

Accelerating Clinical and Translational Research



## nanoHUB.org

ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY







NEEShub

transforming healthcare delivery



INTEGRATED **ENVIRONMENTAL** MODELING

A community center for developing and sharing knowledge and tools for environmental systems anal

GL 3ALHUB Advancing Global Engineering



vscse

VIRTUAL SCHOOL OF COMPUTATIONAL

George E. Brown, Jr. Network for Earthquake Engineering Simulation

Science of Information

NSF Science and Technology Center

ermalHLE





CONNECTING ASSISTIVE TECHNOLOGY CONSUMERS PROFESSIONALS, INNOVATORS, AND PROVIDERS

Monday, April 4, 2011

iemhub

a CIEM project

COLLABORATION FOR PHARMACEUTICAL ENGINEERING AND SCIENCE

Collaborative volcano research and risk mitigation

#### Improved Simulation Through Collaboration

Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory • NYSERNet

#### EERHUB

Collaboratory for Engineering Education Research





MANUFACTURING

## The Greatest and Best Use of Cyberinfrastructure: High-Performance Collaboration



Daniel E. Atkins W.K. Kellogg Professor of Community Informatics, Professor of EECS, Associate VP for Research Cyberinfrastructure University of Michigan <u>atkins@umich.edu</u>





## HUBzero

In a larger historical context;
as an object of celebration;
as a system for future development.



#### Personal Privilege and Amazement: From Digiclock to Petascale Grid Communities



1964 - Digiklok



1949-62 Illiac I



1956-68 Illiac II



1960-68 Illiac III

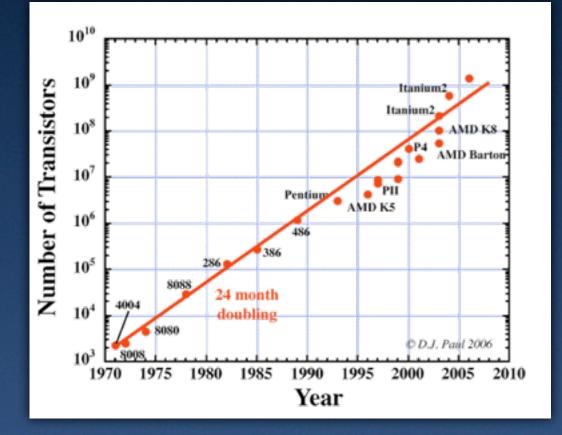


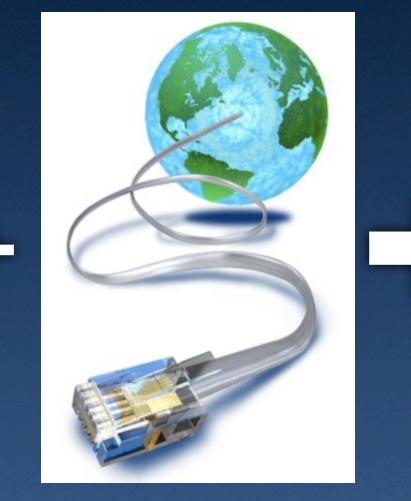
1972-82 - Exp. Machines



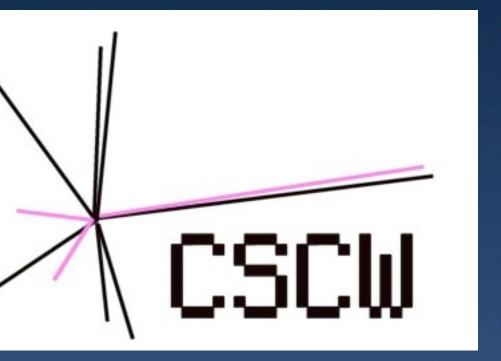
1956-68 Illiac IV

## The Marriage of Computing and Communication









## Personal Privilege and Amazement: From Digiclock to Petascale Grid Communities



1983- CAEN



1993-School of Information **Information School Movement** 

Alliance for

1997- Kellogg ACT

Community Technology



2001-03 CI Adv. Panel



1983- Collaboratory Research • UARC • SPARC



2006- NSF Office of Cyberinfrastructure



#### 1990- UM Digital Lib Project



## **Towards a National Collaboratory**



#### An Invitational Workshop at the Rockefeller University March 17-18, 1989

http://ai.eecs.umich.edu/people/conway/CSE/CollabTech/CollabTechWorkshop.html



#### NATIONAL COLLABORATORIES

Applying Information

Science and Tole

#### 1993 NRC Report

http://www.amazon.com/National-Collaboratories-Information-Technology-Scientific/dp/0309048486

