

Multi-scale Atmospheric Modeling in a Cyberinfrastructure Era

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Outline

- MMF Requirements
 - Computation
 - Data
 - Networking
- Cyberinfrastructure Implications

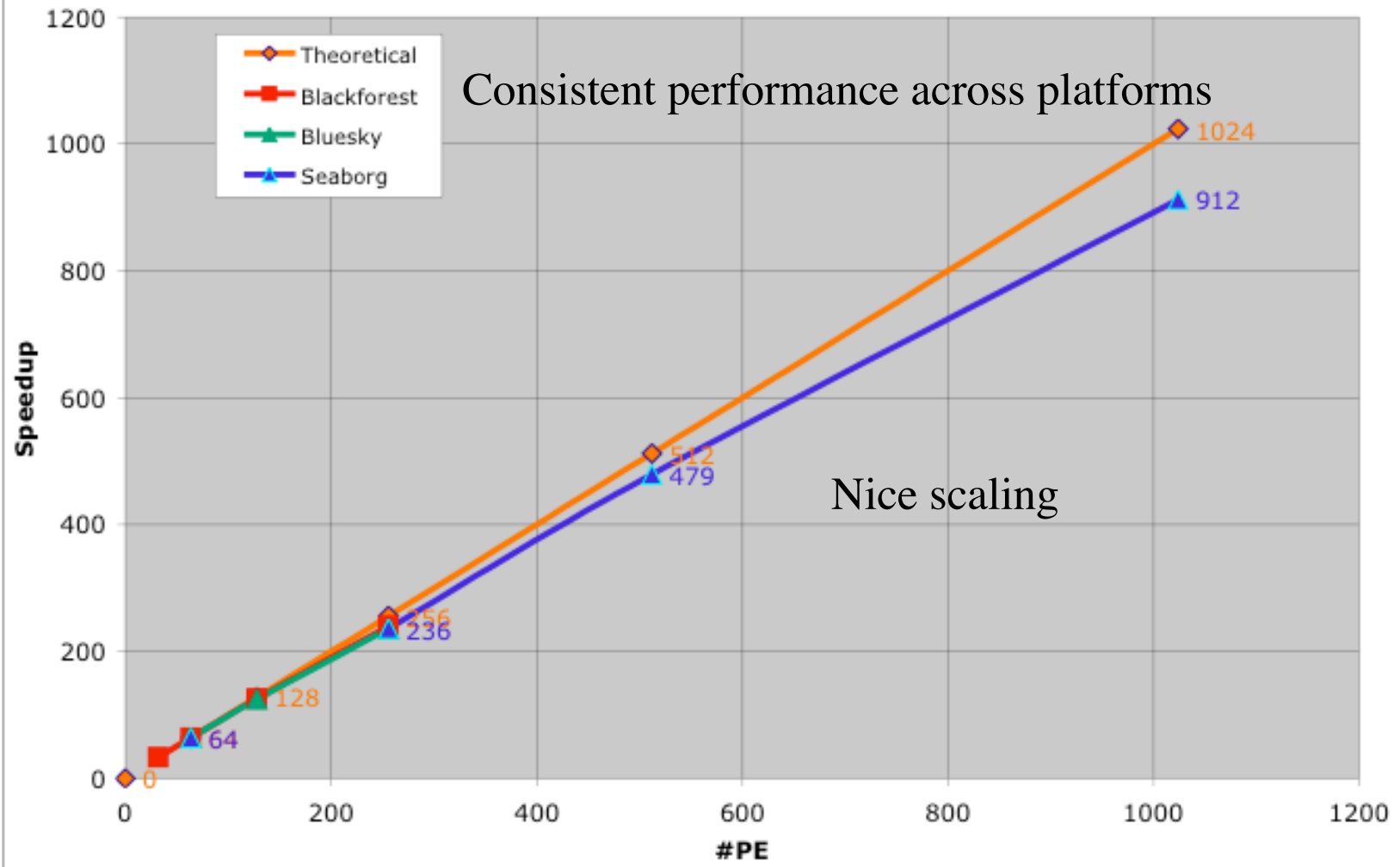
MMF Computational Requirements

	Year(s)				
	2001	2002	2003	2005-06	2009-10
Simulated Duration (years)	1	1	See Plot For Current Results	100s	1000s
Performance (wall-clock days per simulated year)	20	1.5		Configuration dependent	
Number of Processors	64	512			

MMF Computational Requirements (cont.)

- Extrapolating from today's technology
 - 100 simulated years on NCAR's Bluesky today
 - 150 days on 512 PE (of 1216 PE available)
 - 24/7 availability, no errors, no restarts, no problems
- Things are a bit better with some new results ...

Speedup for various computers



MMF Computational Requirements (cont.)

- Still requires better-than-linear scaling
 - 2 runs per year at that rate but we also need
 - developmental versus production runs (ratio?)
 - ensembles (i. e., N)
 - intermediate-scale development and testing
 - Cannot commit an arbitrary number of processors sufficiently often using existing (or near) resources and approaches

Cyberinfrastructure implications

- distributed experiments (i.e., \mathbb{N})
- centralized vs distributed?
- distribution of software and data
- aggregation of results

\parallel^N : Higher-order Parallelism

- Grid computing
 - Divide and conquer (old standby)
 - Maybe it's still the answer but does it scale?
 - Staging
 - Queuing
 - Synchronization
 - Many system engineering challenges
 - Data management
 - Network capacity
 - Configuration management
- How do you address the human and organizational aspects?



