Science Gateways on the TeraGrid

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Outline

- Brief introduction to the TeraGrid
- Making the TeraGrid useful for Science Gateway communities

The TeraGrid

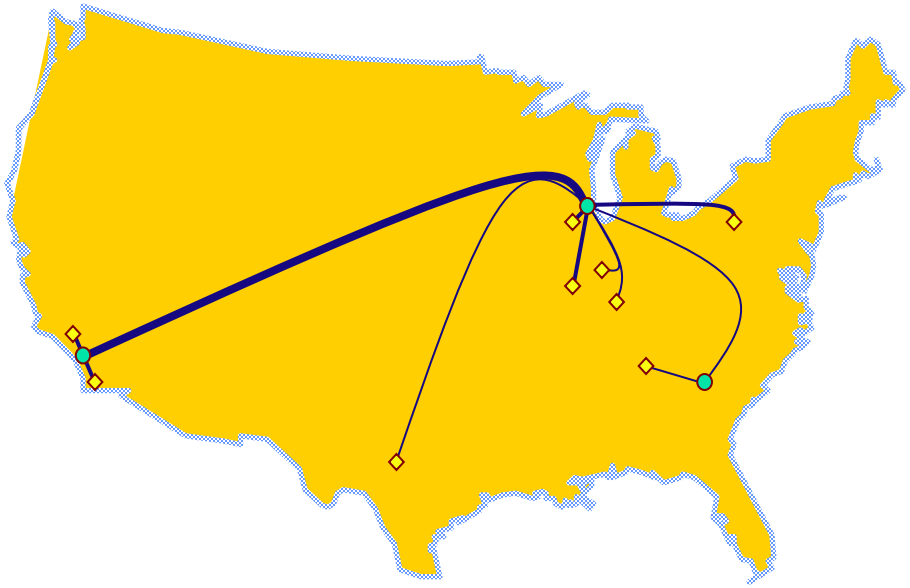
- A major paradigm shift for HPC resource providers
- Make NSF resources useful to a wider community

- *Strength through diversity!*

The TeraGrid Strategy

- Building a distributed system of unprecedented scale
  - 40+ teraflops compute
  - 1+ petabyte storage
  - 10-40Gb/s networking
- Creating a unified user environment across heterogeneous resources
  - Single user support resources.
  - Single authentication point
  - Common software functionality
  - Common job management infrastructure
  - Globally-accessible data storage

- **Create a *unified* national HPC infrastructure that is both *heterogeneous* and *extensible***



"Grid-Like" Usage Scenarios *Currently Enabled by the TeraGrid*

TeraGrid is in its infancy!

- "Traditional" massively parallel jobs
  - Tightly-coupled interprocessor communication
  - storing vast amounts of data remotely
  - remote visualization
- Thousands of independent jobs
  - Automatically scheduled amongst many TeraGrid machines
  - Use data from a distributed data collection
- Multi-site parallel jobs
  - Compute upon many TeraGrid sites simultaneously

Science Gateways
A new initiative for the TeraGrid

- Science communities increasingly building their own cyberinfrastructure: "Science Gateways".
  - Provides an easy-to-use solution for community computational needs.
  - Both software and hardware
- Science Gateways will
  - increase overall science throughput by making computers easier to use for knowledge discovery.

Science Gateways
A new initiative for the TeraGrid

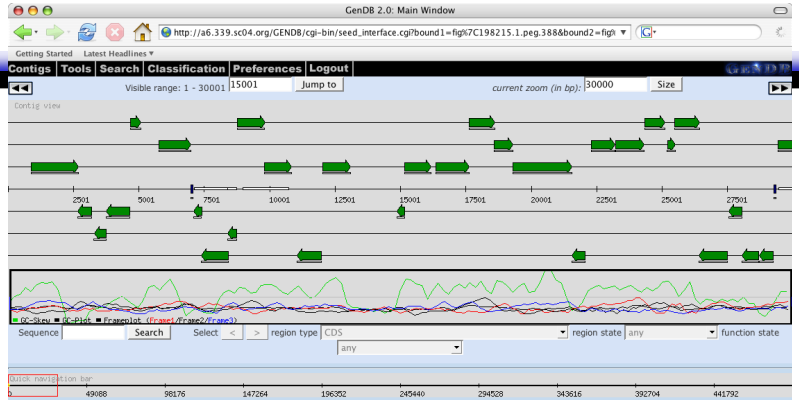
- But many will often have computing needs that far exceed their own capacity.
- The **TeraGrid** can provide massive computing resources to these communities on demand.
- Science Gateways can use the TeraGrid to
  - provide community-tailored access to massive compute resources at no additional cost
- Goals:
  - *Integration* and *interoperability.*