## From Executive Summary of National Collaboratories...

The fusion of computers and electronic communications has the potential to dramatically enhance the output and productivity of U.S. researchers. A major step toward realizing that potential can come from combining the interests of the scientific community at large with those of the computer science and engineering community to create integrated, tool-oriented computing and communications systems to support scientific collaboration. Such systems can be called "collaboratories."

## The University of Michigan Upper Atmospheric Research Collaboratory (UARC)

#### http://www.crew.umich.edu/research/ research\_uarc.html



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## The Initial Facility at Sondrestrom, Greenland

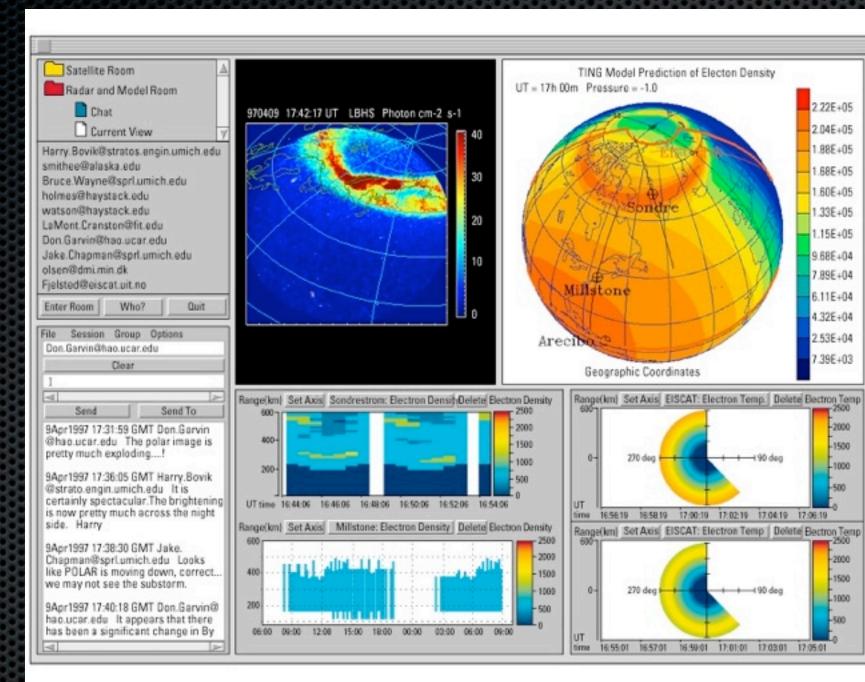




## UARC Interface Real-time instruments computational models

#### dynamic work rooms

team chat



University of Michigan

Archival data

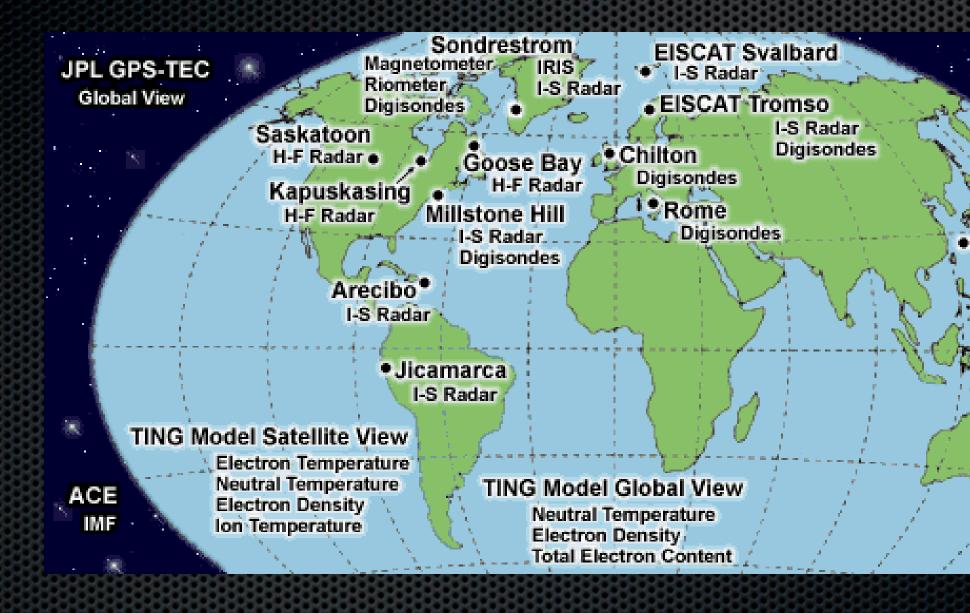
Journals

Monday, April 4, 2011