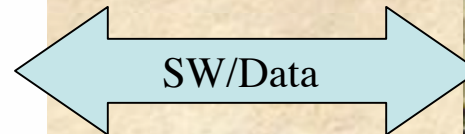
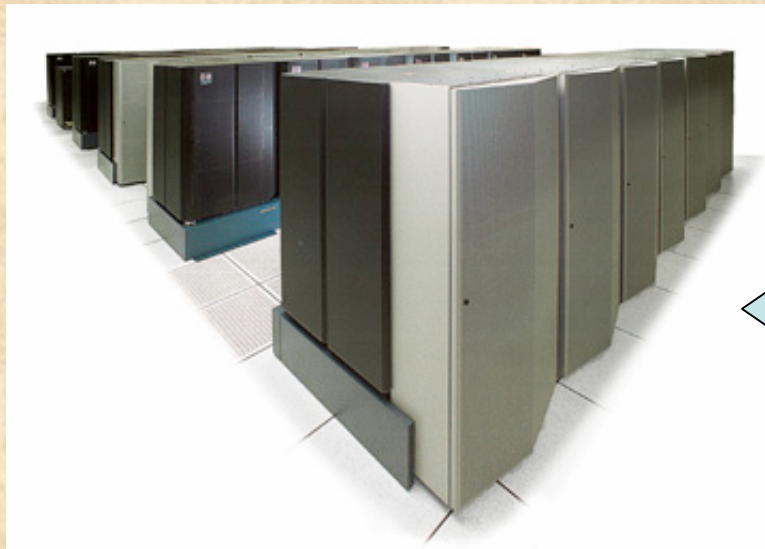
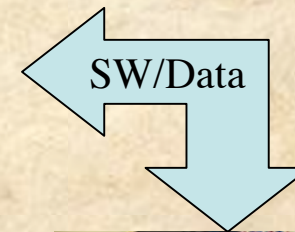
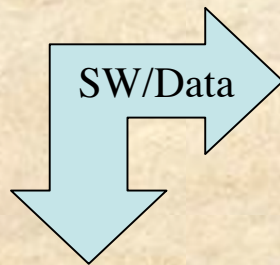
Cyberinfrastructure Implications

- What's the Right Mix?

Workstation



- How should they be connected?



7/19/2003 Mainframes?

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Clusters? 9

New SDSC Resources

- DataStar
 - 128 x 8 Power4, 1.5GHz, 16GB processors (01/2004)
 - 10 x 32 Power4, 1.7GHz, 128/256GB processors (now)
- Teragrid/Itanium
 - Cluster of 256 x 2, Madison 1.5GHz, 4GB processors
 - Cluster of 128 x 2, Madison 1.3GHz, 4GB processors
 - Both in house (operational 01/2004)
- Parallel File Systems
 - 5GBps (sustained)
 - 10GBps (peak)
 - To both of these machines

New SDSC Resources

- Fast Storage
 - 600 TB SAN (backbone)
 - Fiber channels to every node of both machines
 - And to Teragrid network (viz, external network)
- Tape Subsystem
 - ~2PB fast tape
 - ~2GBps transfer rate
 - Automatic migration from disk to tape according to disk quota management (and back)
 - Long-time parking of output data for post-processing
- Network
 - Phase 1: 40Gbps (to NCSA, lower to Argonne, CalTech)
 - Phase 2: 6 other institutions

Lessons-learned from Collaborative Code Development?

- Joint experiments with community codes require inter-organizational and interdisciplinary collaboration
 - Scientists knowing the physics and phenomena
 - Programmers with architectural expertise and comprehension of the domain language
 - Sympathetic system administrators
 - Principal Investigators who are good managers

Regional Spectral Model

Example

- Joint code development and experiments
 - SDSC
 - Scripps Institution of Oceanography Climate Research Division
 - NOAA National Center for Environmental Prediction
- Goals
 - 10-12 km resolution of atmospheric processes (esp. ppt)
 - distributed access to common resources for joint experiments
 - preparing code to run on the Earth Simulator

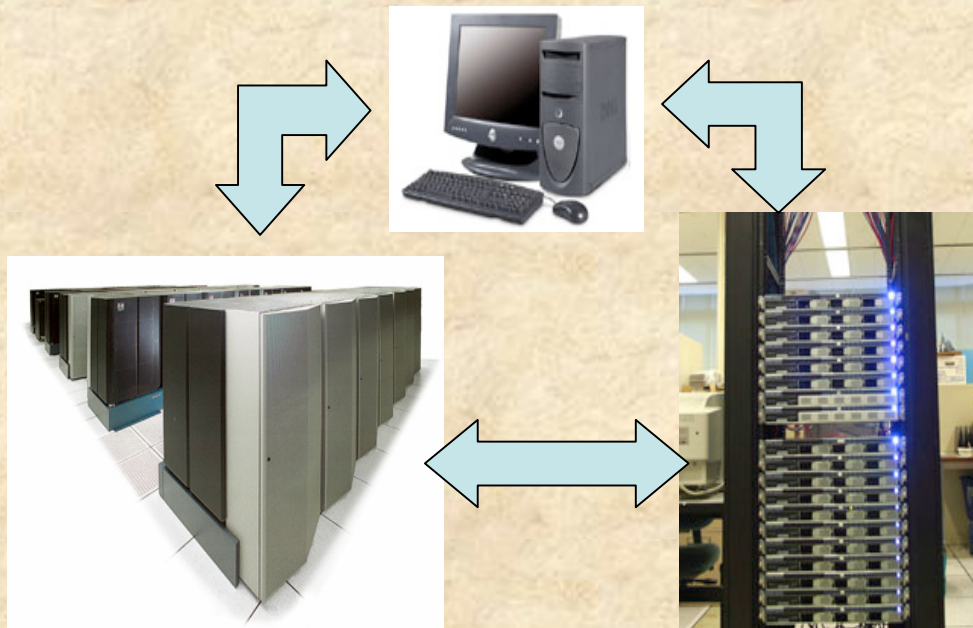
Regional Spectral Model (cont.)

- New community code resource
 - Supported platforms (i.e., build environments)
 - Power 3 / Power 4
 - Intel Architecture 32 / 64 (clusters)
 - SX-6 (Earth Simulator)
- Configuration management
 - Open source development model
 - Multiple developers (NOAA, SIO, SDSC)
 - Train domain-scientists in these techniques
 - Code changes versus CVS baseline
 - Test suites executed before ‘commit-to-baseline’

Biggest Issue (for now)

- Race between ‘stable baseline’ and new physics (i.e., new code)
 - Multiple platforms
 - Multiple build environments
 - Multi-processor (small n) testing
 - Multi-processor (big N) production
- Keeping a community code relevant
 - There will always be a lag
 - How much is too much?

