Computational Science Portals: Grid Portal Toolkit (GridPort)

Mary Thomas Computational Science Portals Group San Diego Supercomputer Center University of California at San Diego

> Presented at CERN Geneva, Switzerland



Outline

- Introduction/Background/Motivation
- The GridPort Toolkit
- GridPort-Based Portals
 - HotPage
 - Other application Portals
- Web Services based portals
- Future Work



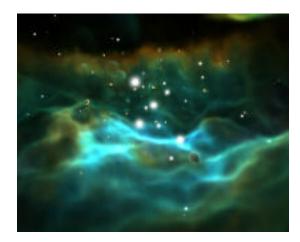








Broad-based Impact



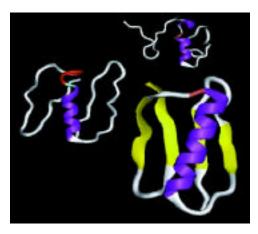
Viewing the Orion Nebula Developed for Hayden Planetarium American Museum of Natural History using NPACI Scalable Volume Visualization Tools



Distributing Large-scale calculations of CHARMM Using Legion



Developing scalable simulation infrastructure to enable breakthrough science

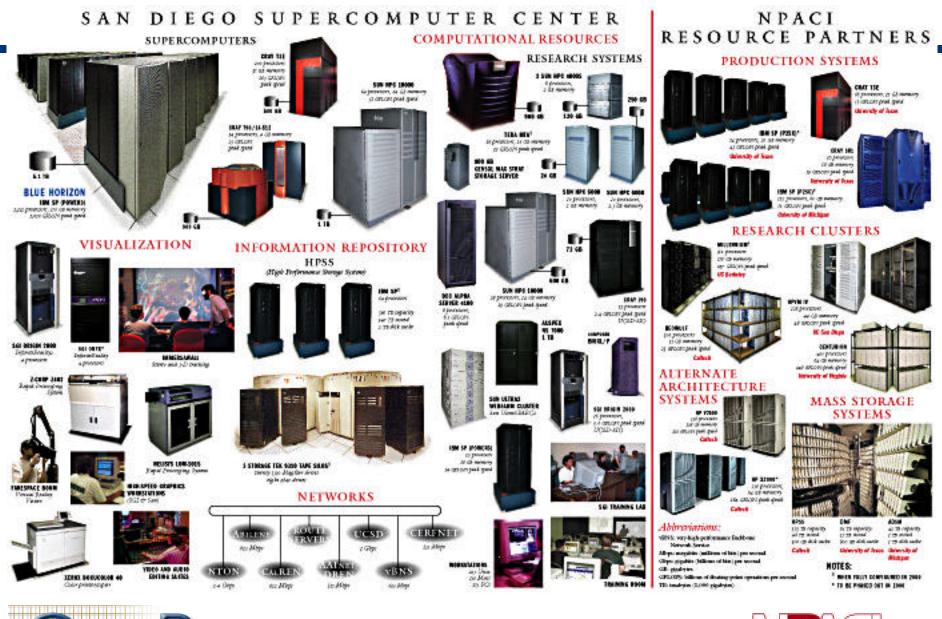




Increasing access through the GridPort Toolkit and Genie Portal









Portals for Computational Science

- Computational science environment is complex:
 - Users now have access to a variety of distributed resources (compute, storage, etc.).
 - Interfaces to these resources vary and change often
 - Policies at sites sometimes differ
 - Using multiple resources can be cumbersome
- Portals can provide simple interfaces
 - Portals are web based and that has advantages -
 - Users know & understand the web
 - Interface to middle-tier infrastructure of the Grid
 - Users can be isolated from resource specific details
 - Uniform interface isolates system changes/differences
 - Not and end-all solution
 - But good for community models, small projects, etc.





The GridPort Toolkit

- Based on the architecture developed for the NPACI HotPage
- Focus on computational scientists and application developers
- Comprised of a set of simple, modular services and tools
- Support application level, customized science portals development
- Facilitate seamless web-based access to distributed compute resources and grid services
- Built with commodity technologies
- Sits on top of the middle-tier of the Grid -
 - An interface to these services for web





GridPort Toolkit Design Concepts

- Key design idea:
 - Any site should be able to host a portal
 - Any user should be able to create their own portal if they have accounts and certificate
- Key Requirements:
 - Base software design on infrastructure provided by World Wide Web:
 - use commodity technologies wherever possible
 - avoid shell programs/aapplications/applets
 - GridPort Toolkit should not require that additional services be run on the HPC Systems
 - reduce complexity -- there are enough of these already
 - so, leverage existing grid research & development

- GSI security (considering Kerberos, secure ID)