# annotation Session replay



# Evolved into a Network of Instruments (one global instrument)



University of Michigan

POLAR UVI VIS PIXIE

 Okinawa Digisondes



## UARC Patterns of Communication

#### Pattern of Communication, UARC Campaign, April 9, 1997



Monday, April 4, 2011

University of Michigan

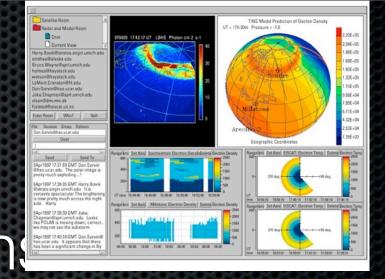
1998 Smithsonian Science Award



Vignettes from UARC/SPARC Shared, tele-instruments & expertise. Rapid response, opportunistic campaign. • Multi-eyes, complementary expertise. Isolated instruments became a global instrument chain. Cross-mentoring/training. New & earlier opportunities/exposure for grad students. Enhanced participation. Legitimate peripheral participation.



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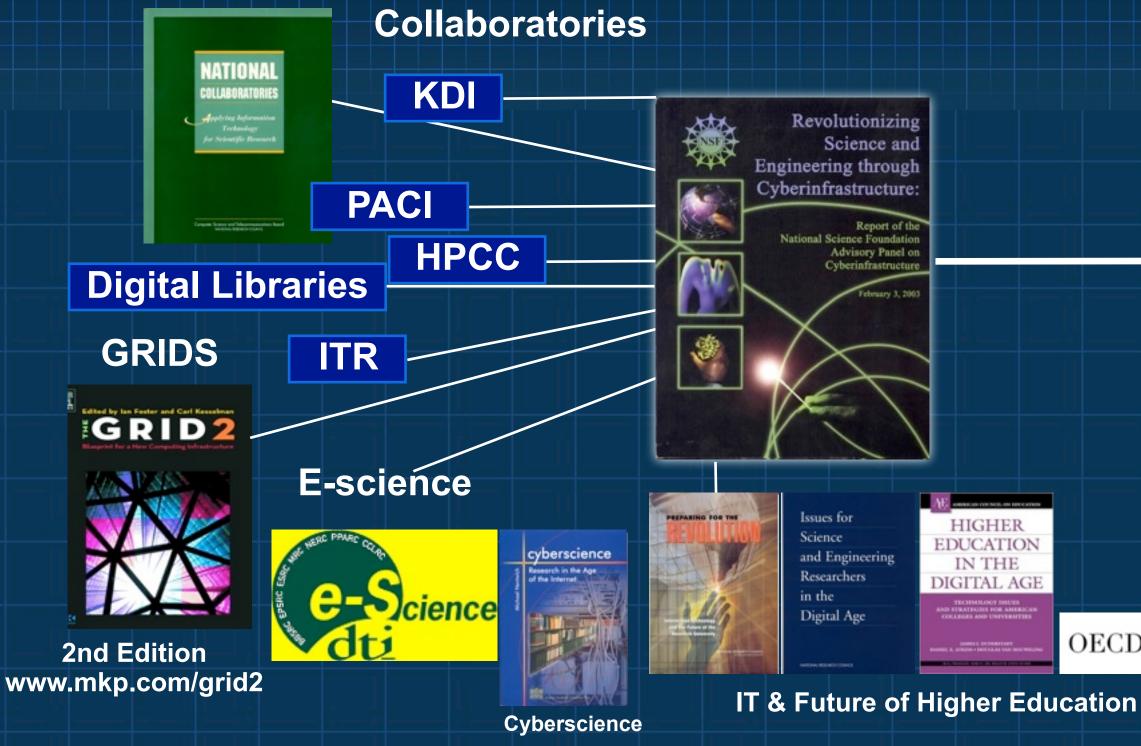


- Support for authentic, inquiry-based learning at UG and pre-college level.
- Distributed workshops for post-campaign data analysis.
- Session re-play for delayed participation. • Data-theory closure.





