinfrastructure (both resources and services), intellectual capacity, and academic environment in support of high-end computing- and data-intensive research activities that ensures UM leadership as a 21<sup>st</sup> century research institution.*

Adopted by ORCI Steering Committee, April xx

# The UM CIRRUS Research Computing Project

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- CIRRUS - Computation and Information Resources (for) Research as a Utility Service
- The centerpiece of our innovation in the provisioning of research cyberinfrastructure.
- Goal is to provide a *portfolio* of integrated research computing services that are mission effective, financially efficient, and environmentally friendly.

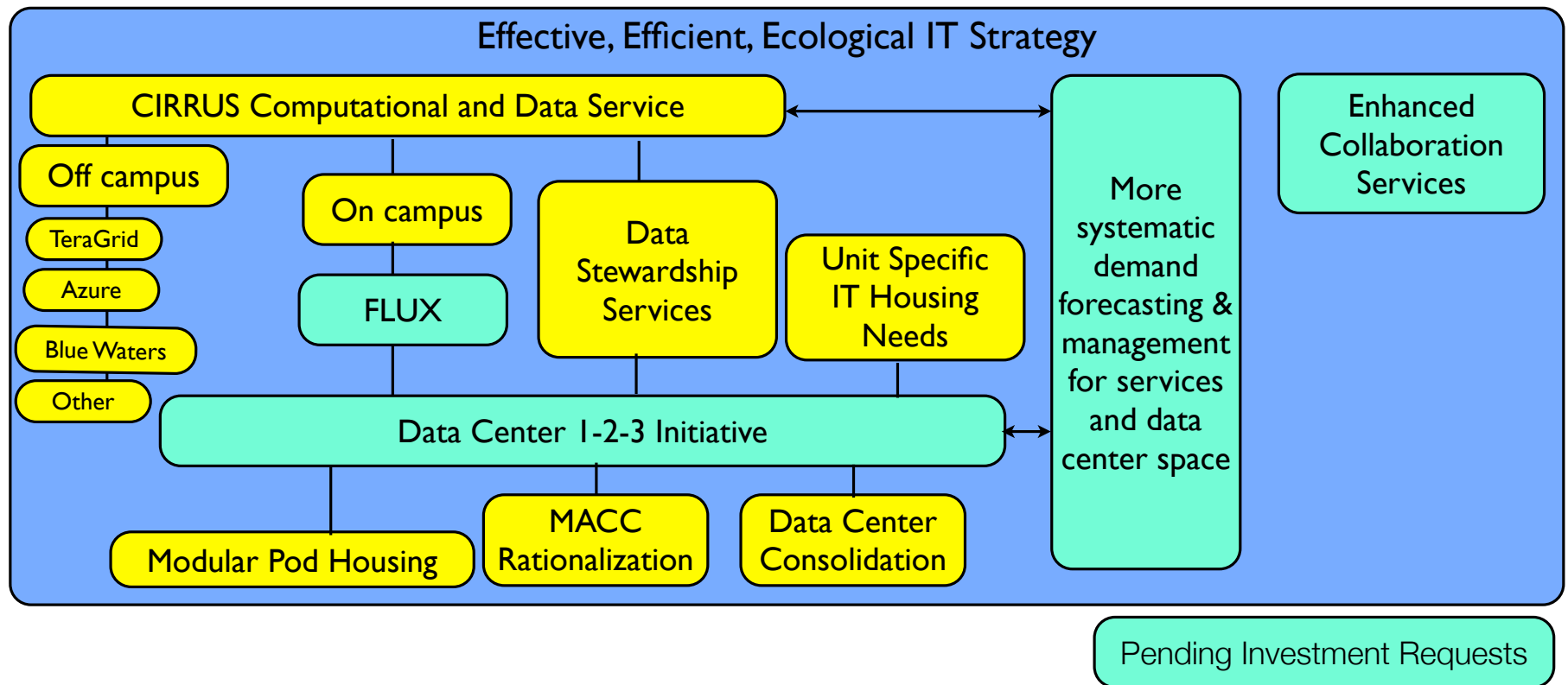
D. E. Atkins • [atkins@umich.edu](mailto:atkins@umich.edu)



# CIRRUS

Computation and  
Information Resources (for)  
Research as a Utility  
Service

## Part of NextGen Michigan Roadmap and Pending Investment Requests for IT Council Consideration



# Exploring Use of Pod Optimized Performance Datacenters

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<https://research.umich.edu/blogs/ci/>

