



The NGS Grid Portal

David Meredith

NGS + Grid Technology Group, e-Science Centre,

Daresbury Laboratory, UK

d.j.meredith@dl.ac.uk





NGS Portal

The NGS portal can be used to access and interact with the HPC and Data resources available on the Grid via SSO (Certificates + myproxy):

- Browse for different applications available on a Grid this includes your own personal applications and preconfigured applications available on a particular Grid (e.g. the NGS is currently publishing applications within the NGS portal to be made easily available for its users).
- Submit/monitor compute jobs/applications.
- Access and move data around the Compute and Data Grid (Gridftp, srb).





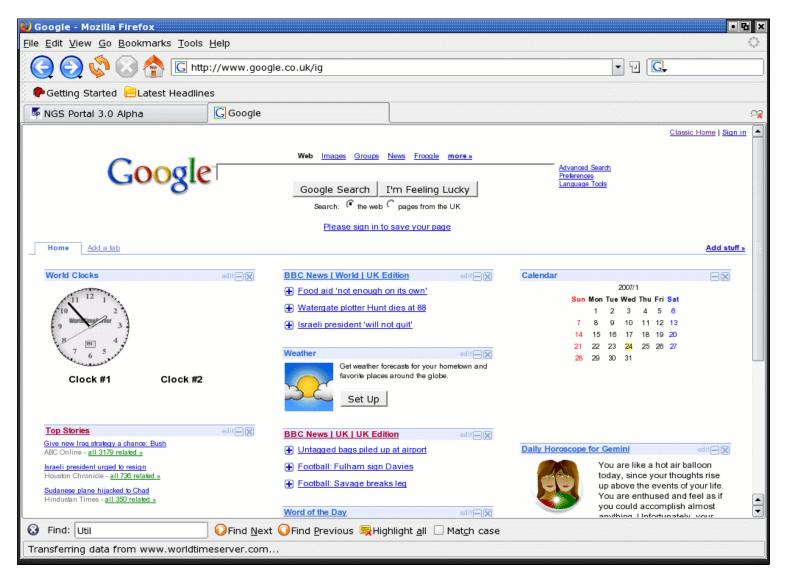
Portal and Portlets

- The NGS Grid portal extends a JSR-168 compliant portal container which hosts a selection of 'portlets.'
- Portlets are online-accessible applications that are hosted and managed within the portal container.
- The list of portlets that are deployed to the portal make up the portal's overall functionality (users may be interested only in a selection of portlets)
- Main Benefit: Portlets facilitate the sharing and re-use of applications (168-compliant 3rd party portlets can be used within a portal as required).
- NGS and CCLRC e-Science Centre are developing a collection of portlets designed for the Computational and Data Grid.
- The NGS portal is a current implementation of these Grid portlets.





