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The NGS Grid Portal

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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).





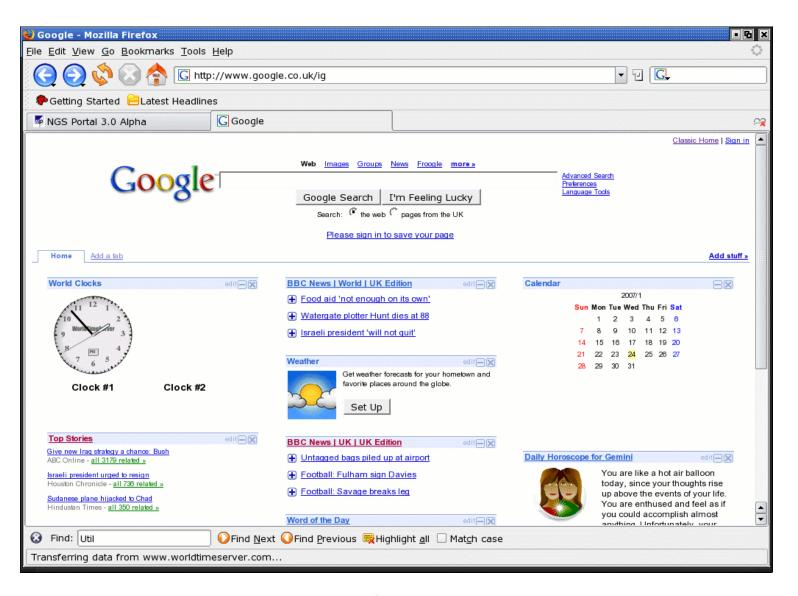
Portal and Portlets

- 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 within a 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.





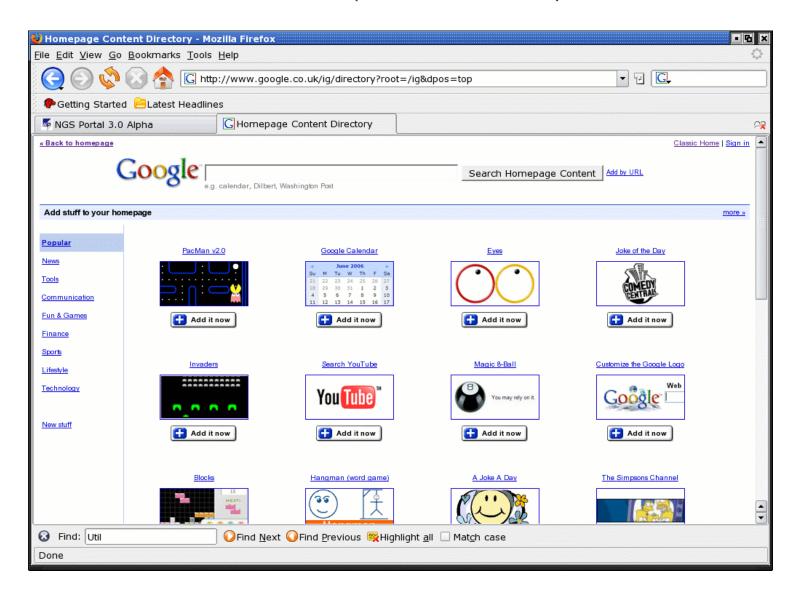
A Famous Portal + Portlets







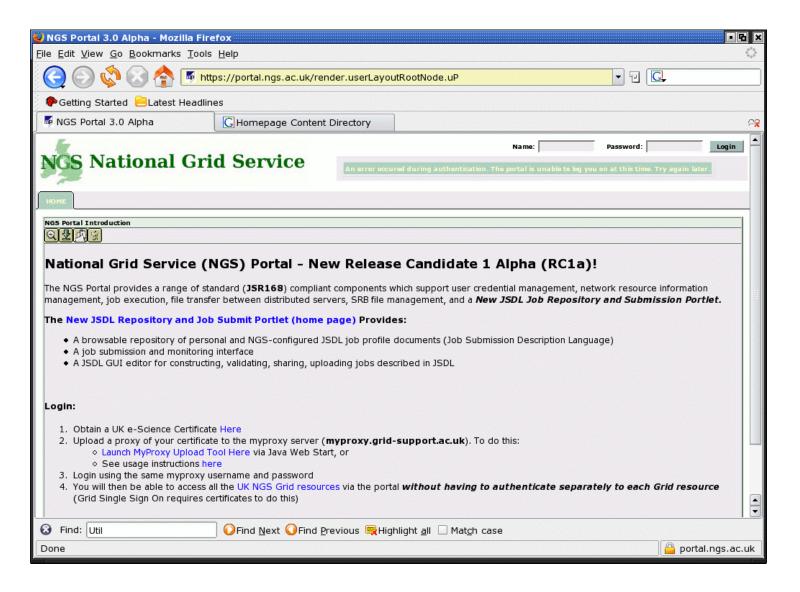
Select Portlets of Interest (customisation)







NGS portal







After Login – Grid portlets

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NGS JSDL Job Submission Portlet (Release Candidate 1 - RC1) • Loaded Grid proxy credentials ok	
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JSDL Repository / Job Submit Portlet

- 1. 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> <jsdl-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>

- 1. 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.
- 4. 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.'