## Cyberinfrastructure Genealogy & Movement



D. E. Atkins • University of Michigan • atkins@umich.edu



## NSF Blue Ribbon Advisory Panel on Cyberinfrastructure

Daniel E. Atkins, Chair University of Michigan Kelvin K. Droegemeier University of Oklahoma

Stuart I. Feldman

Hector Garcia-Molina Stanford University

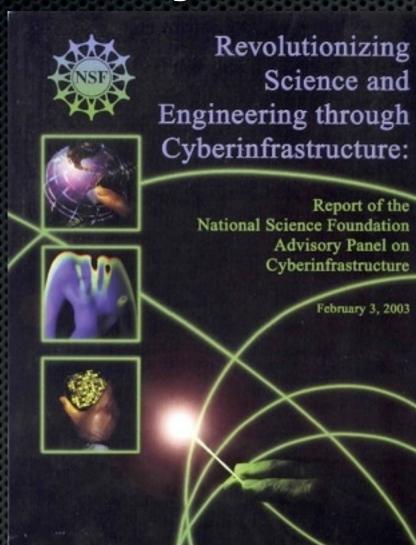
Michael L. Klein University of Pennsylvania David G. Messerschmitt

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



## Now 100's of Reports on CI-enabled Research

Cyberinfrastruc	Ice Foundation	s About OCI					
Cyberinfrastructure - stimulating advances in 21st century science and engineering							
About OCI	High Performance Computing	Get OCI Updates					
View OCI Staff Directory		by Email					
Search OCI Staff Directory	OCI has released a new HPC Resource Solicitation, PD 11-1155. Proposals are due March 7, 2011. An updated version of the benchmark site will be provided by PC and the Solicitation of the benchmark site will be provided by PC and the Solicitation of the benchmark site will be provided by PC and the Solicitation of the benchmark site will be provided by PC and the Solicitation of the benchmark site will be provided by PC and the Solicitation of the benchmark site will be provided by PC and the Solicitation of the benchmark site will be provided by PC and the Solicitation of the benchmark site will be provided by PC and the Solicitation of the benchmark site will be provided by PC and the Solicitation of the benchmark site will be provided by PC and the PC and th	Additional OCI Resources					
General Information About OCI	available by December 27, 2010. For a list of FAQs please see <u>HPCFAQ</u> . For solicitation information please see <u>High Performance</u> <u>Computing System Acquisition: Enhancing the Petascale Computing</u>	Cyberinfrastructure Vision for 21st Century					
Career Opportunities	Environment for Science and Engineering (NSF 11-511) Posted December 7, 2010.	Discovery Long-Lived Digital Data					
Advisory Committee	(NSF 11-511) Posted December 7, 2010.	Collections: Enabling					
Budget Excerpt	Strategic Technologies for CI (STCI)	Research and Education in the 21st Century					
Proposals and Awards Proposal and Award Policies and Procedures Guide Introduction Proposal Preparation and	OCI has released a new Strategic Technologies for Cyberinfrastructure (STCI) program description, PD 11-7684. The next window for proposal submissions is January 3, 2011 - January 18, 2011. Please see <u>http://www.nsf.cov/funding/pom_summ.jsp?</u> pims.id=5034758org=OCI8sel_org=OCI8/rom=fund for additional information and STCI program proposal submission instructions.	Reports and Workshops Relating to Cyberinfrastructure and Its Impacts A Process-Oriented Approach to Engineering Cyberinfrastructure					
Submission Grant Proposal Guide		OCI Presentations					
Grants.gov Application Guide Award and Administration	New Deputy Director (Acting), OCI	International Research Network Connections (IRNC)					
Award and Administration Guide	(Acting) for the Office of Cyberinfrastructure (OCI).	Cyberenvironment Project Management:					
Award Conditions	Scientific Software Innovation Institutes	Lessons Learned					
Other Types of Proposals Merit Review		Publications See All					
NSF Outreach	Software is an integral part of the computation paradigm for supporting innovation and discovery in science and engineering, and is a primary	Report of Blue-Ribbon Advisory Panel on					
Policy Office	modality for realizing NSF's Cyberinfrastructure Framework for 21st Century	Cyberinfrastructure					
Awards OCI Award Search Active OCI Awards Discoveries	Science and Engineering (CF21) <sup>1</sup> / <sub>4</sub> vision. In order to nurture, accelerate and sustain this critical mode of scientific progress, NSF has established the crosscutting Software Infrastructure for Sustained Innovation (SI2) program <sup>2</sup> , a long-term Investment with the overarching goal of transforming innovations in research and education into sustained software resources that are an integral part of the cyberinfrastructure. Scientific Software Innovation Institutes (S2I2) will be the anchors of the SI2 program and will focus on the establishment of long-term community-wide hubs of sustained software excellence.	Frequently Asked Questions: Regarding High Performance Computing System Acquisition: Enhancing the Petascale Computing Environment for Science and Engineering (NSF 11-511)					