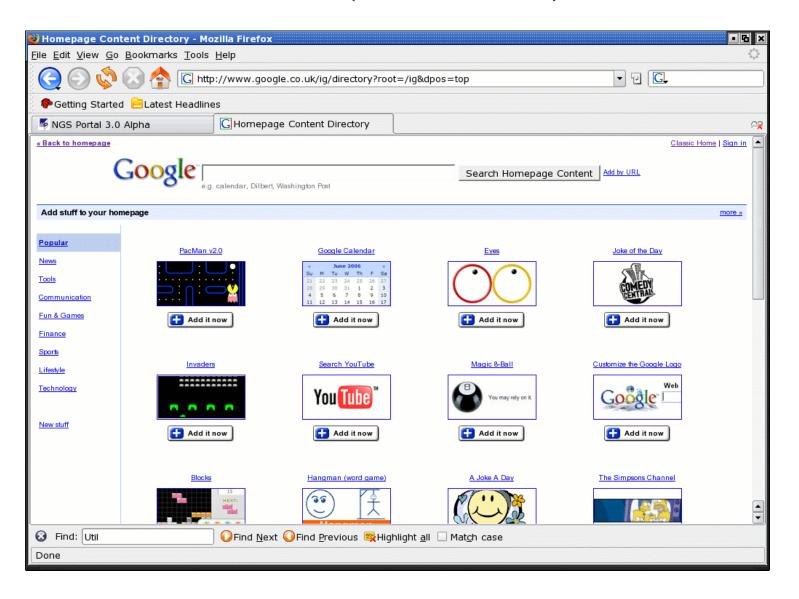
A Famous Portal + Portlets







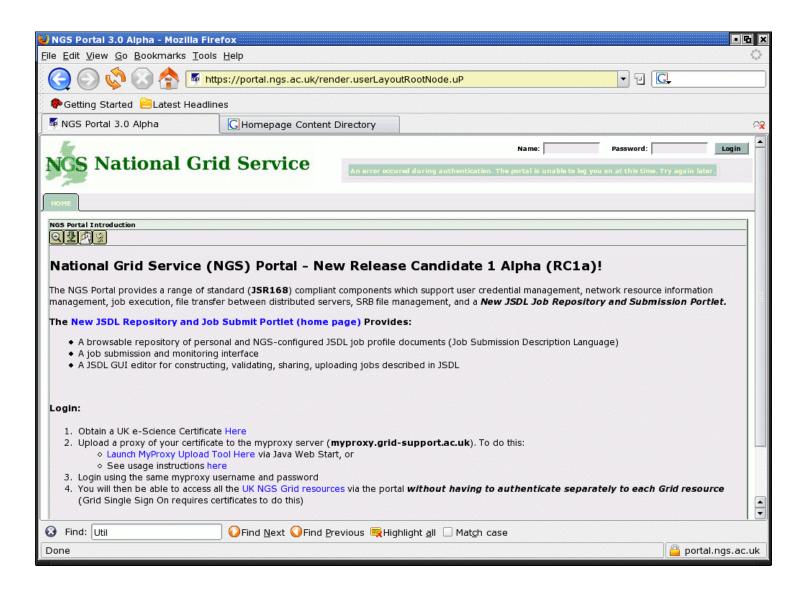
Select Portlets of Interest (customisation)