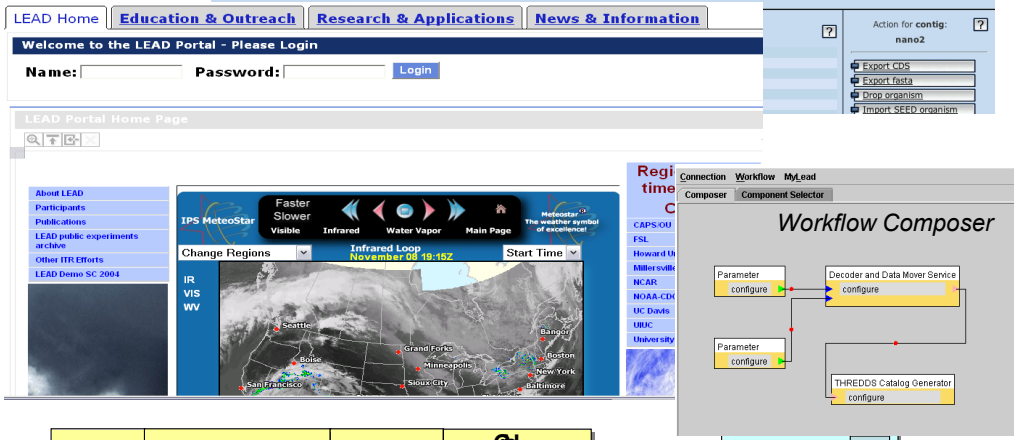
Three Types of Science Gateways

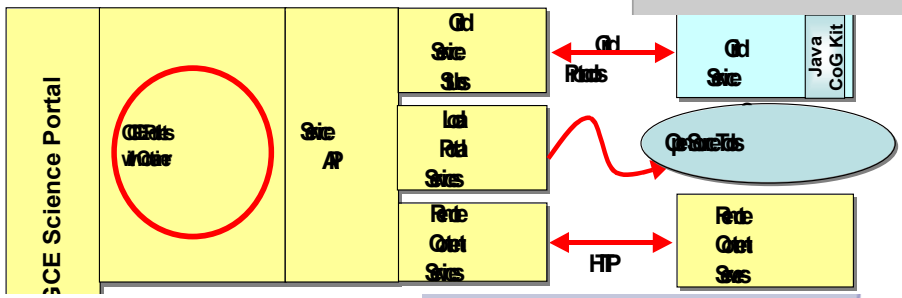
- Web-based Portals
  - User interacts with community-deployed web interface.
  - Runs community-deployed codes
  - Service requests forwarded to TeraGrid resources
- Bridges to Community Grids
  - Jobs forwarded seamlessly between science community grids and TeraGrid
- Service Gateways
  - Application programs running on users' machines but access services in TeraGrid (and elsewhere)

Types of Gateways: *Web-Based Portal*

- A portal is a gateway to a set of distributed services accessible from a Web browser or desktop tools
- Example: GEON
- Provides single point of access to:
  - Grid authentication
  - Community-deployed data
  - Community-deployed services (e.g. Synseis)
- Seamlessly forwards service requests (and data?) to TeraGrid resources







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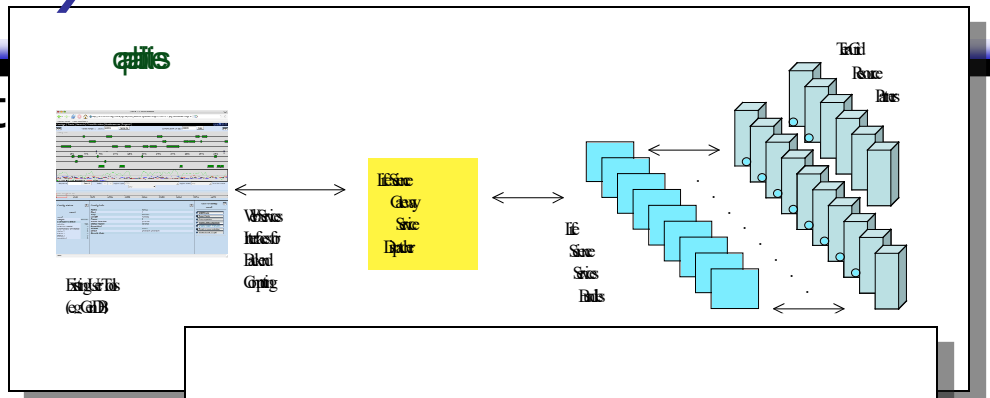
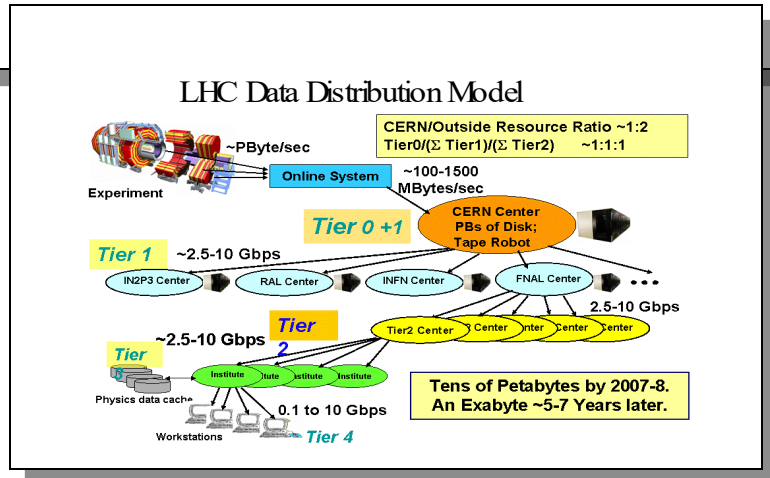
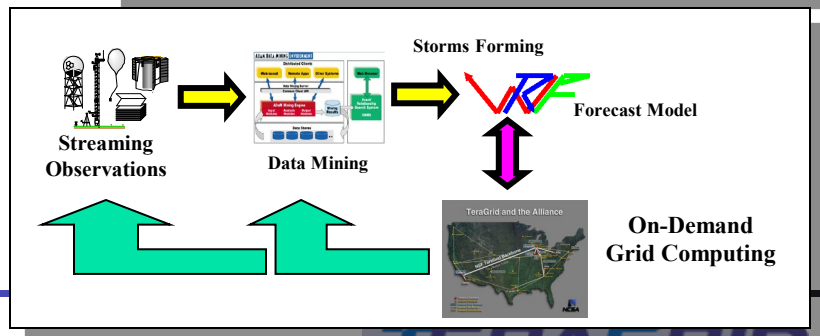
Types of Gateways:
Bridges to Community Grids