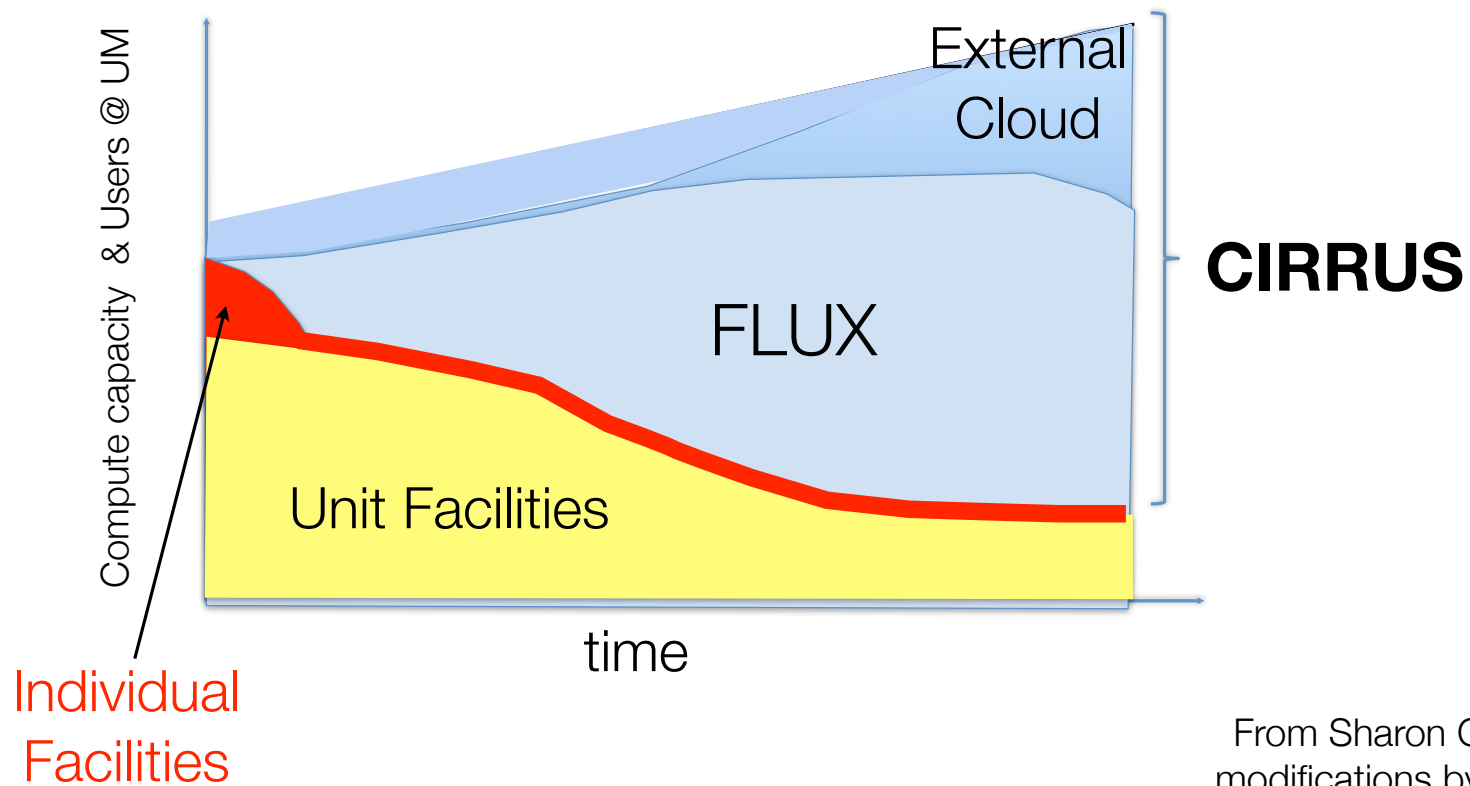


The screenshot shows the header of the ORCI Blog Site. On the left is a large yellow 'M' logo. To its right, the text reads 'Computational Discovery & Cyberinfrastructure at U-M' in white, with 'News and information from the Office of Research Cyberinfrastructure' below it. The main content area features a post titled 'Want to explore a very large Microsoft cloud for research computing? Let us know!' posted on February 17th, 2010 by OVPR-CI. The categories are 'Funding Opportunities' and 'Resources'. The post text begins with 'In case you missed our post about Microsoft teaming with NSF to offer free access to research computing, there is also supplemental and EAGER funding available. From the NSF'. To the right of the post is a search bar with a 'Search' button and an 'Archives' section listing posts by month: February 2010 (7), January 2010 (5), December 2009 (2), October 2009 (1), and September 2009 (2).