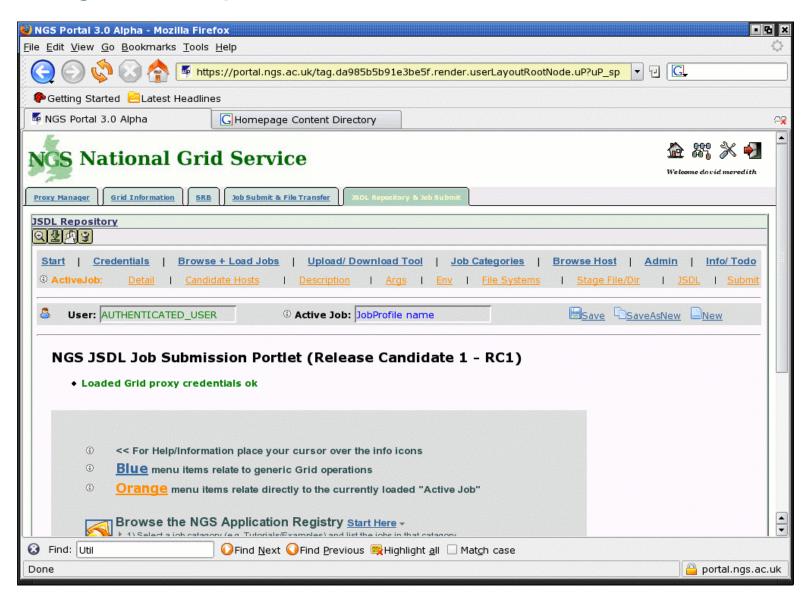
NGS portal







After Login – Grid portlets







JSDL Repository / Job Submit Portlet

- A browsable JSDL database of personal and shared JSDL job profile documents (Job Submission Description Language, i.e. 'job recipes/templates').
 - JSDL can be browsed for, selected and loaded in order to run applications on the Grid (loaded either 'out-of-the-box' or, more usually loaded and modified/tweaked as required).
 - JSDL can be searched for by category of interest in the portal (e.g bioinformatics, chemistry, tutorials/examples).
 - JSDL documents can be pre-configured and published by the portlet administrator(s) to be made available to all other users.
- 2. A JSDL GUI editor for constructing, validating, sharing, uploading jobs described in JSDL.
- 3. A Grid job submission and monitoring application (currently, only Globus but more Grid middleware providers are being added, e.g. GridSam/WSRF).





JSDL – Job Submission Description Language

```
<jsdl:Application>
       <jsdl:ApplicationName>gnuplot</jsdl:ApplicationName>
       <jsdl-posix:POSIXApplication>
         <isdl-posix:Executable>
           /usr/local/bin/gnuplot
         </isdl-posix:Executable>
         <jsdl-posix:Argument>control.txt</jsdl-posix:Argument>
<jsdl-posix:Argument>DavesControlFile.txt</jsdl-posix:Argument>
         <jsdl-posix:Input>input.dat</jsdl-posix:Input>
         <jsdl-posix:Output>output1.png</jsdl-posix:Output>
       </jsdl-posix:POSIXApplication>
    </isdl:Application>
    <jsdl:Resources>
       <jsdl:IndividualPhysicalMemory>
<jsdl:LowerBoundedRange>2097152.0</jsdl:LowerBoundedRange>
       </jsdl:IndividualPhysicalMemory>
       <jsdl:TotalCPUCount>
         <jsdl:Exact>1.0</jsdl:Exact>
       </jsdl:TotalCPUCount>
    </isdl:Resources>
```

- XML Schema language for describing compute jobs in a platform independent language (XML).
- 2. Is agnostic of middleware no dependencies on Globus, WSRF, gLite (portal that is generic and not tied to any particular set of Grid technologies).
- 3. GGF / OGF Standard.
- JSDL documents can be validated against the JSDL and JSDL POSIX XSD Schema to ensure its correctness



JSDL – Job Submission Description Language XSD Schema

```
<xsd:complexType name="Environment Type">
    <xsd:simpleContent>
         <xsd:extension base="xsd:string">
             <xsd:attribute name="name" type="xsd:NCName" use="required"/>
             <xsd:attribute name="filesystemName" type="xsd:NCName" use="optional"/>
             <xsd:anyAttribute namespace="##other" processContents="lax"/>
         </xsd:extension>
    </xsd:simpleContent>
</xsd:complexType>
<xsd:complexType name="Argument_Type">
    <xsd:simpleContent>
         <xsd:extension base="xsd:normalizedString">
             <xsd:attribute name="filesystemName" type="xsd:NCName" use="optional"/>
             <xsd:anyAttribute namespace="##other" processContents="lax"/>
         </xsd:extension>
    </xsd:simpleContent>
</xsd:complexType>
```



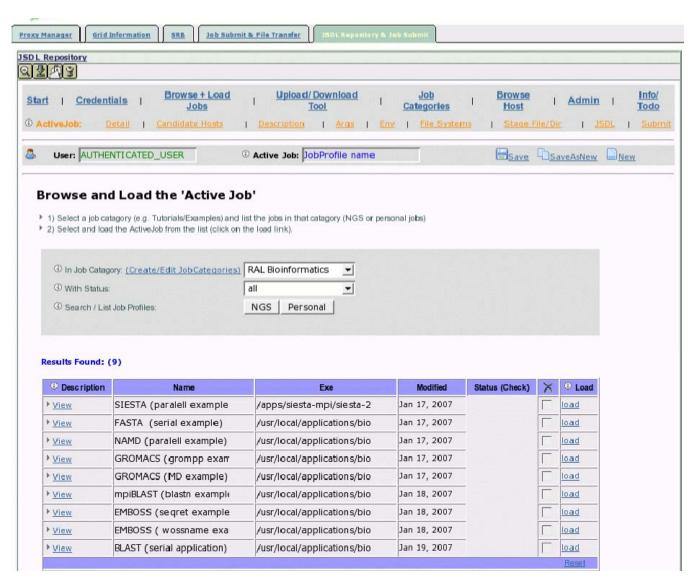


JSDL Repository / Database

Select category of interest – e.g. 'RAL Bioinformatics.'