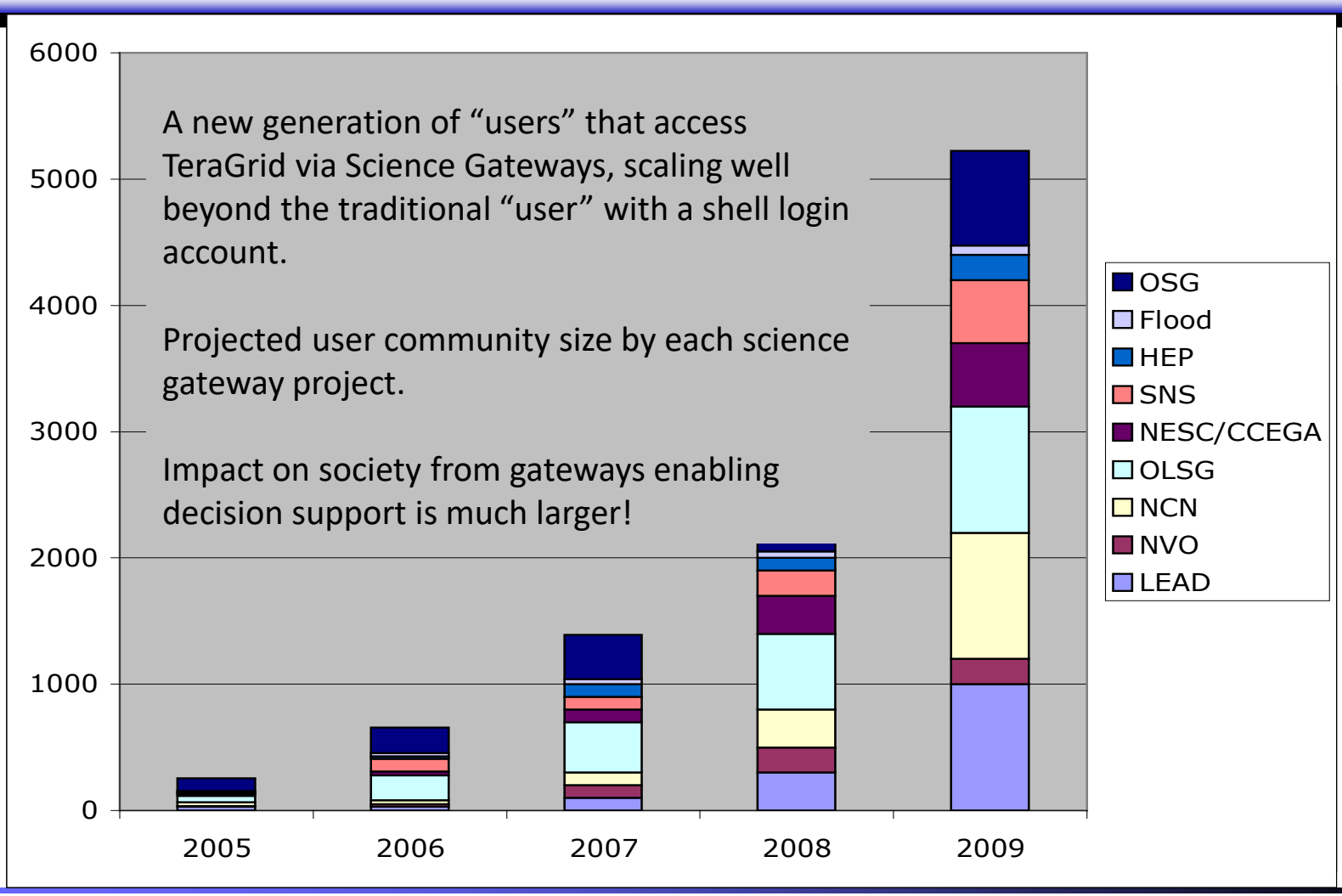
- Many Community Grids already exist or are being built
  - NEESGrid, LIGO, Earth Systems Grid, NVO, Open Science Grid, etc.
- TeraGrid will provide a service framework to enable access in ways that are transparent to their users.
  - The community maintains and controls the Gateway
- Different Communities have different requirements.
  - NEES and LEAD will use TeraGrid to provision compute services
  - LIGO and NVO have substantial data distribution problems.







Science Gateways
An expanding user base



Science Gateways
A new ~~initiative~~ for the TeraGrid
Challenge

- Heterogeneity
  - Software stacks - every gateway is a "custom job".
  - Resources - different architectures at local, national and international levels
  - Users- from HPC developer to K-12 student
  - Security policies
- How can "centers/Institutions" like the TeraGrid provide and operate in this heterogeneous world?
- Working with Gateways, TeraGrid is starting to answer that question
  - Identifying important generic CyberInfrastructure services
  - Providing those services to communities.