ORCI Blog Site to Help Share Information and Build Community



## A Vision of HPC @ UM



From Sharon Glotzer with  
modifications by Dan Atkins

# Cyberinfrastructure Framework for 21st Century Science & Engineering (CF21)

NSF-wide Cyberinfrastructure Vision  
People, Sustainability, Innovation, Integration

# Five Challenges

## ❖ Computing Technology

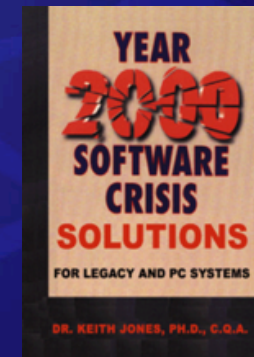
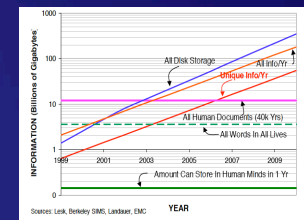
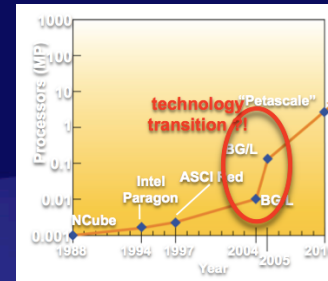
- Multicore: processor is new transistor
- Programming model, fault tolerance, etc
- New models: clouds, grids, GPUs,... where appropriate

## ❖ Data, provenance, and visualization

- Generating more data than in all of human history: preserve, mine, share?
- How do we create "data scientists"?

## ❖ Software

- Complex applications on coupled compute-data-networked environments, tools needed
- Modern apps:  $10^6+$  lines, many groups contribute, take decades



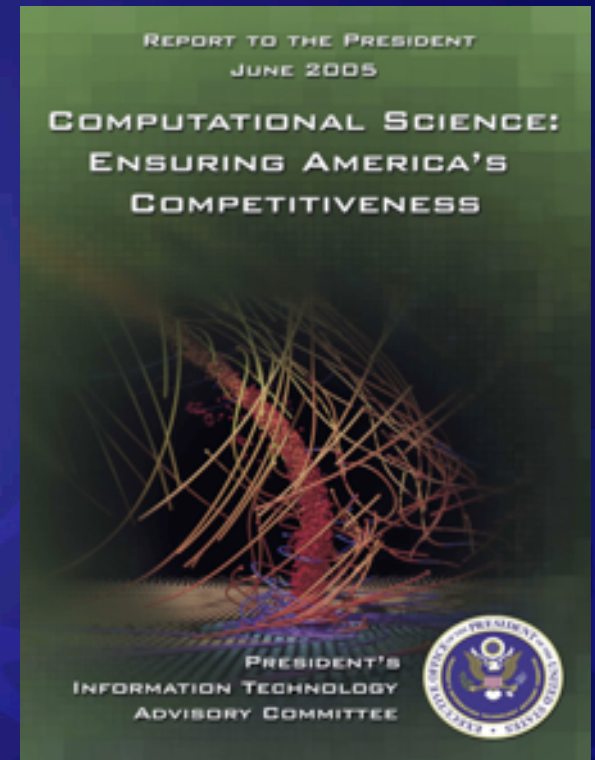
## Five Crises con't

### ❖ Organization for Multidisciplinary Computational Science

- "Universities must significantly change organizational structures: multidisciplinary & collaborative research are needed [for US] to remain competitive in global science"
- "Itself a discipline, computational science advances all science... inadequate/outmoded structures within Federal government and the academy do not effectively support this critical multidisciplinary field"

### ❖ Education

- The CI environment is becoming more **complex** and more **fundamental** for research
- How do we develop a workforce to provide leadership, expertise and support ?