Browsing the JSDL database for public and personal job profiles.

List jobs, read job descriptions and load a job to initialise the 'Active Job.'



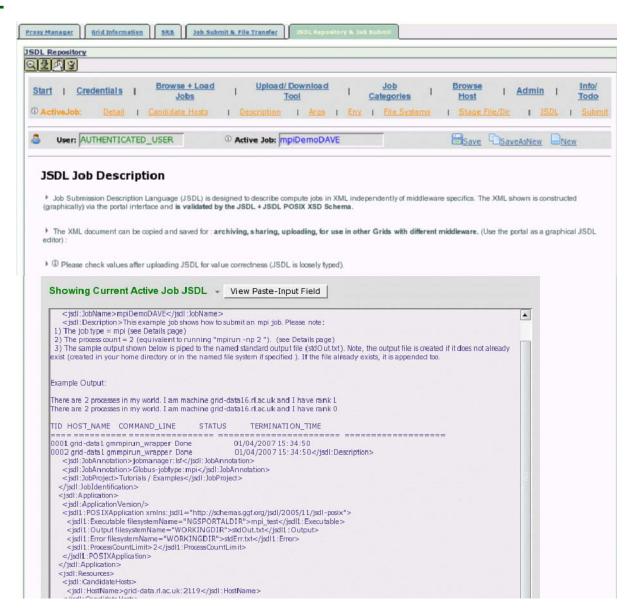




Active Job's JSDL

The Active Job JSDL is automatically created, updated and validated by the portal by changing parameters in the portal GUI.

The portlet acts as a JSDL GUI editor





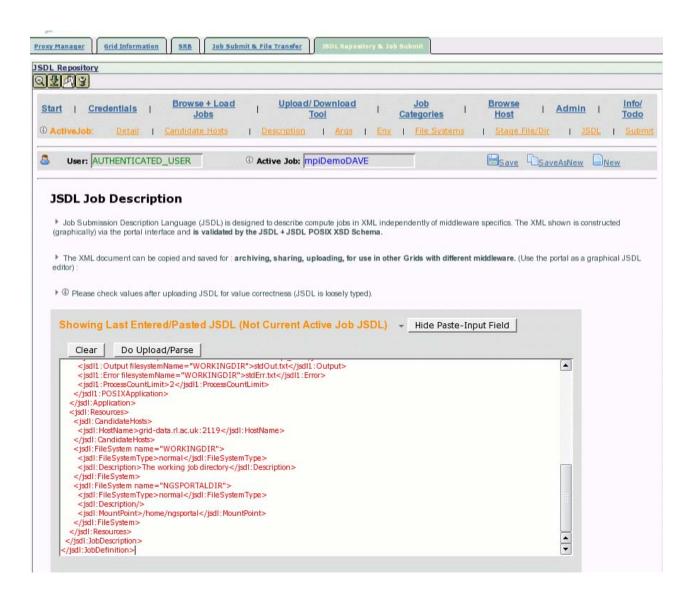


Upload / Share JSDL

JSDL documents can be uploaded to the portal in order to initialise the Active Job.

Validation errors and messages are displayed in the interface when uploading JSDL.

The portlet allows the sharing of job profiles and JSDL between users and user communities.







Active Job Detail

Input fields are filled out for pre-configured applications.

Changes to the parameters in the GUI will update the generated JSDL automatically.