Initial Focus on 10 Gateways

Science Gateway Prototype	Discipline	Science Partner(s)	TeraGrid Liaison
Linked Environments for Atmospheric Discovery (LEAD)	**Atmospheric**	Droegemeier (OU)	Gannon (IU), Pennington (NCSA)
National Virtual Observatory (NVO)	**Astronomy**	Szalay (Johns Hopkins)	Williams (Caltech)
Network for Computational Nanotechnology (NCN) and "nanoHUB"	**Nanotechnology**	Lundstrum (PU)	Goasguen (PU)
National Microbial Pathogen Data Resource Center (NMPDR)	**Biomedicine and Biology**	Schneewind (UC), Osterman (Burnham/UCSD), DeLong (MIT), Dusko (INRA)	Stevens (UC/Argonne)
NSF National Evolutionary Biology Center (NESC), NIH Carolina Center for Exploratory Genetic Analysis, State of North Carolina Bioinformatics Portal project	**Biomedicine and Biology**	Cunningham (Duke), Magnuson (UNC)	Reed (UNC), Blatecky (UNC)
Neutron Science Instrument Gateway	**Physics**	Dunning (ORNL)	Cobb (ORNL)
Grid Analysis Environment	**High-Energy Physics**	Newman (Caltech)	Bunn (Caltech)
Transportation System Decision Support	**Homeland Security**	Stephen Eubanks (LANL)	Beckman (Argonne)
Groundwater/Flood Modeling	**Environmental**	Wells (UT-Austin), Engel (ORNL)	Boisseau (TACC)
Science Grid [GrPhyN/ivDGL/Grid3]	Multiple	Pordes (FNAL), Huth (Harvard), Avery (Uflorida)	Foster (UC/Argonne), Kesselman (USC-ISI), Livny (UW)

Timelines - Fall, 2005

- Deploy 3 prototype portals
  - LEAD, Bioinformatics, Evolutionary Biology
- Define work plan and application characteristics
  - NVO, nanoHub, Neutron Science
- Port/install software
  - Homeland Security, Flood Analysis, OSG
- Re-Analyze Gateway needs
- Draft Gateways Primer document

Gateways Primer Outline:

Defining generic cyberinfrastructure services

- 1. Introduction
- 2. Science Gateway in Context
  - a. Science Gateway (SGW) Definition(s)
  - b. Science Gateway user modes
  - c. Distinction between SGW and other TeraGrid user modes
- 3. Components of a Science Gateway
  - a. User Model
  - b. Gateway targeted community
  - c. Gateway Services
  - d. Integration with TeraGrid external resources (data collections, services, …)
  - e. Organizational and administrative structure
- 4. TeraGrid services and policies available for Science Gateways
  - a. Portal middleware tools (user portal and other portal tools)
  - b. Account Management (user models, community accounts,)
  - c. Security environment (security models)
  - d. Web Services
  - e. Scheduling services (and meta-scheduling)
  - f. Community accounts and allocations
  - g. Community Software Areas
  - h. All traditional TeraGrid services and resources
  - i. Ability to propose additional services and how that would interact with TeraGrid operations
- 5. Responsibilities and Requirements for Science Gateways
  - a. Interaction with and compatibility with TeraGrid communities
  - b. Control procedures
    - i. Community user identification and tracking (map TeraGrid usage to Portal user)
    - ii. Use monitoring and reporting
    - iii. Security and trust
    - iv. Appropriate use
- 6. How to get started
  - a. Existing resources
    - i. Publication references
    - ii. Web areas with more details
    - iii. Online tutorials
    - iv. Upcoming presentations and tutorials
  - b. Who to contact for initial discussions
  - c. How to propose a new Gateway
  - d. How to integrate with TeraGrid Gateways efforts.
  - e. How to obtain a resource allocation