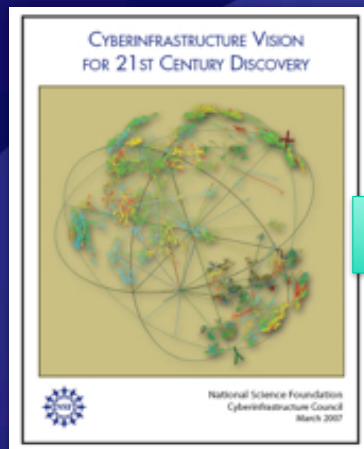
## Some observations

- ❖ Science and Scholarship are team sports
  - Competitiveness and success will come to those who can put together the best team, and can marshal the best resources and capabilities
- ❖ Collaboration/partnerships will change significantly
  - Growth of dynamic coalitions and virtual organizations
  - International collaboration will become even more important
- ❖ Ownership of data plus low cost distribution fuels growth and number of data systems
  - Growth in both distributed systems and local systems
  - More people want to access more data
  - Federation and interoperability become more important

## More observations

- ❖ More discoveries will arise from search approaches
  - Mining vast amounts of new and disparate data
  - Collaboration and sharing of information
- ❖ Mobility and personal control will continue to drive innovation and business
- ❖ Gaming, virtual worlds, social networks will continue to transform the way we do science, research, education and business
- ❖ The Internet has collapsed six degrees of separation and is creating a world with two or three degrees.

What is Needed?  
An **ecosystem**, not just components...



*NSF-wide CI  
Framework for 21<sup>st</sup>  
Century Science &  
Engineering*

People, Sustainability, Innovation, Integration

# Cyberinfrastructure Ecosystem

## Expertise

Research and Scholarship  
Education  
Learning and Workforce Development  
Interoperability and operations  
Cyberscience

## Organizations

Universities, schools  
Government labs, agencies  
Research and Medical Centers  
Libraries, Museums  
Virtual Organizations  
Communities

## Scientific Instruments

Large Facilities, MREFCs, telescopes  
Colliders, shake Tables  
Sensor Arrays  
- Ocean, environment, weather, buildings, climate. etc

## Computational Resources

Supercomputers  
Clouds, Grids, Clusters  
Visualization  
Compute services  
Data Centers

**Discovery  
Collaboration  
Education**

## Data

Databases, Data repositories  
Collections and Libraries  
Data Access; storage, navigation  
management, mining tools,  
curation

## Software

Applications, middleware  
Software development and support  
Cybersecurity: access, authorization,  
authentication

## Networking

Campus, national, international networks  
Research and experimental networks  
End-to-end throughput  
Cybersecurity

**Maintainability, sustainability, and extensibility**



# ACCI Task Forces

Campus Bridging:  
Craig Stewart, IU  
(BIO)

Data & Viz: Tony  
Hey, , Dan Atkins

- ❖ Completion by end of year
- ❖ Advising NSF
- ❖ Conducting Workshop(s)
- ❖ Recommendations
- ❖ Input to NSF informs CF21 programs, 2011-12 CI Vision

Software: David  
Keyes, Columbia/  
KAUST (MPS)

Computing: Thomas  
Zacharia, ORNL/UTK  
(DOE)

Education & Workforce:  
Alex Ramirez, CEOSE

Grand Challenge  
Communities/VOs:  
Tinsley Oden, Austin  
(ENG)

## CF21 Impact on Data

- ❖ All science is becoming data-dominated
  - Experiment, computation, theory
- ❖ Totally new methodologies
  - Algorithms, mathematics
  - All disciplines from science and engineering to arts and humanities
- ❖ End-to-end networking becomes critical part of CI ecosystem
- ❖ How do we train “data-intensive” scientists?
- ❖ Data policy and sustainability becomes critical!



## **US NSF Data and Visualization Strategy Task Force**

Co-chairs Tony Hey and Dan Atkins; Member: Liz Lyon

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- Charge: Examine the increasing importance of data and their visualization in driving grand challenge science, engineering, education.
- Emphasis: Value of the data, complexity, and organic aspects. The role of data in research, the value of metadata and ontologies for integration, etc.
- Goal: Catalyze a network of science and engineering data collections that is open, extensible and sustainable. Enable multiple fields of science and engineering research and education -- including new types of data-driven computational science, interdisciplinary research and cross-disciplinary education.

## 12. Towards functionally complete, four-quadrant, research environments

- ▶ Pursue capacity for collaborative, international, interdisciplinary team science to occur routinely in “functionally complete, four-quadrant environments” built upon e-infrastructure.
- ▶ “A four-quadrant environment” refers to a blended virtual-physical environment in which the activities of a group can flow easily between all four quadrants in a 2-by-2 matrix with same versus different for the two dimensions of both time and place. It subsumes the concept of virtual research environment.
- ▶ “Functionally complete” means that the environment supports access to all the people, the information and data services, the observatories and facilities, the computational services, and the collaboration and communication services necessary for a scientific team (or more generally, a community of practice) to carry out its work.