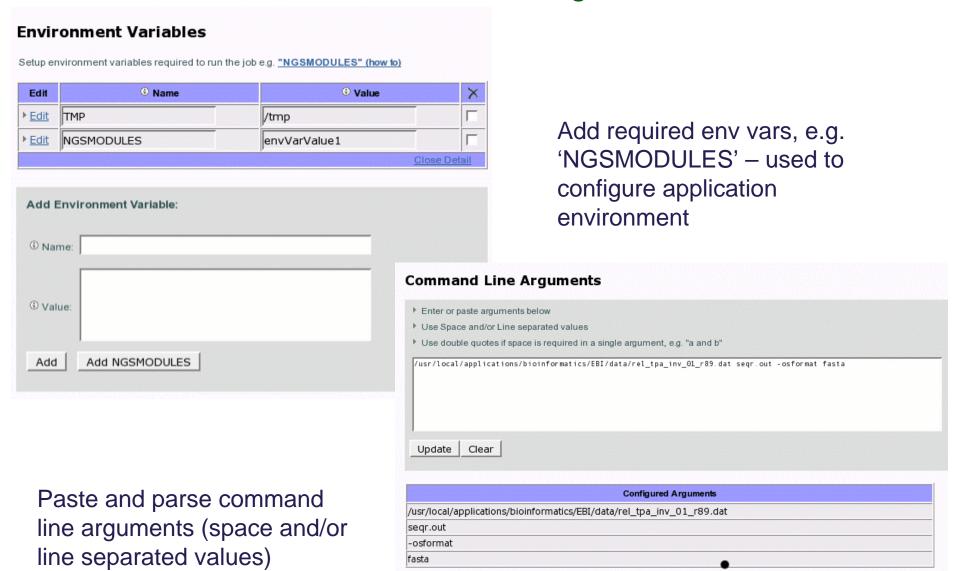
Input fields are taken from the JSDL and JSDL-POSIX extension schemas.

① > JSDL Job Identification:			
① Job Name:	mpiDemoDAVE		① + JSDL Application: ① App Name:
Job Catagory: ▶ <u>Select</u>	Tutorials / Examples		
① Job Description:	▶ <u>Job Description</u>		App Version:
⊕ ► JSDL Job Resources:			
Execute Host+Port:			[grid-data.rl.ac.uk:2119]
Job Manager:			lsf
Resource Count:			
			<u>'</u>
① Min + Max Mem (MB):			
File Systems + Stage Data:			► <u>File Systems</u> ► <u>Stage Data</u>
⊕ > JSDL POSIX Extensions:			
WORKINGDIR (Mount Point Pat	h):		<clear td="" ⊕<=""></clear>
Create New (Use Optional N		!	<create td="" workingdir="" ©<=""></create>
Use optional name)			
_ x >			to the <u>File_System_Mount_Point</u> OR Full path oduce valid JSDL executable element) ▼
③ Executable Or Script:		NGSPORTALDIR	_ y mpi_test
		/home/ngsportal/mpi_t	est
⑤ File Paths: Std In/Out/Error Files: (Specify paths Relative to <u>File System Mount Points</u> - Recommended) (Can also specify a Full path starting with ") ▼			
		(Can also specify a Full WORKINGDIR	path starting with ?) →
③ Input File (Must Exist):			
9		WORKINGDIR	▼ stdOut.txt
Output File (Created if not e	exist):	std Out.txt	
0-	🥦	WORKINGDIR	▼ stdErr.txt
Error File (Created if not ex	ist):	stdErr.txt	
A CONTROL CONTROL CONTROL OF THE		mpi ▼ 2	
③ JobType + ProcessCount:		TIPI - 1 2	
③ Wall Time:			
Arguments + Environment: Environment		► Environment ► Ar	<u>quments</u>
Update Active Job Profile			
1			