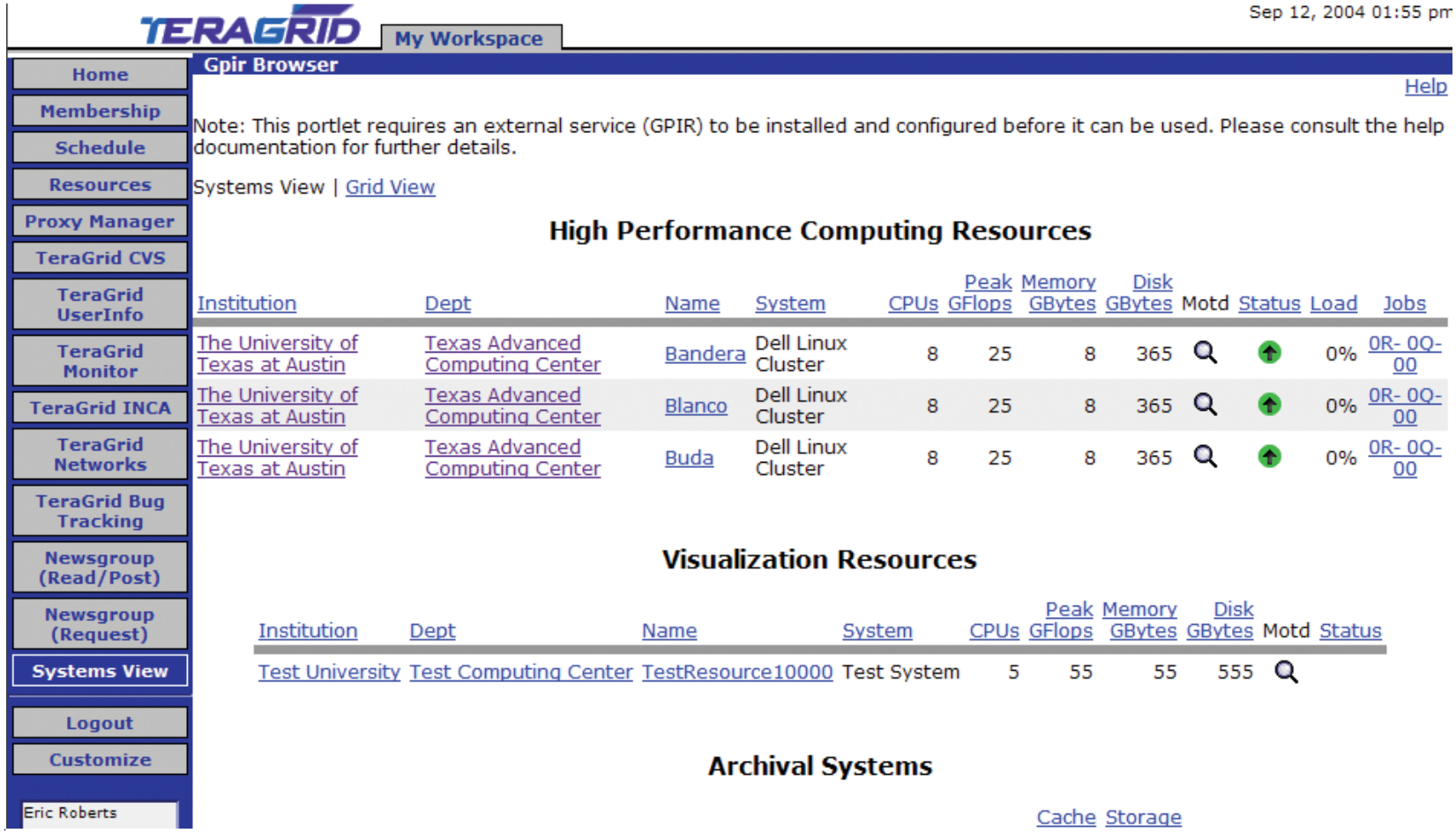
Spring, 2006

- Integrate TeraGrid compute resources
  - LEAD, nanoHUB, Bioinf., Evo. Bio., HEP, OSG
- Prototypes
  - web/grid services (Bioinformatics)
  - Data archive hosting (Neutron Science)
  - Data federation models with compute support (Evolutionary Biology)
  - Application hosting services, initial compute resource brokering and data federation. Test for security, scalability.
- Explore authentication methods (NVO)