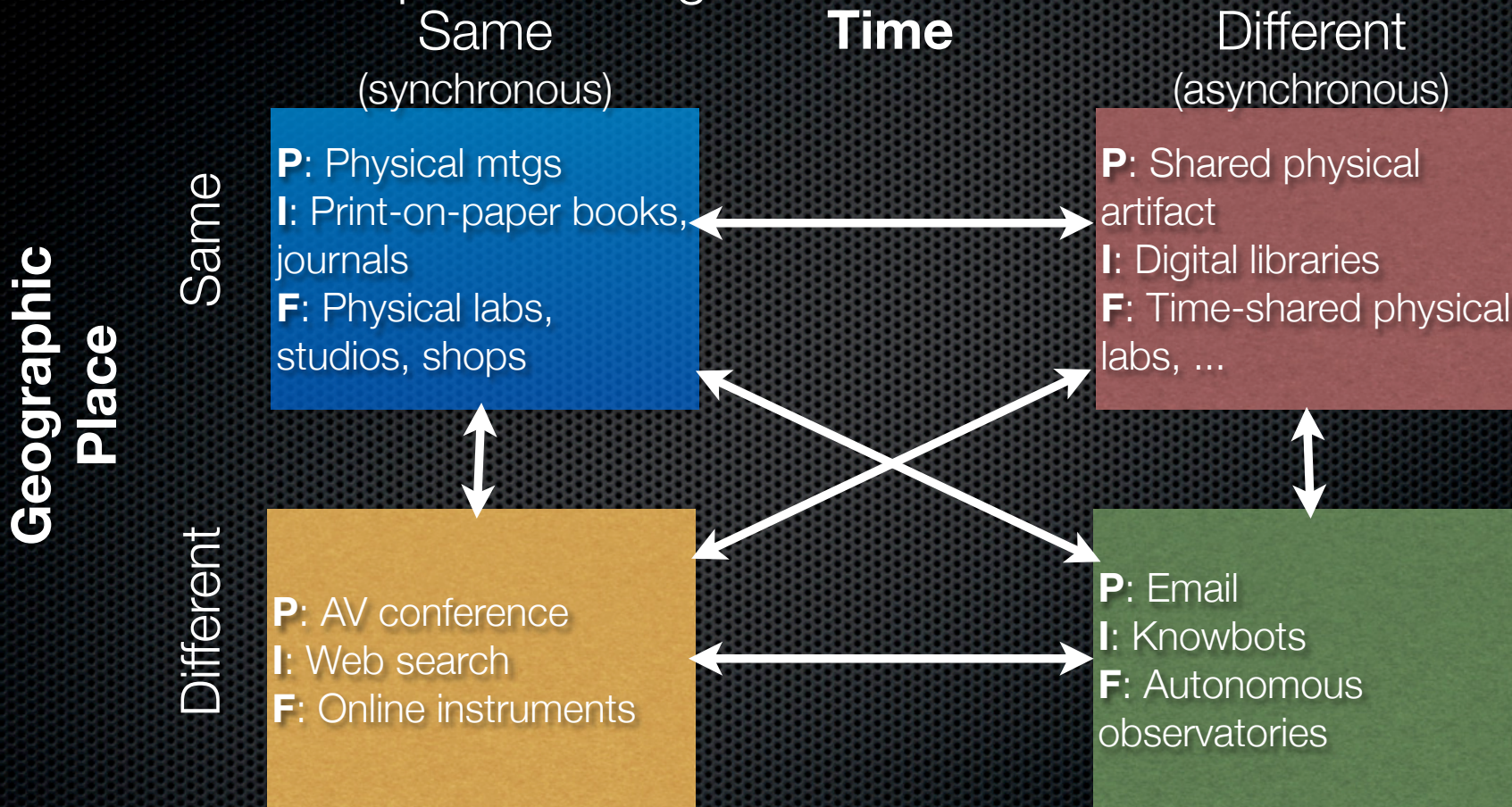
Four Quadrant Organizations (virtual + physical organizations) offer additional modes of interaction between People, Information, and

		Time	
		Same (synchronous)	Different (asynchronous)
Geographic Place	Same	<b>P:</b> Physical mtgs <b>I:</b> Print-on-paper books, journals <b>F:</b> Wet labs, studios, shops	<b>P:</b> Shared physical artifact <b>I:</b> Library reserve <b>F:</b> Time-shared physical labs, ...
	Different	<b>P:</b> AV conference <b>I:</b> Web search <b>F:</b> Online instruments	<b>P:</b> Email <b>I:</b> Knowbots <b>F:</b> Autonomous observatories