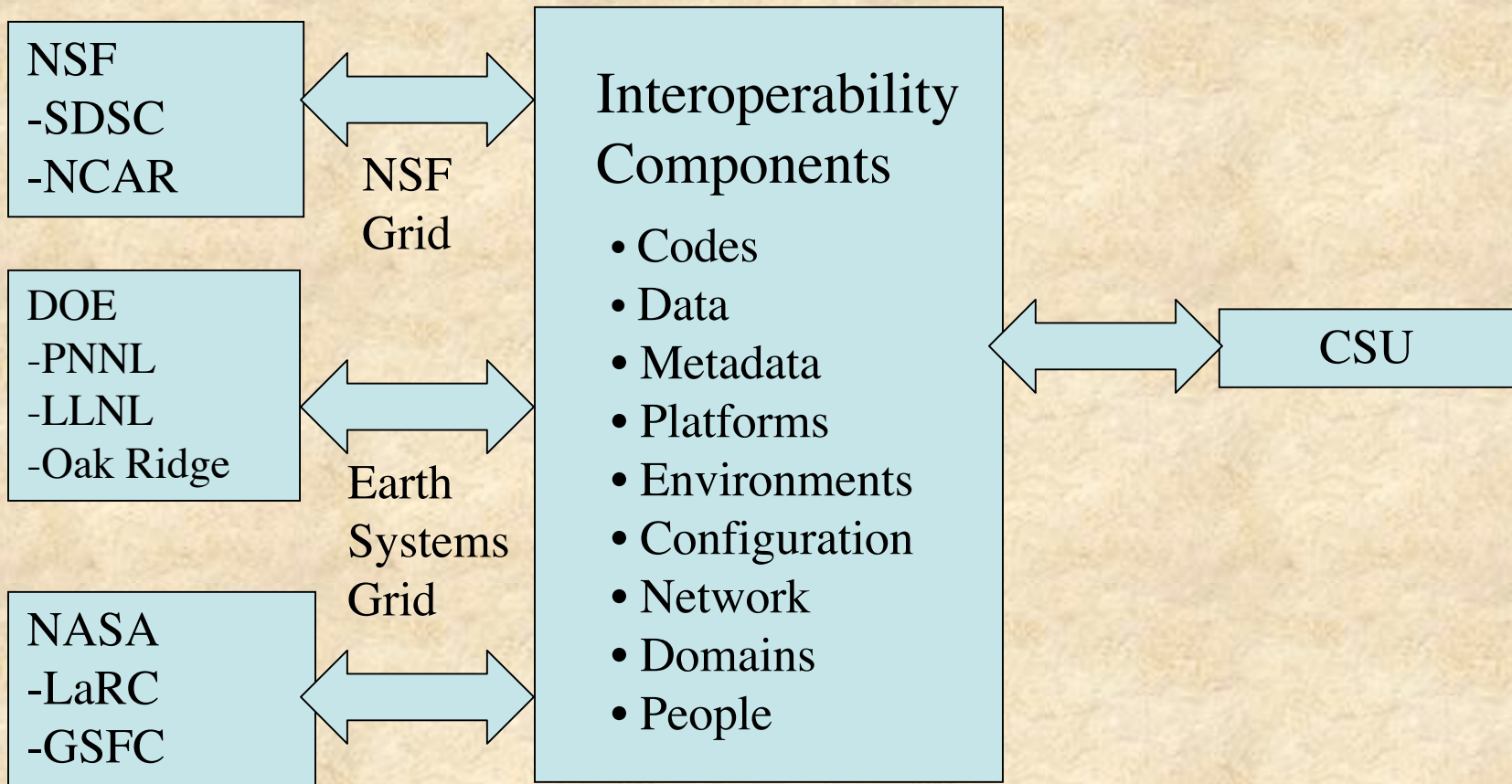
Cyberinfrastructure Implications



‘Intangible’ Tradeoffs

- Interoperability
- Logistics

Cyberinfrastructure for MMF

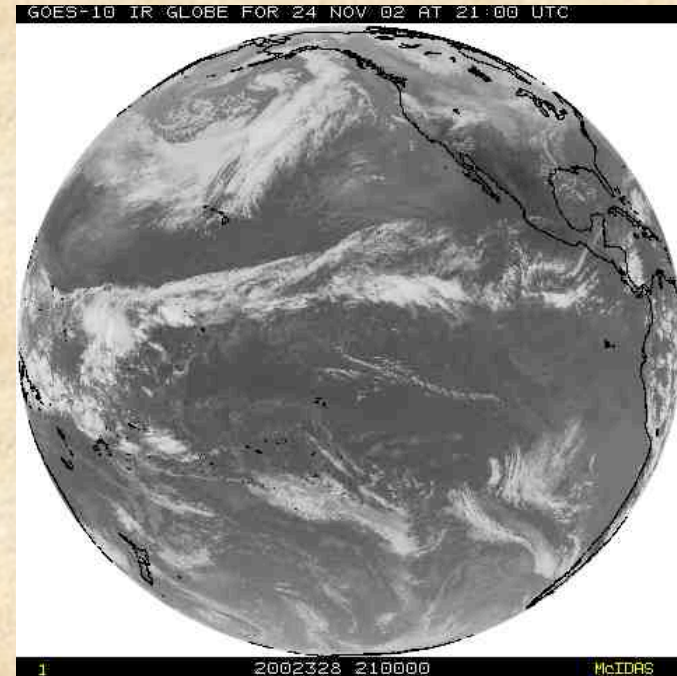
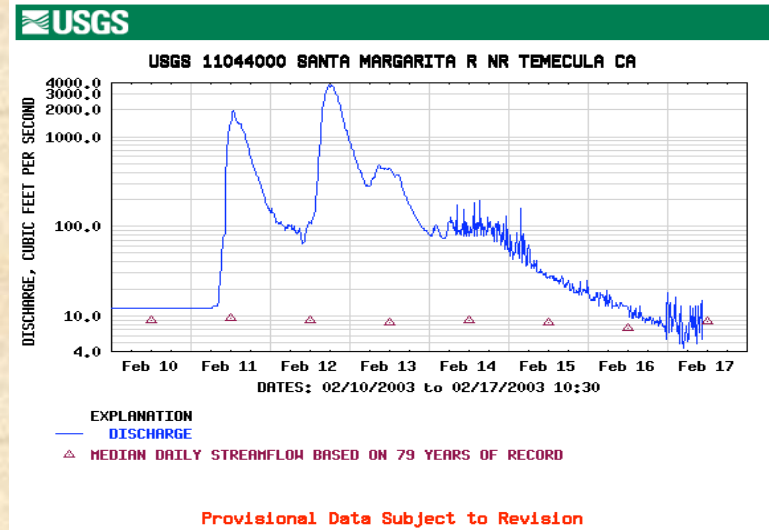
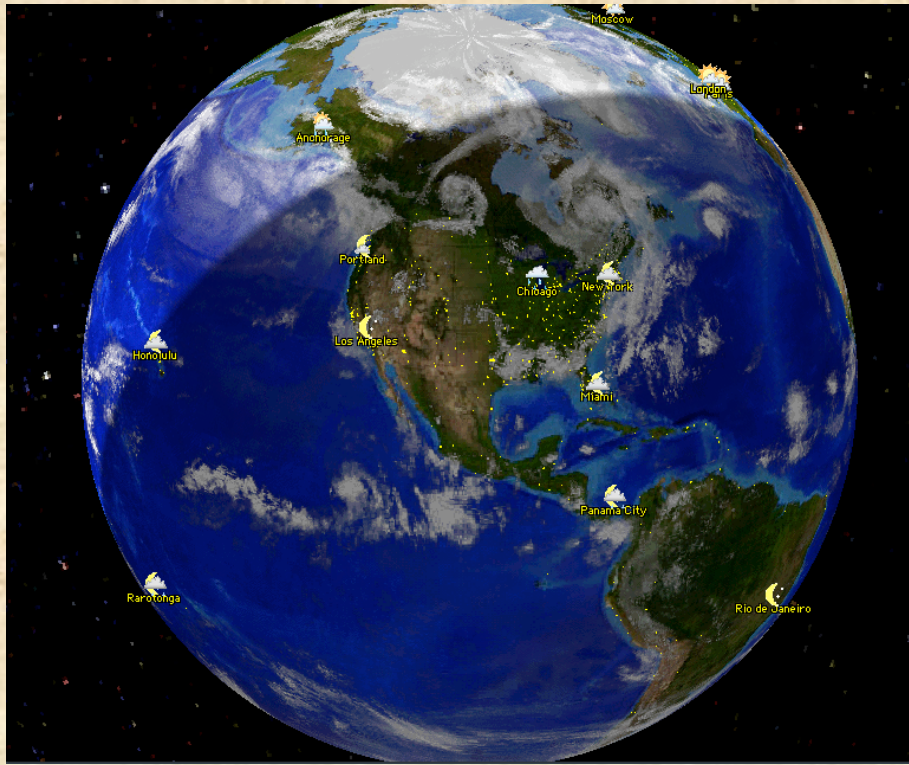


Cyberinfrastructure Implications

- Wide range of resource requirements
 - Development vs. production
 - Painless migration between them
 - Empirical data
 - verification and
 - validation
- Convenient access to resources for ‘many’ users
 - Dedicated resources or small queuing delays
 - Interactive atmosphere of trust and tradition
- High bandwidth, convenient, collegial interaction

Cyberinfrastructure Implications (cont.)

- Better-than-linear scaling requires organizational parallelism as well as architectural parallelism
 - A higher-degree of standardization is required as the number of participants grows
 - Configuration management becomes a critical, joint, cooperative activity