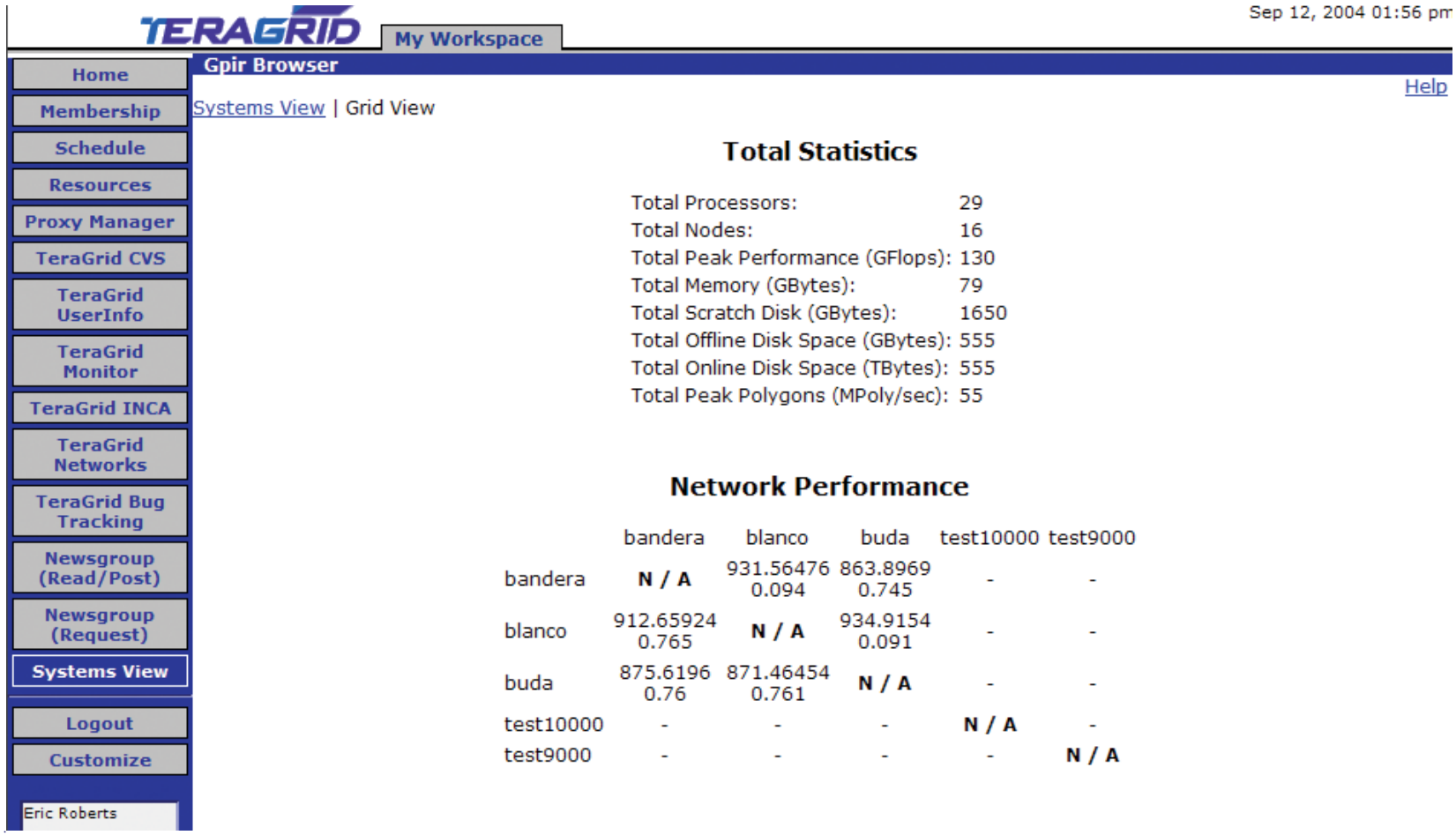
Summary

- TeraGrid offers Science Gateways the ability to extend their compute power on demand.
- Supporting Science Gateways is important to the TeraGrid.
- TeraGrid is starting to work closely with ~10 Science Gateway communities to define and implement common services.
- Prototype gateways deployed in ~1 year

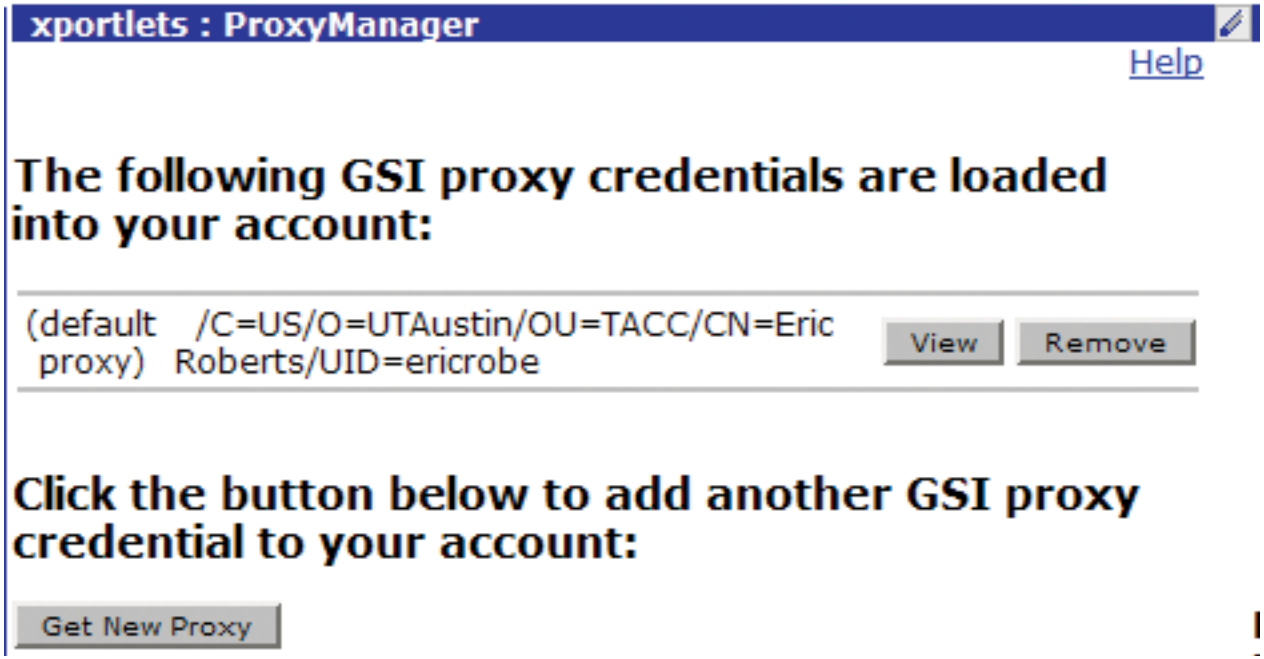
Portal Example: The TeraGrid Portal!