#### http://www.nsf.gov/dir/index.jsp?org=OCI

#### **Research Guides**

Inhereity Cyberin Last update

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	Library					
-	entry of Michigan Library > 1 berinfrastructure and			frastructure and Resea	arch Rasources	
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	Walcome		What is for	han al a firm attended to a 7		
Welcome				What is Cyberinfrastructure?		
This research guide is designed to provide links to literature related to cybernfrastructure and e- Science. Questions? Prease contact Ye LI, Devid Carter or Valerie Waldron.			"Cyberinfrastructure consists of computing systems, d storage systems, advanced instruments and data repositories, visualization environments, and people, linked by high speed networks to make possible scholarly innovation and discoveries not otherwise possible." – from UTIS Knowledge Base (What is Cyberinfrastructure?, IU)			
Coline Videos on Cyberinfrastructure			acience and eng researchers will	"Cyberinfestructure is poised to revolutionize many science and engineering disciplines. Individual researchers will have the power of the work's highest performance digital resources at their disposal."- hor Cyberinfestructure (A Special Report, NSF)		
The NSF Cyderinfrastructure Initiative: Vision and Implementation Towards Learning and Discovery.						
			Cyberinfrastructure is often discussed together with e- Science, which include any science fields share team and networked research approaches.			
			NSF Cyberinfrastructure-TEAM (CI- TEAM) Related URLs			
			Connerts (0)			
		ce Foundation				
rewarded Daniel Alkins for his unique contributions to high-performance computing and distributed			NSF Publications on Cyberinfrastructure and Data Sharing			
	mitworld mit edu Geoscience in Cyderinfrastru	pture				
			100000	Revolutionizing 1 Engineering Thre Cyberinfrastructu Blue-Ribbon Adv Cyberinfrastructu 2003. Also called	sugh re: Report of isory Panel on re , January	
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Colaboration RE I CERTILAR RE				Cyberinthastructu Century Discover		
	HUBzero allows you to create dy that connect a community in scie and educational activities. HUBzer 	rtific research no siles combine		Fostering Learnin Networked World Cyberlearning O Challenge , June	: The portunity and	
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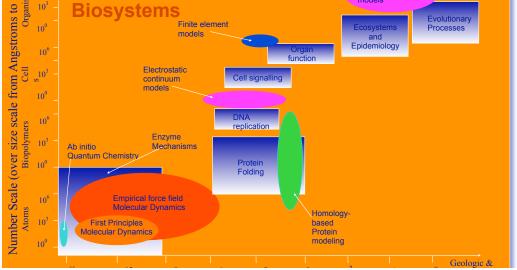
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November 2006

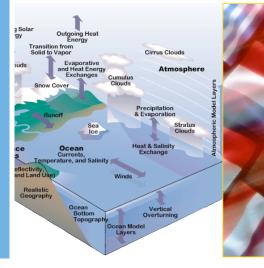
ssing the Power of Dis



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.



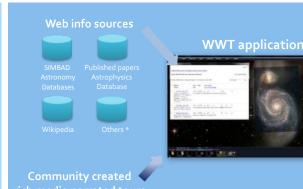
The accompanying requirement for multi-disciplinary, multi-investigator, multi-institutional approach (often international in scope).