Data Loading

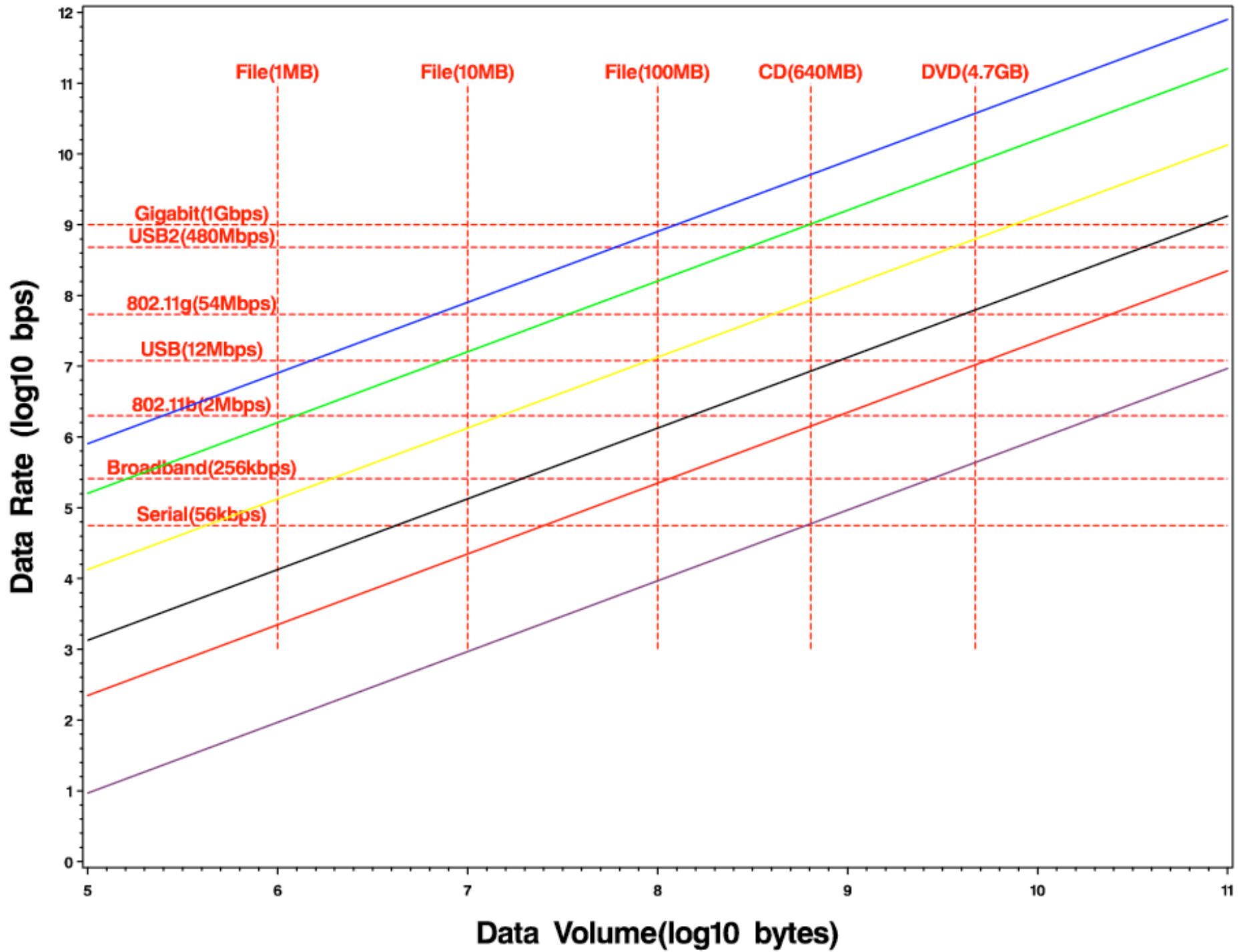
Staging, Execution, Analysis

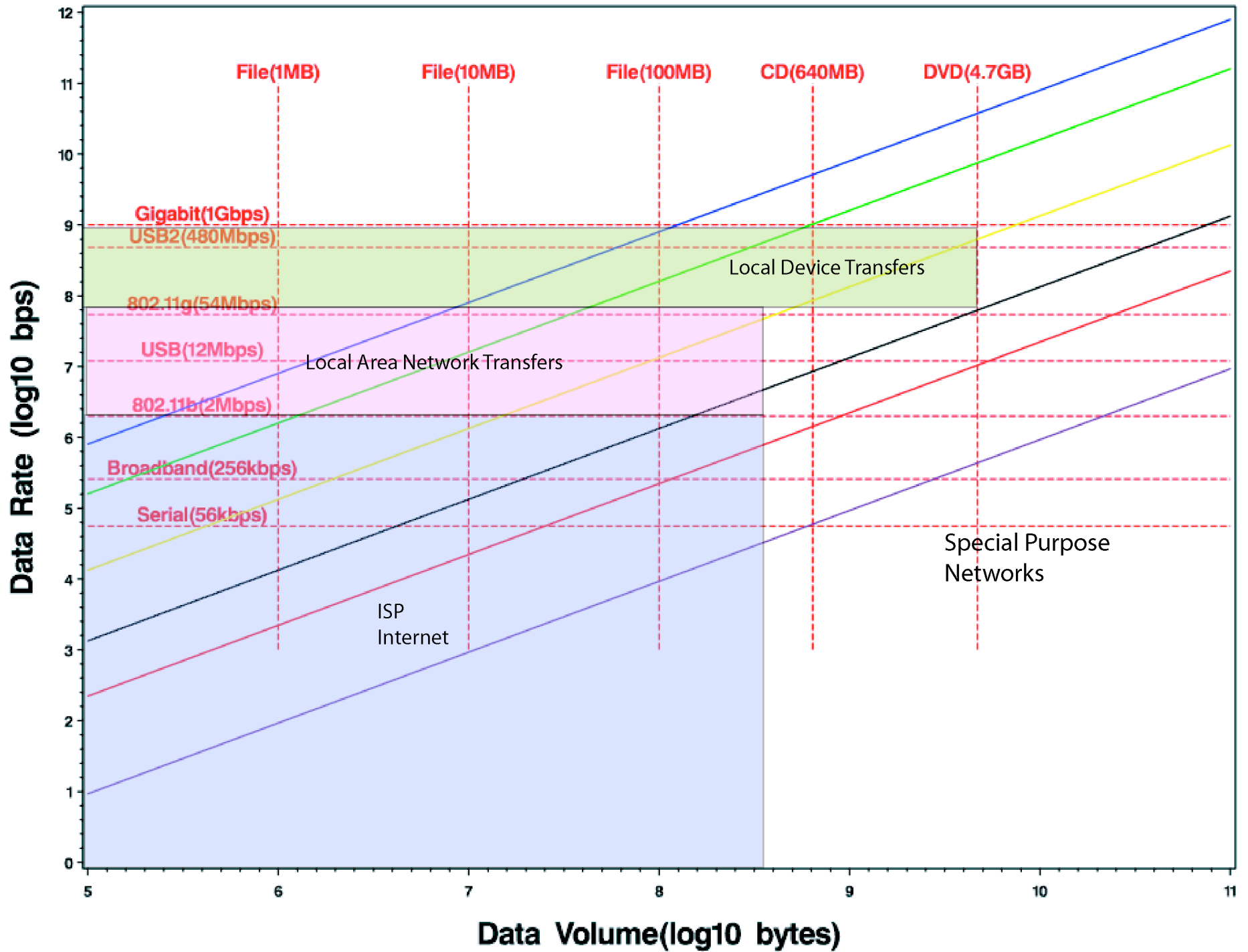
- Staging (outbound)
 - Initialization : 0.1 Gbytes to each cluster then disseminated to each node
- Execution (held locally)
 - Data assimilation : 0.2 GBytes x nodes/cluster x clusters
 - Model output: Cloud Resolving Model @ 8192 grid cells
 - 1 year x (5 space-time, 6 prognostic, 10 diagnostic variables)
 - 10 Terabytes roughly per cluster (say 256 nodes)
- Analysis (inbound)
 - 10 Terabytes/run x number of clusters