Environment Variables / Arguments







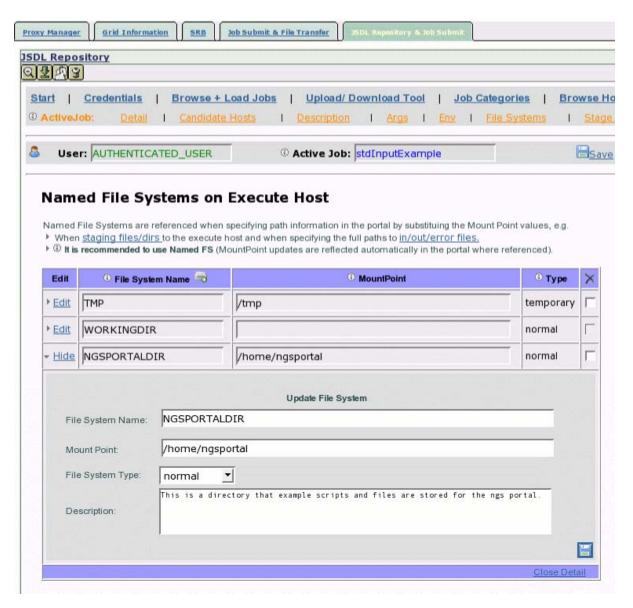
Named File Systems

Named file systems used to declare mount points that are required on the consuming system.

File system names are referenced throughout the portlet (and JSDL doc) for substituting mount points where required.

Changes to a FS mount point will be updated automatically throughout the portal/JSDL.

Used when specifying path info e.g., locations to files/dirs, stage data locations etc.







Stage Data

Compile a list of required data (i.e. data that should be copied to the consuming system from remote locations across the Grid prior to job execution).

Data is staged relative to named file systems.

The source URI can be either specified manually or, more normally, browsed for in the 'Browse Host' page.



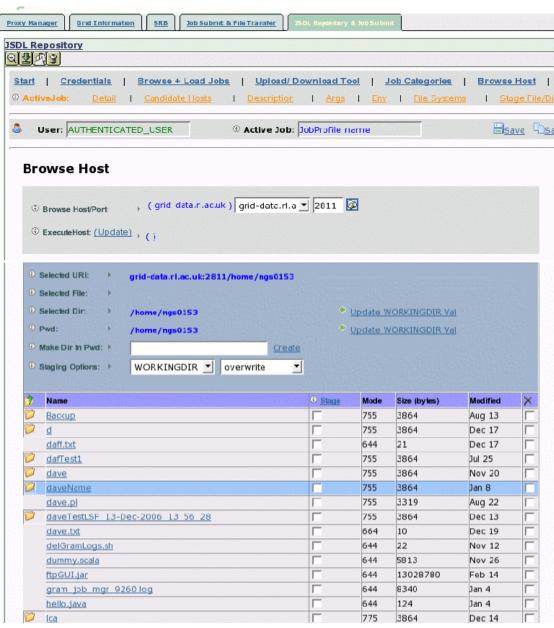




Browse Hosts

Browse remote Grid hosts for stage data.

Select files and directories that should be copied to the consuming system via GsiFtp (more protocols to be supported inc srb, ftp, webdav).



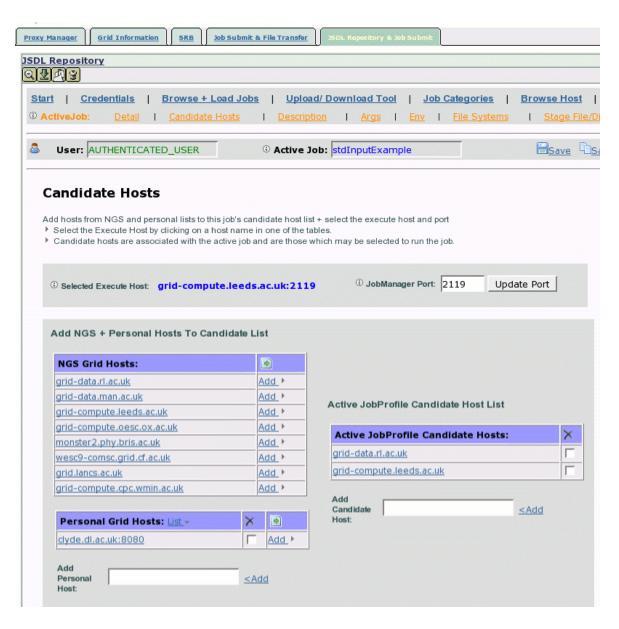




Candidate Hosts

Candidate hosts are consuming systems that can be nominated to run the Active Job.