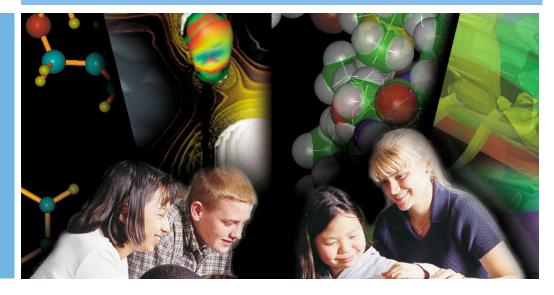
The high data intensity and heterogeneity from simulations, digital instruments, sensor nets, and observatories.



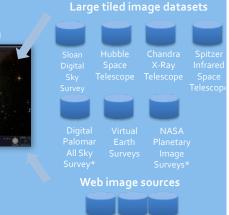
The increased scale and value of data and demand for semantic federation, active curation and long-term preservation of access.



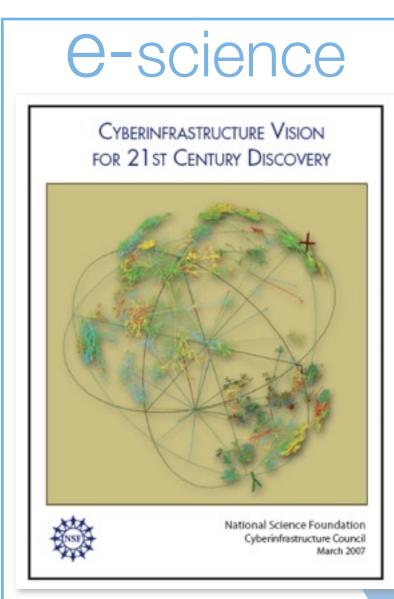
Produced by astronomers, astrophysicists & educators om: Harvard, Space Telescope, Chandra, Spitzer, Adler, NOAO, Hayden, Johns Hopkins, Cal Tech et al.



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



Multiple data sources By object, wavelength, format, etc.needed



Cl-enabled

science

### Community (Virtual) Environments

### High Performance Computing

Data & Visualization/ Interaction

#### Learning & Work Force Needs & Opportunities

Note: Many other reports on discipline-specific visions of and drivers for e-Science are available at <u>www.nsf.gov/oci</u>



### NSF CIF-21: What we Need is a Cyberinfrastructure Ecosystem, not just Components

#### 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

#### Computational Resources

Supercomputers Clouds, Grids, Clusters Visualization Compute services **Data Centers** 

#### Collaboration in Discovery 8 Learning

#### 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

#### Maintainable, sustainable, and extensible

#### **Scientific Instruments**

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

#### Data

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

## **CIF-21 FY 12 Focus Areas**

**Data-Enabled Science**  Community Research Networks New Computational Infrastructure Access and Connections to Cyberinfrastructure Facilities

## **CIF-21 Community Research Networks...**

New cyberinfrastructure tools and changes in the research process have enabled community research networks to address complex, multi-disciplinary problems of societal concern such as competitiveness, security, economic development, and well-being. Community research networks enable people and organizations to perform everyday research functions more effectively by building on and integrating diverse resources, knowledge, and abilities. NSF has a long history of investing in community research networks such as the iPlant collaborative, the Southern California Earthquake Center, the SRS Data Enclave, and the nanoHUB. Cyberinfrastructure links these combinations of people, organizations, instrumentation, physical facilities, computers, data, and software, but few scientists know how to select and assemble these components into a functioning community research network. Focused investments in socio-technical analyses advance understanding of how to develop virtual organizations, and under what conditions they can foster innovation in science, engineering and education. Such investments are necessary to harness the full potential and promise offered by virtual organizations.

## **Celebrating Hubzero**

In contrast to early collaboratory projects such as UARC that were "hard-wired" for particular project, Hubzero is a platform -- a meta collaboratory -- that can be tailored to many different domain specific projects. For example:



HUBzero is having international impact on science and engineering research and learning.

ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

D. E. Atkins • atkins@umich.edu

 HUBzero through a web-based portal reduces the barrier of entry to the use of high-performance computing for modeling, simulation, and prediction. It also draws upon multiple resources, both local and remote including the TeraGrid.

 HUBzero is intentionally designed to support both research and education.