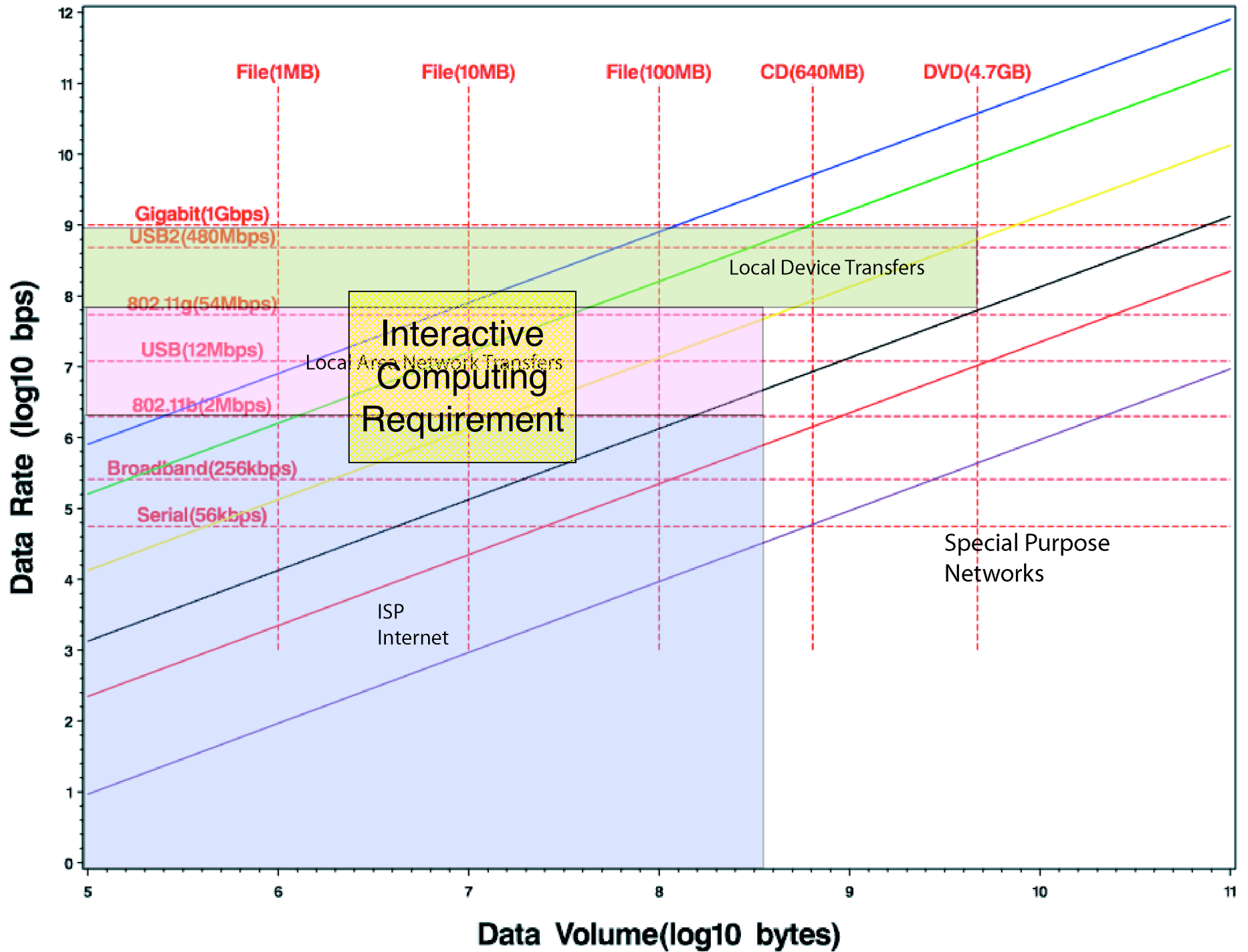
Cyberinfrastructure Implications

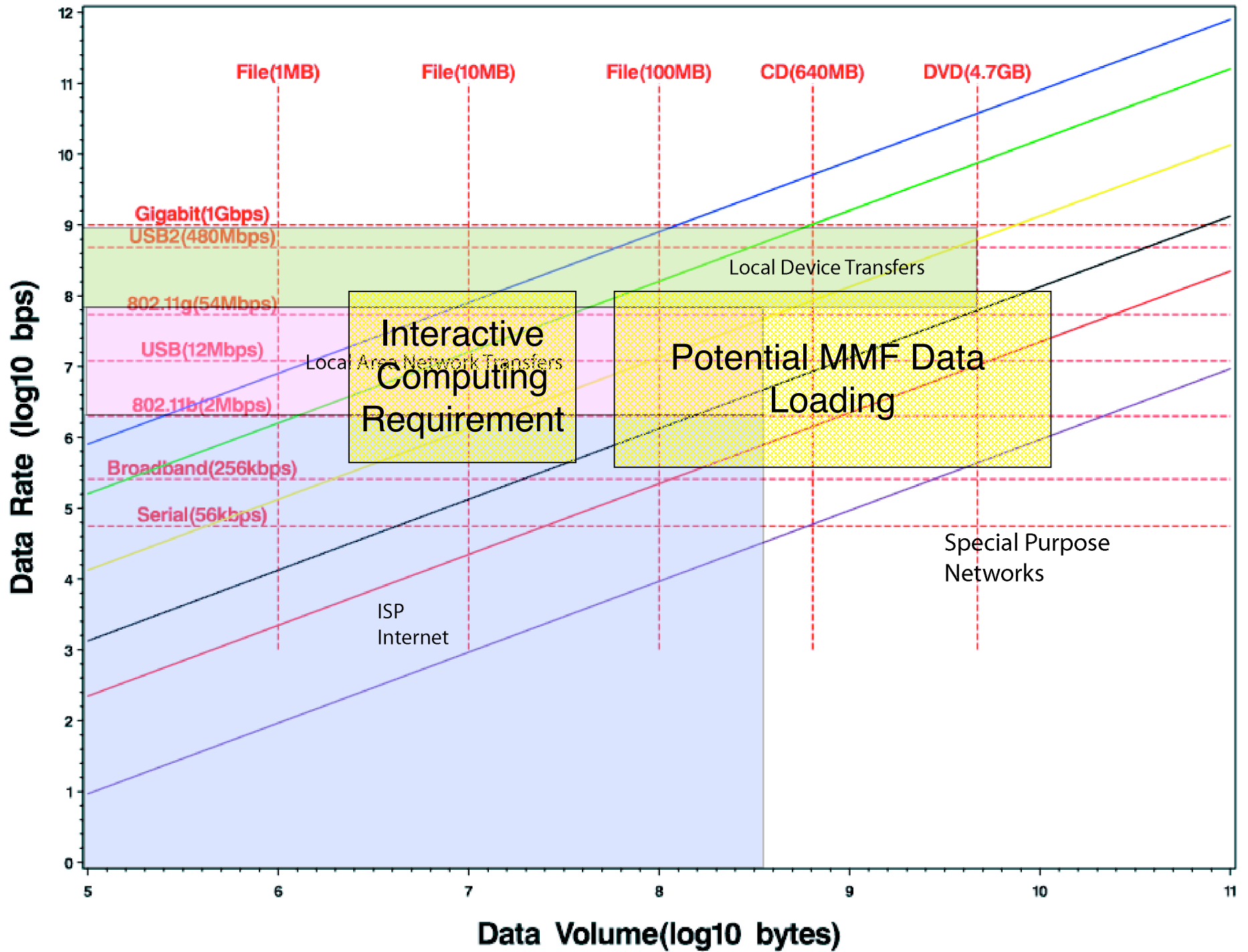
- Reality check
 - This implies that big fractions of a petabyte must be moved per run
 - Potentially 10's of petabytes per experiment (i.e., ensembles)
 - Analysis, Re-analysis
 - Archival
- Maybe not, but there's a catch to move less
 - Some form of data extraction on a space-time basis must otherwise exist everywhere