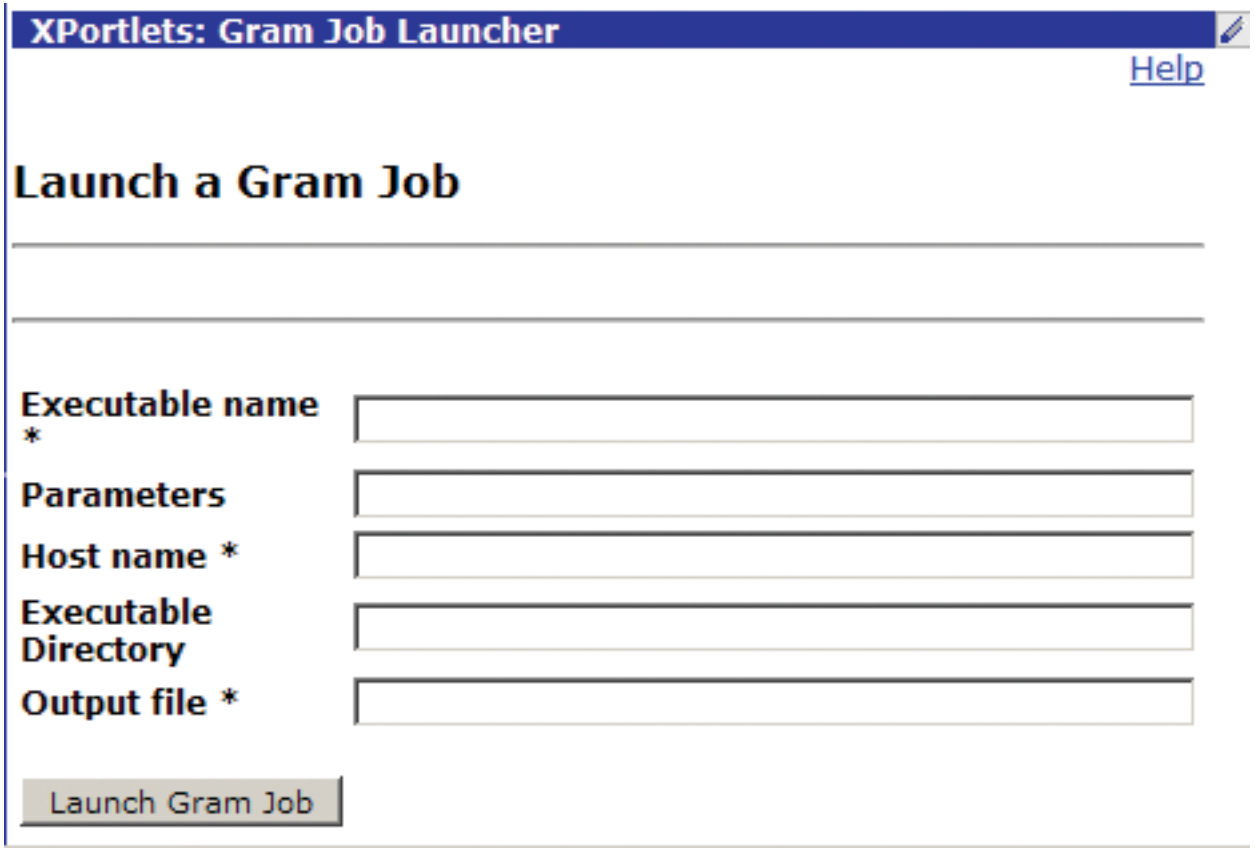
Grid Networking Status



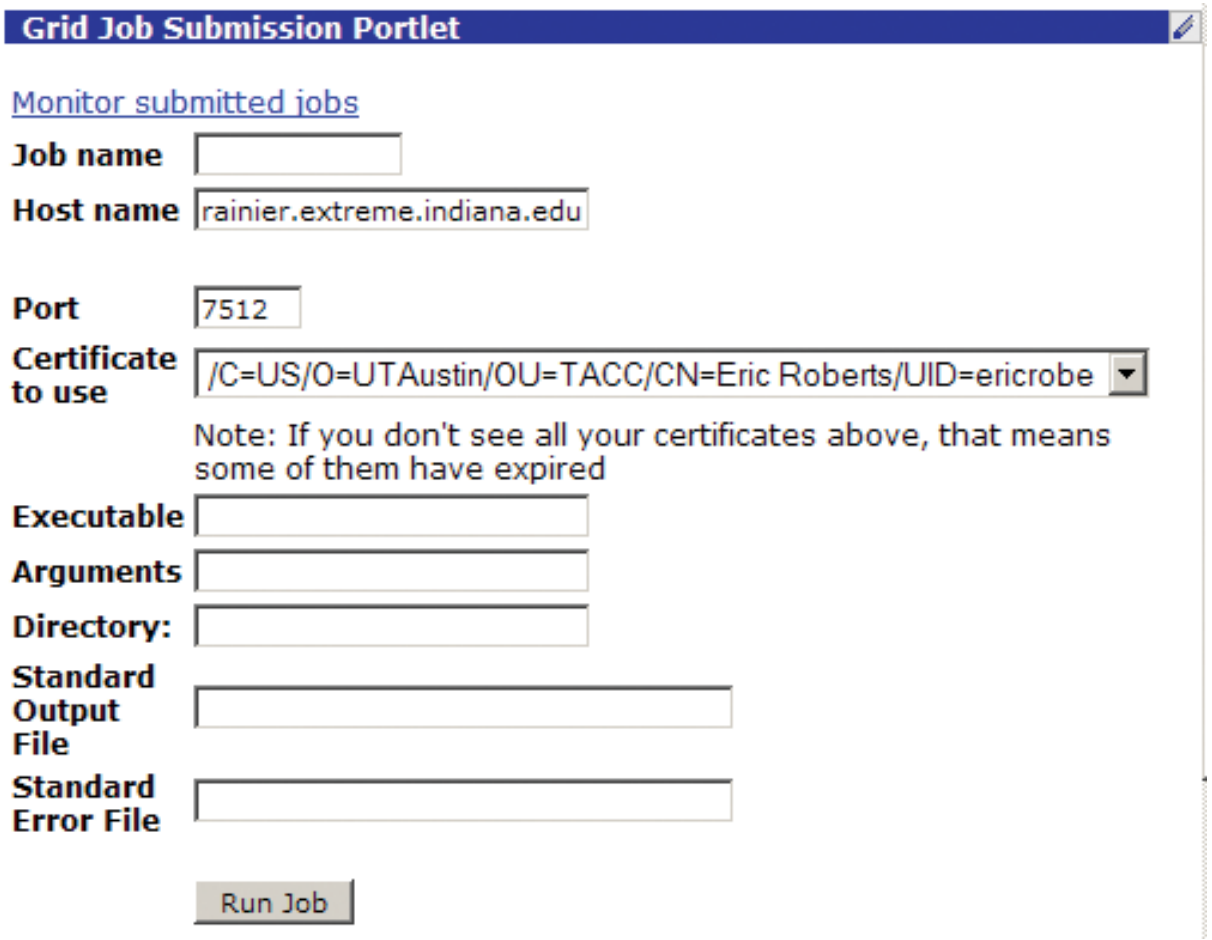
Manage Proxies



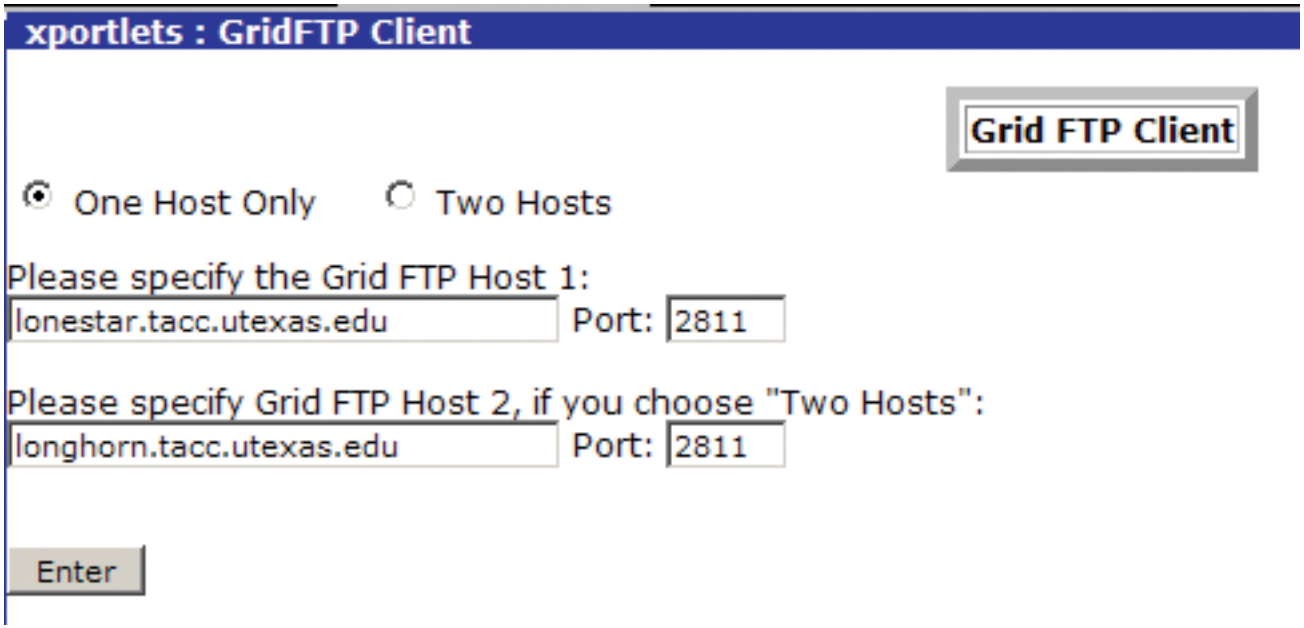
Remote Command Execution



Job Submission



File Management



TeraGrid Resources

	ANL/UC	Caltech	IU	NCSA	ORNL	PSC	Purdue	SDSC	TACC
Compute Resources	Itanium2 (0.5 TF) IA-32 (0.5 TF)	Itanium2 (0.8 TF)	Itanium2 (0.2 TF) IA-32 (2.0 TF)	Itanium2 (10 TF) SGI SMP (6.5 TF)	IA-32 (0.3 TF)	XT3 (10 TF) TCS (6 TF) Marvel (0.3 TF)	Hetero (1.7 TF)	Itanium2 (4.4 TF) Power4 (1.1 TF)	IA-32 (6.3 TF) Sun (Vis)
Online Storage	20 TB	155 TB	32 TB	600 TB	1 TB	150 TB		540 TB	50 TB
Mass Storage			1.2 PB	3 PB		2.4 PB		6 PB	2 PB
Data Collections			Yes	Yes			Yes	Yes	Yes
Visualization	Yes		Yes			Yes	Yes		Yes
Instruments		Yes	Yes		Yes				
Network (Gb/s,Hub)	30 CHI	30 LA	10 CHI	30 CHI	10 ATL	30 CHI	10 CHI	30 LA	10 CHI

TeraGrid Resource Partners