 HUBzero encourages openness in sharing codes, courseware, and data (?).

HUBzero has done better than most in financial sustainability.

## **Knowledge Communities CI Model**

The key figure of merit for the application of IT in research, learning and practice should be the extent to which it enhances the effectiveness of knowledge communities engaged in learning, discovery, and practice.

Developments in CI-enabled science now point the way to creating and nurturing cyberinfrastructure to enable groups to work together in functionally-complete, four-quadrant organizations.

 The overarching goal is "high performance collaboration" not just high performance computing.



#### Learning Research

#### **CI-enabled, All Quadrant Knowledge Communities**

#### **Professional Practice**

#### Learning to Learning

#### Four Quadrant Organizations (virtual organizations) offer additional modes of interaction between People, Information, and Facilities Time Different Same (synchronous) (asynchronous) Physical + Virtual, **ST-SP DT-SP** Same **P**: Physical mtgs **P**: Shared Not Physical vs. Virtual Geographic Place I: Print-on-paper notebook books, journals I: Library reserves F: Physical labs, **F**: Time-shared studios, shops physical labs, ...

**ST-DP P**: AV conference I: Web search F: Online instruments

Different

**DT-DP P**: Email I: Knowbots F: Autonomous observatories

**P**: People I: Information **F**: Facilities, instruments

## **Some Attributes of 4-Quadrant Communities**

- These all quadrant organizations are not just conversing about people and doing work, they are also sharing objects to observe, manipulate, and discuss. They therefore can incorporate **both** explicit and tacit knowledge creation and transfer.
- Conversations themselves (the collaborative sessions) can be captured and used later as an object of conversation and reflection.
- Enables engagement in open learning, exploration, and knowledge creation and to shift more from an authority-based learning model to a discovery-based learning model.
- This model does not make a sharp distinction between learning, teaching, discovery, research, and practice. These are activities all supported in blended ways within the knowledge communities model.

## Game Changers

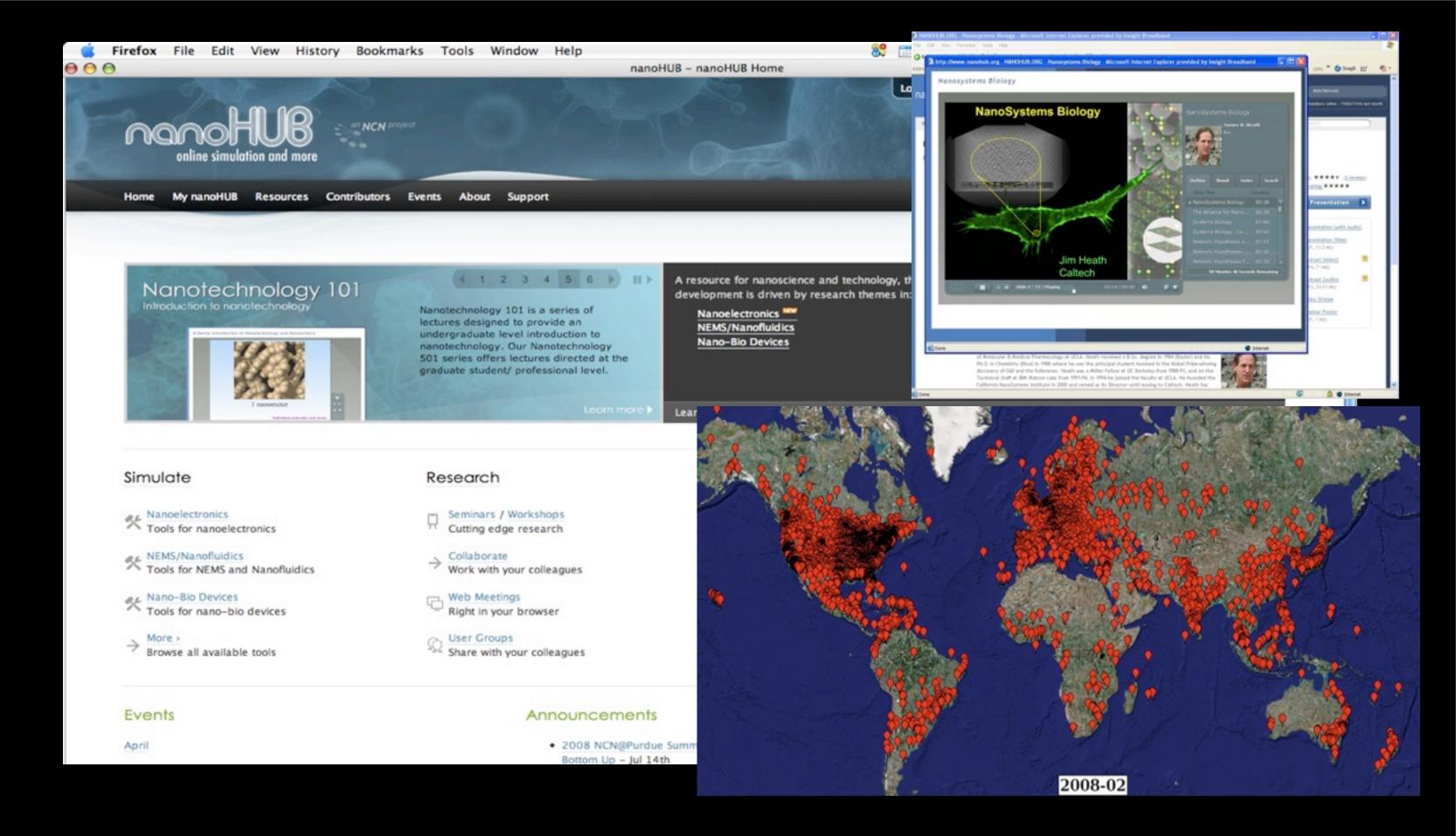
- Game-changing possibilities for "better than being there" organizational forms:
  - decreased time to discovery;
  - decreased time *from* discovery;
  - increased intellectual cross-section and transformational results;
  - enhanced stewardship and return on investment for research infrastructure investments;
  - multi-use: discovery, learning, rapid-response, ....
- A key to economic leadership in a global knowledge-based flat world.