Network Requirements



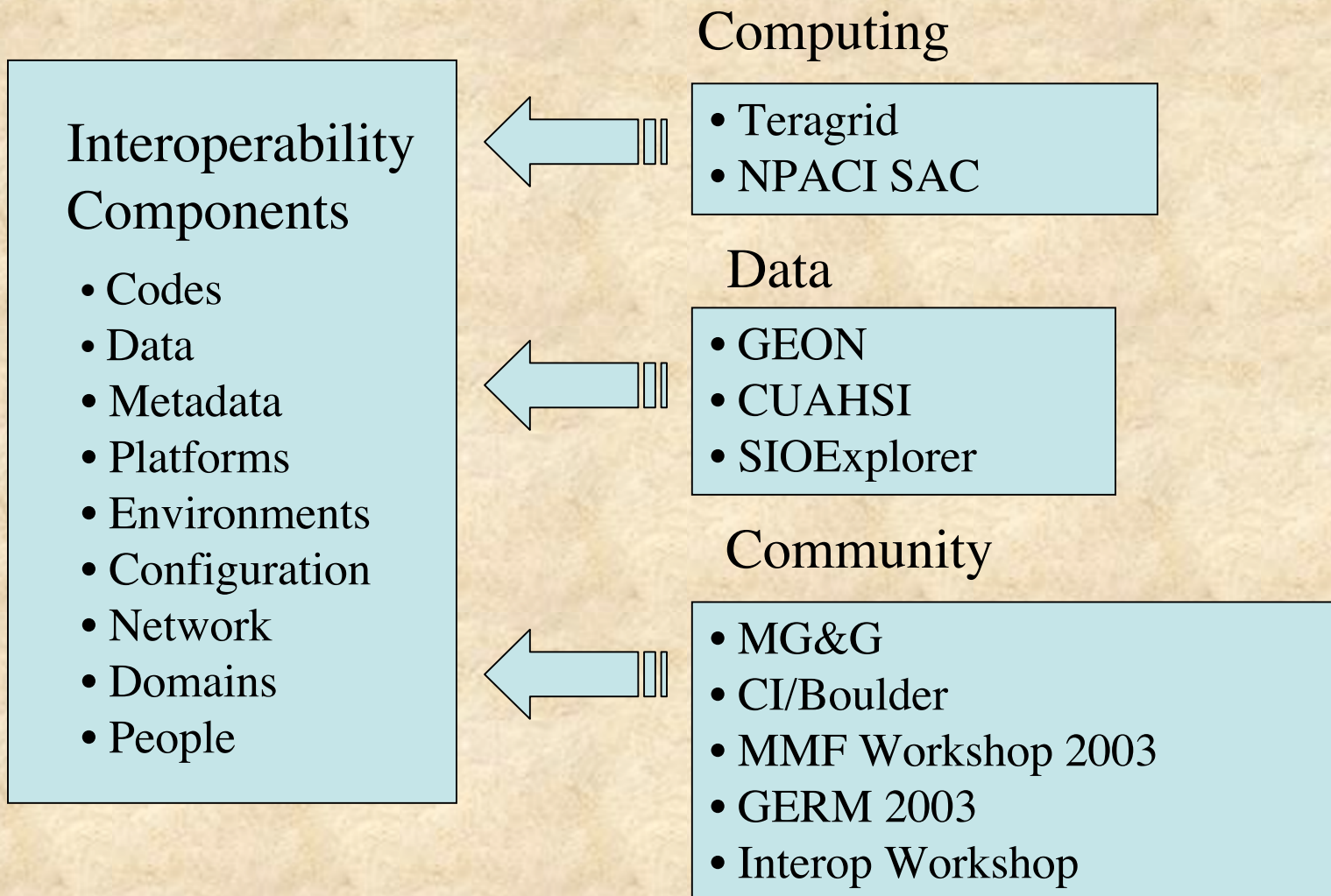






How are we preparing for the Cyberinfrastructure Era?