Technologies Used

- Uses 'commodity' technologies -> Portability
 - contributes to 'plug-n-play' grid
 - Software is easily ported to, and used by other sites.
 - Perl makes it easy to modify and adapt to local site policies, requirements, servers
- Requirements:
 - Communicator and IE (4.0 or greater),
 - HTTP, HTTPS, SSL, HTML/JavaScript, Perl/CGI, SSH
 - Netscape or Apache servers
 - Grid:
 - Globus, GSI, SRB, CACL (SDSC)
- Goal is to design a toolkit that is simple to implement, support, and develop
 - Technology transfer



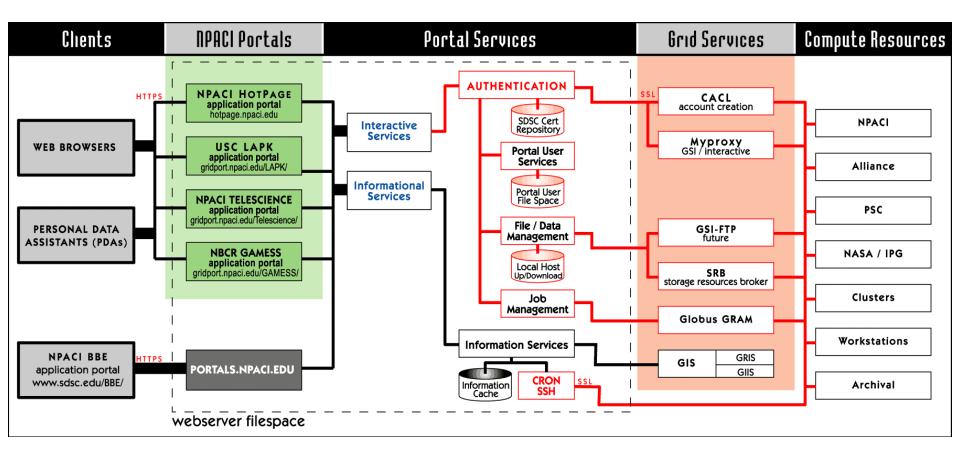
Current Portal Services

- Current features (always adding more)
 - login/logout to grid services (single sign-on)
 - jobs:
 - Submit/cancel jobs to queues
 - monitor jobs and track them
 - web-based batch script builders
 - files:
 - dir listing, file transfer/archival
 - file upload & download
 - SRB integration, default collections for users
 - command execution
 - $\boldsymbol{\cdot}$ any UNIX commands
 - accounts:
 - Personalization





GridPort Architecture





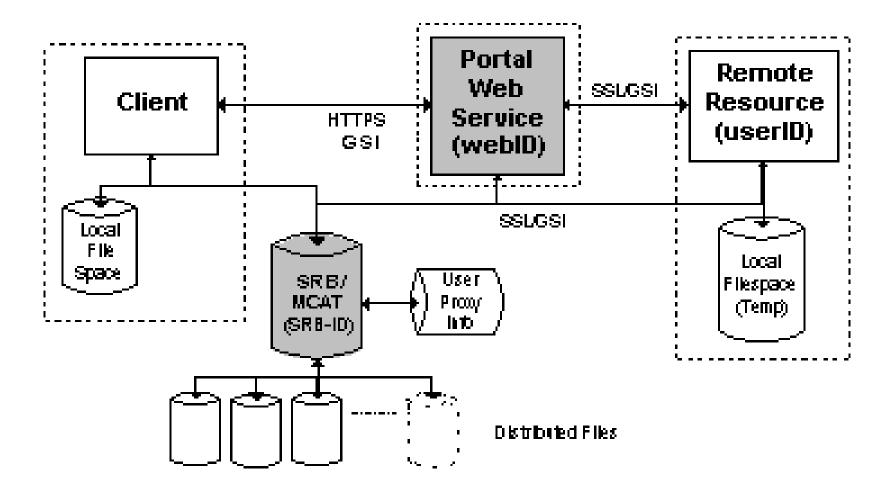


Grid Security at all Layers

- GSI authentication for all portal services
 - transparent access to the grid via GSI infrastructure
 - Security between the client -> web server -> grid:
 - SSL/RC4-40 128 bit key/ SSL RSA X509 certificate
 - authentication tracked with cookies coupled to server data base/session tracking
- Single login environment (another key goal)
 - provides access to all NPACI Resources where GSI available
 - with full account access privileges for specific host
 - use cookies to track state
- Globus used for client requests on resources, but latencies are an issue:
 - Gatekeeper not designed for simple tasks (e.g. "ls")
 - Perl invocation of Globus may be heavyweight (will eval)