#### BEYOND BEING THERE:

UEPRINT FOR ADVANCING THE DESIGN, DEVELOPMENT AND EVALUATION OF VIRTUAL DREANIZATIONS

FINAL REPORT FROM WORKSHOPS ON BULLOW





Monday, April 4, 2011

## **Suggestions & Questions for HUBzero Future**

- Conceptualize HUBzero as supporting all-quadrant collaboratories with a goal to become functionally complete.
- Data-intensive scientific discovery is becoming more prominent is what some call a Fourth Paradigm for Science. What does HUBzero need to do to support this?
- View your core competency as that of enabling others to create collaboratories efficiently and effectively and the community you have builta s aprimary asset, rather than thinking of yourselves more narrowly as the creators and stewards of a particular set of software.

• Many universities are moving to cloud-based collaboration environments now offered by Google and emerging from Microsoft. With this and the previous point in mind, can HUBzero find ways to link with and leverage the Google Apps environment?

The Sakai Foundation is now embarked on creating an open source platform called Sakai 3 that will be a platform for an Open Academic Environments that are built to provide functions need in the university but not as a monolithic system but rather as one that leverages cloudbased services available from others. Might HUBzero be part of this? Be more intentional about the positive impact of HUBzero on STEM education, especially on blended forms of formal and informal learning. Explore, for example, how HUBzero can contribute to visions and directions articulated in the new National Education Technology Policy, the NSF report on Cyberlearning, and the MacArthur Foundation initiatives on Connected Learning.

 Work with the Creative Commons, now with new leadership, to promote appropriate open licensing for codes, data, and scholarly communications. • What is your plan to provide long-term access to (preservation of) all of the the digital objects in your Hubs? This is important for many reasons, perhaps most profoundly to preserve the reproducibility of research results so fundamental to science.

What are metrics of impact of HUBzero built environments and can you establish more data gathering and research to explore these metrics? Could you demonstrate quantitative payoff from investments in the Hubs.

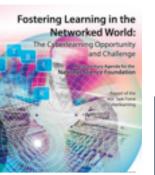


#### e-Humanities & Arts



Science for Development





#### e-Learning



#### e-Development

Monday, April 4, 2011

#### The Research University in the Digital Age

rmation Technology Id the Future of the Research University

PREPARING FOR THE

VATIONAL RESEARCH COUNCIL

## **Questions & Discussion**

Monday, April 4, 2011