Road to Cyberinfrastructure



MMF NPACI SAC

- NPACI Strategic Application Collaboration (SAC) with CSU
 - Porting to Blue Horizon and Teragrid environments
 - Provide performance data for MMF scaling in Grid environment
 - Infrastructure requirements for distributed, collaborative code development
- Establishing
 - joint working relationships
 - data management environment
 - RDTE procedures

NSF Technology Pathfinders

Apply for an NPACI Strategic Collaboration (SAC)

Volume 7, Issue 1

Calendar - Search

Apply for an NPACI Strategic Collaboration (SAC)

Responses due January 31

NPACI NPACI is pleased to announce the opportunities Applications Collaboration (SAC) program. First to enable or significantly enhance research through from six to twelve months between scientists at on the development of new capabilities to collaborate with N on the development of new capabilities to solve scientific problems, with emphasis significant storage, computation, and visualization resources.

These collaborations would include: participation in regular meetings and perhaps contributions to journal publications. In return, research groups would benefit from with performance improvement and algorithmic development, that builds upon the capabilities of present and projected hardware and software. In particular, a strong which can exploit the new opportunities enabled by the TeraGrid. For more info www.teragrid.org/about.html.

Internet zone

NPACI and the Alliance to build the TeraGrid

Address: http://www.npaci.edu/teragrid/

NPACI

Building the TERAGRID

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NCSA, SDSC, Argonne, and Caltech to build world's most powerful computational infrastructure

The National Science Foundation (NSF) has awarded \$53 million to four U.S. research institutions to build and deploy a distributed terascale facility (DTF). The DTF will be the largest, most comprehensive infrastructure ever deployed for scientific research—with more than 13.6 teraflops (trillions of calculations) capable of modeling a trillion of molecules.

The four research National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign, the National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign, the National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign, and the National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign.

NPACI
SDSC

EarthRef.org

Address: http://earthref.org/

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Geochemical Earth Reference Model

Chemical characterization of the Earth, its major reservoirs and the fluxes between them

GERM

Goldschmidt Conference
 GERM and MARGINS Pressure (HP) to Ultra-High Pressure (UHP) Cycling in Convergent Plate Boundaries

Metadata Proposal Geochemistry
 GERM Workshop Lyon 2003
 Data Sharing in Earth Sciences
 What's New

http://humw.whoi.edu/DBMWorkshop

Address: http://humw.whoi.edu/DBMWorkshop/

Marine Geology & Geophysics Database Management Workshop, May 14-1

Sponsored by The National Science Foundation and The Office of

National Science Digital Library

Address: http://nsdl.org/reader/user/Login/RootNode.jsp

NSDL Educational resources for science, technology, engineering and mathematics. Funded by the National Science Foundation.

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New in the Library

Analytical Sciences DL

The ASDL is an electronic library that collects, catalogs and links web-based information or discovery material (URLs) pertinent to innovations in curricular development and supporting resources in the analytical sciences.

SAMPLES FROM THE COLLECTION:
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 Sample Item 2 from ASDL
 Mathematics Preprint Server
 Networked Comp. Science Tech. Ref. Lib.
 Geotech. Rock & Water DL
 Math Forum
 SciCentral - Southwest SciCentral Search

Organizing Committee

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- [Final Workshop Report \(2.9 Mgbtve pdf file\)](#)
- [Final Workshop Report \(7.3 Mgbtve pdf file\)](#)
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- [Go to Workshop Presentations](#)

Purpose:

The purpose of this workshop was to develop a coordinated data management strategy for digital geoscience data sets.

GEON: The Geosciences Network



Two testbeds
Broad range of geoscience data sets

- IT: SDSC, Penn State, San Diego State University
- Geosciences: Arizona State University, Bryn Mawr College, Cornell University, Rice University, UNAVCO, University of Arizona, University of Idaho, University of Missouri, University of Texas El Paso, University of Utah, Virginia Tech
- Education and Outreach: DLESE, Cornell, UNAVCO
- Agency Partner: USGS

GEON THE GEOSCIENCES NETWORK

http://www.cuahsi.org/

Address: http://www.cuahsi.org/

CUAHSI
 Consortium of Universities for the Advancement of Hydrologic Science, Inc.

Mission

To foster advancements in the hydrologic sciences, in the broadest sense of that term, by:

- Developing, prioritizing and disseminating a broad-based research and education agenda for the hydrologic sciences derived from a continuous process that engages both research and applications professionals;
- Identifying the resources needed to advance this agenda and facilitating the acquisition of these resources for use by the hydrologic sciences community; and
- Enhancing the visibility, appreciation, understanding and utility of hydrologic science through programs of education, outreach, and technology transfer

Announcements

- The EAO committee is soliciting the membership on future activities.
- The agenda of the Membership Conference call June 3, 2003 is summarized in a [press release presentation](#).
- CUAHSI is advertising for a [hydrologic scientist](#) in Washington DC.
- A [posting](#) to discuss the Synthesis Center will be held July 10-12 in Santa Barbara, CA. RSVP by June 29.

SIOExplorer - Home

Address: http://sioexplorer.org/

SIOExplorer - Home

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Cyberinfrastructure is Not Just 'Bits and Boxes'

- Human infrastructure
 - People
 - Interdisciplinary, multi-lingual, multi-cultural
- Broad-base of expertise
 - Across institutions
 - Across disciplines
 - Across systems
- Leveraging existing investments provides foundation for future CI

Summary

- MMF is a well-behaved, challenging computational task
 - New physics and phenomena at better resolution
 - Existing code scales well and performs consistently
 - Climate-scale, distributed experiments pose exciting cyberinfrastructure challenges
 - We are learning today to handle these challenges
- MMF provides an outstanding application at the right stage of code development (i.e., early)

Backup

Network Requirements

- Collaborative, interdisciplinary research requires joint access to common information and resources
 - Data includes empirical and derived data and model results
 - Analysis tools
 - RDTE environment
 - Research, Development, Testing and Evaluation
 - Compilers, hardware, build-environments
 - Especially important in a transient user/developer population (i.e., academia) due to spin-up time
- Standard trade-off between computing and communications
 - ‘Compute it there, transfer it here’
 - Cycles vs. bandwidth

Definitions of Interoperability

- IEEE
 - Ability of two or more systems or components to
 - exchange information and to
 - use the information that has been exchanged
- ISO
 - Attributes of software that bear on its ability to interact with specified systems