Physical + Virtual,  
Not Physical vs.  
Virtual

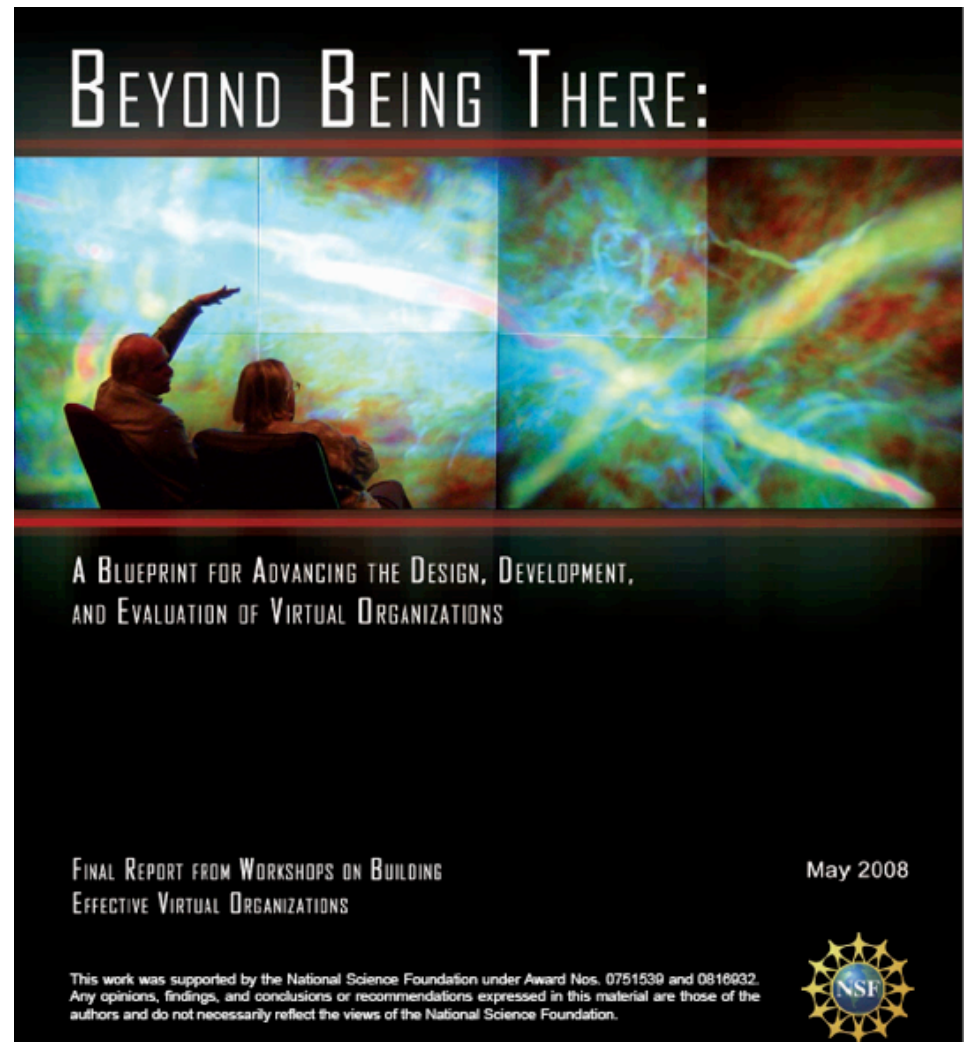


Need to discover how to best map collaborative workflows onto various paths through these collaboration states.



# Beyond Being There: A Blueprint for Advancing the Design, Development, and Evaluation of Virtual Organizations

Available at:  
[www.ci.uchicago.edu/  
events/VirtOrg2008/](http://www.ci.uchicago.edu/events/VirtOrg2008/)



# CF21 Impact on Virtual Organizations

- ❖ What constitutes effective virtual organizations? How do they enhance research and education; what about production and innovation?
- ❖ Multi-disciplinary approach
  - Anthropology, complexity sciences, CS, decision and management sciences, economics, engineering, organization theory, organizational behavior, social and industrial psychology, public administration, sociology
- ❖ Broad variety of qualitative and quantitative methods
  - Ethnographies, surveys, simulation studies, experiments, comparative case studies, network analyses.
- ❖ Grounded in theory, rooted in empirical methods







## What Can JISC and CNI Independently and Together Do to Help?

e-Science

Discussion & Questions