GridPort Use of SRB







Applications running on GridPort

- Current applications in production:
 - NPACI HotPage (also @PACI/NCSA)
 - https://hotpage.npaci.edu
 - LAPK Portal: Pharmacokinetic Modeling (live demo of Pharmacokinetic Modeling Portal)
 - https://gridport.npaci.edu/LAPK
 - GAMESS (General Atomic and Molecular electronic Structure System)
 - https://gridport.npaci.edu/GAMESS
 - Bays to Estuaries Project (Don Sutton)
- Application portals under development:
 - Telescience (Ellisman)
 - https://gridport.npaci.edu/Telescience





HotPage View: Job Submission

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Informational Services

- Vertical portal to NPACI Resources and Services:
 - News/events within NPACI
 - Documentation, training , news, consulting
 - Simple tools:
 - application search systems information
 - generation of batch scripts for all compute resources
 - Network Weather System
- Provides dynamic information -
 - real-time information for each machine (or summaries) such as:
 - Status Bar: live updates/operational status/utilization
 - Machine Usage: summary of machine status, load, queues
 - Queues Summaries: displays currently executing and queued jobs
 - Node Maps: graphical map of running applications mapped to nodes
 - Network Weathering System: connectivity information between a user's local host and grid resources



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Interactive Services

- Users have direct access to accounts on resources
 - single entry point to all NPACI resources on which a user has accounts/allocations
- Requires portal account, and authentication
 - secure access to compute and storage resources (GSI)
- Standard menus for each machine
 - allows user to perform common Unix tasks:
 - create, submit, monitor, cancel or delete jobs
 - view output
 - compile and execute code
 - manipulate and view files, navigate through file systems
 - use system commands: chmod, mv, ls, cat, mkdir, cp, rm
 - perform file transfer:
 - upload/download/archive files
 - archiving and retrieving data between local host and HPC system
 - managing accounts and allocations (via Webnewu)



Laboratory for Applied Pharmacokinetics (LAPK) Portal

- Users are Doctors, so need extremely simple interface
- Must be portable run from many countries
- Need to hide details such as
 - Type of resources (T3E), file storage, batch script details, compilation,UNIX command line
- Uses gridport.npaci.edu portal services/capabilities:
 - File upload/download between local host/portal/HPC systems
 - Job Submit:
 - submission (builds batch script, moves files to resource, submit jobs)
 - Job tracking: in the background portal tracks jobs on system and moves results back over to portal storage when done
 - Job cancel/delete
 - Job History: maintains relevant job information
- Major Success:
 - LAPK users can now run multiple jobs at one time using portal.
 - Not possible before because developers had to keep codes & scripts simple enough for doctors to use on T3E



LAPK Job Submit and Job History

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GridPort and Web Services

- New architecture for Grid portals is emerging:
 - Workshop held at SDSC (May '01) to discuss this.
 - Grid Portals Markup Language/XML
- Similar to 'web services' model that is currently evolving in commercial world:
 - Sun Jxta, IBM WebSphere Microsoft .NET
 - XML/SOAP/UDDI/WSDL
 - Client may be a web page/portal or another application or portal
- Allows separation of the function of hosting client from the service or application being used
- Key project goal:
 - Allow scientist to write local portals





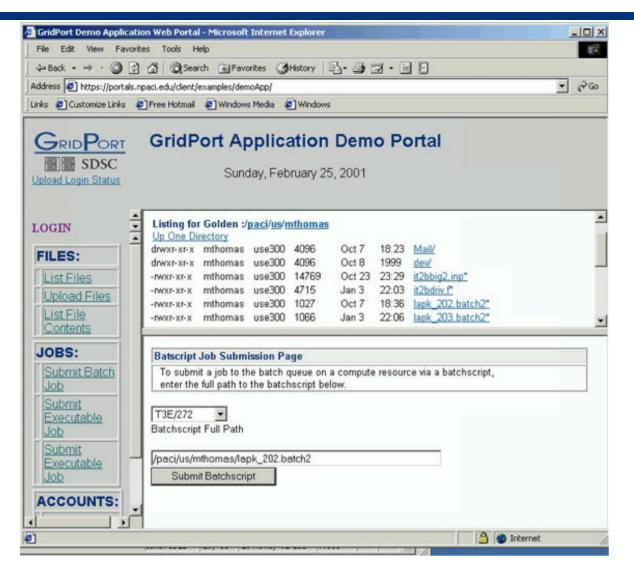
Web Services Expt: GridPort Client Toolkit

- Focus on medium/small applications and researchers
- Choose simple protocol (HTTP/CGI/Perl)
- Application website can be located on any server.
- Connection to portal services is through the GCT:
 - https://portals.npaci.edu/client/tools/FUNCTIONS
 - Inherits all existing portal services running on portal
- Ease of use:
 - Do not have to install complex code to get started:
 - webservers, no Globus, no SSH, no SSL, no PKI, etc.
 - Do not have to write complex interface scripts to access these services (we've done that already)
 - Do not have to fund advanced web development teams
- Client has local control over project, including filespace, etc.
- Integration to existing portals can be done:
 - Bays to Estuaries project