The candidate host list can be compiled from a personal host list and from a default host list (available to all users).

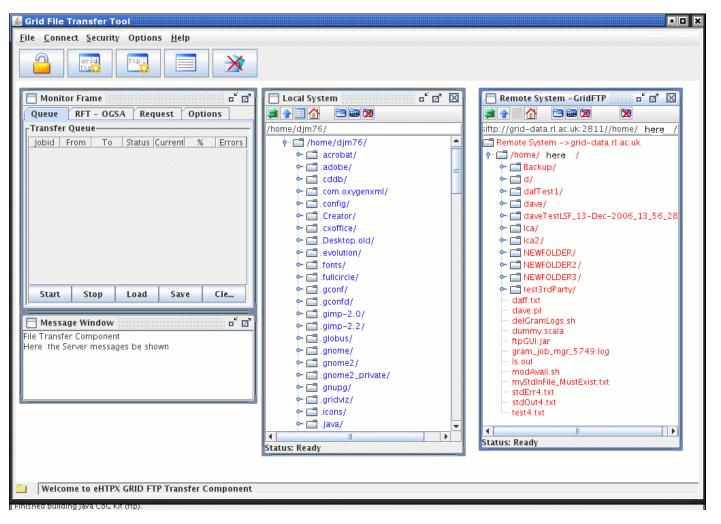






GridFtp Upload / Download / File Transfer Tool

Transfer files to/from your desktop and a remote Grid ftp server via 'drag-n-drop' – akin to Windows explorer for the Grid







Summary

- Core of the application is designed to be generic and not tied to any particular set of Grid technologies (facilitated using JSDL). Middleware dependencies emerge at job-submit/monitor time when the specifics of the middleware have to be accommodated (e.g. parsing the JSDL into RSL, adding mw-specific parameters, e.g. RSL JobType).
- 2. Application can be deployed as a JSR-168 portlet or as a standalone Web application. This helps deployment e.g. openPortal that was designed to show users what is available before having to 'log-in' (encourage users).
- 3. Currently, application only supports Globus, but GridSAM will be added shortly (more on GridSAM next few days).



NGS National Grid Service

TODO / Future

- 1. Extend application to support more Data Grid + Web protocols for data staging (SRB, WebDav). This will involve browsing / interacting with different data protocols in the interface (e.g. browse SRB), but deciding who actually performs the stating is currently being decided (manage in application, or leave to job submission service). Crossing protocols adds some complexity.
- Growing list of improvements / suggestions to refine interface HCI (Human computer interaction).
- 3. Extend the interface for Data visualisation via the portal interface.
- 4. Release the portlets for use in other projects / Grids.
- 5. Longer term Extend the portlet to support the registration of new interfaces, i.e. register application specific interfaces designed for specific applications. (Note, new interfaces will build JSDL in same way will use underlying portlet functionality in same way).
- 6. A portal is only as good as the underlying deployed infrastructure.... portal development often involves debugging the underlying consuming systems and middleware





Software Stack

JSF (Java Server Faces) interface + MVC control layer (Http session and request scope data)

Spring v2.0 managed business objects (singleton + prototype injected object graphs, declarative transaction demarcation, data source management).

C3p0 db connection pooling

ORM (object relational mapping) - JPA (Java persistence API) + Hibernate 3.2 for domain model.

Java CogKit for Globus API

Apache XMLBeans for JSDL xml-object data binding framework