GridPort Client Toolkit: DemoApp







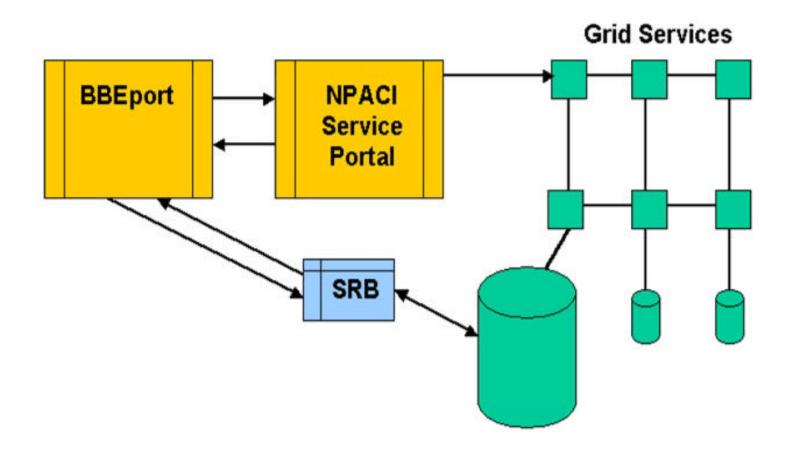
Basin, Bays to Estuaries (BBE) Portal

- Community model: scientific portal for conducting multi-model Earth System Science (ESS):
 - Simulations are run to forecast the transport of sediments within the San Diego Bay area during a storm.
- Technology developed for the BBE project:
 - Website located on BBE webserver/machine
 - Uses SRB for file management (GSI)
 - Perl/CGI
- Uses GCT for all interactive functions:
 - minimal effort required to modify code
 - roughly 14 tests needed to integrate GCT
 - four new perl scripts required





Basin, Bays to Estuaries (BBE) Portal







Services Implemented in GCT

- Authentication:
 - Login
 - Logout
 - Check authentication state

- Files:
 - Upload from local host
 - Download to local host
 - FTP move FILE
 - View Portal FILEpace (?)

- Jobs:
 - Sumbit jobs to queues
 - Cancel jobs
 - Execute commands (command like interface)
- Commands:
 - Pwd
 - Cd
 - Whoami
 - Etc.





Future Work

- Evaluate Servlet technologies: why?
 - Faster than Perl process invocation
 - Rapid integration to databases, schemas, etc.
 - Integrate with JINI and new broker
 - Collaboration with Sun & CAL(IT)2 project
- Implement portal broker in Java
 - Choose services based on conditions such as user, resource, security methods, etc.
- Develop data portal capabilities:
 - Integrate SRB for file management
 - All portal accounts get collection
 - Java and Perl libraries
 - Use for maintaining state/status information



Future Work (cont.)

- Continue to develop Web services
 - Develop XML schemas
 - Evaluate using SOAP/WSDL, etc.
 - architectures
 - Collaborate with GGF/GCE:
 - GCE Testbed plan underway between
 - USA: PACI, Alliance, NASA, Jefferson lab, PNNL, others
 - Europe: Daresbury, Cactus, others?
- Continue to develop personalization features
- Develop Advanced Tools:
 - JobBuilder, JobTracker, JobCompiler, FileStager
- Collaborations:
 - User portal collaboration: NSF (PACI, NASA, PSC, Argonne), PNNL, Globus, others)
 - Global Grid Forum/Grid Computing Environments (GCE)
 - metascheduling projects
 - Grid accounts





GridPort Team

- A Collective Effort
- SDSC Staff:
 - Mary Thomas
 - Steve Mock
 - Kurt Mueller
 - Maytal Dahan (former intern)
 - Cathie Mills (former intern)
- Student Interns:
 - Ray Regno
 - Chris Garsha
 - Kathy Seyama



- Cadre of other SDSC services and people
- Collaborators: User Portal Collaboration
 - Globus/Argonne
 - SRB
 - NCSA/Alliance
 - NASA/IPG
 - LBL
 - Univ. of Texas
 - Univ. of Indianna (Gannon)
 - Don Sutton (UCSD)
 - Daresbury (UK)



References

- GridPort Toolkit Website
 - https://gridport.npaci.edu
- NPACI HotPage User Portal
 - HotPage: https://hotpage.npaci.edu
 - Accounts: http://hotpage.npaci.edu/accounts
- Downloads
 - GridPort Toolkit
 - NPACI HotPage
 - GCT Portal (frames based)
 - http://gridport.npaci.edu/download
- Contact:
 - Use comment form located on HotPage