DL Repository							
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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

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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.

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<jsdl: FileSystemType>normal</td><td>SDL (Not Current Active Job JSDL) Hide INGDIR">stdOut.txt GDIR">stdErr.txt SesCountLimit> 9 '> SystemType> bory SystemType></jsdl:></jsdl:></jsdl:></jsdl:></jsdl:></jsdl:></jsdl1:>		





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.

⊕ ► JSDL Job Identifcation	:	③ ▶ JSDL Application:
③ Job Name:	mpiDemoDAVE	App Name:
④ Job Catagory: ▶ <u>Select</u>	Tutorials / Examples	App Version:
Job Description:	• Job Description	App version.
③ ▶ JSDL Job Resources:		
Execute Host+Port Select From Candidat	e Host List	[grid-data.rl.ac.uk:2119]
③ Job Manager:		Ist
Resource Count:		
O		
① Min + Max Mem (MB):		
④ File Systems + ④ Stage Data:		File Systems Stage Data
③ ▶ JSDL POSIX Extension	s.	
WORKINGDIR (Mount Point Pate	100	<clear td="" ③<=""></clear>
10		<create td="" workingdir="" ③<=""></create>
③ Create New (Use Optional National	ame): J	
		elative to the <u>File System Mount Point</u> OR Full path both produce valid JSDL executable element) ▼
③ Executable Or Script:	NGSPORTAL	
	/home/ngsporta	/mpi_test
③ File Paths: Std In/Out/Error Files		elative to <u>File System Mount Points</u> - Recommended) a Full path starting with /) →
	WORKINGD	
Input File (Must Exist):		
	WORKINGD	IR 🔄 stdOut.txt
Output File (Created if not e	stdOut.txt	
© Error File (Created if not exi		IR _∫stdErr.txt
Choi the (created if horex)	stdErr.txt	
③ JobType + ProcessCount:	mpi 💌	2
③ Wall Time:		
④ waii Time: ④ Arguments + Environment:) Environment	→ Arguments
- Algumenta + Environment.	- Environment	
Update Active Job Profile		





Environment Variables / Arguments

Environment Variables

Add Environment Variable:

Setup environment variables required to run the job e.g. "NGSMODULES" (how to)

Edit	③ Name	O Value	\times
Edit	ТМР	/tmp	Г
Edit	NGSMODULES	envVarValue1	Г

Add required env vars, e.g. 'NGSMODULES' - used to environment

③ Name:	
^① Value:	c

configure application

Command Line Arguments
Enter or paste arguments below
▶ Use Space and/or Line separated values
▶ Use double quotes if space is required in a single argument, e.g. "a and b"
/usr/local/applications/bioinformatics/EBI/data/rel_tpa_inv_OL_r89.dat seqr.out -osformat fasta
Configured Arguments
/usr/local/applications/bioinformatics/EBI/data/rel_tpa_inv_01_r89.dat
seqr.out
osformat
asta

Paste and parse command line arguments (space and/or line separated values)





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.



Named File Systems on Execute Host

Named File Systems are referenced when specifying path information in the portal by substituing the Mount Point values, e.g. When staging files/dirs to the execute host and when specifying the full paths to in/out/error files.

③ It is recommended to use Named FS (MountPoint updates are reflected automatically in the portal where referenced).

Edit	File System	m Name 🔫	MountPoint O Type	×
Edit	ТМР		/tmp tempora	у Г
Edit	WORKINGDIR		normal	Γ
Hide	NGSPORTALDI	R	/home/ngsportal normal	Г
	le System Type:	normal	<u> </u>	
M	ount Point:	/home/ngs	portal	
De	escription:	This is a dir	ectory that example scripts and files are stored for the ngs portal.	





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).

у Ма	nager Srid Information SRB Job Submit & File Transfe	15DL Repository		nt.		
I D	epository					
	N3		· · · · · · · · · ·		· · · · · · · · · · · · ·	
tart	Credentials Browse + Load Jobs Upl	oad/ Download To		ob Categories	Browse	Host
Acti	tiveJob: <u>Detail</u> I <u>Candidate Hosts</u> I <u>Descr</u>	iption I <u>Args</u>	I <u>Env</u>	I <u>File Syste</u>	<u>ms</u> I <u>Sta</u>	ige Fil
						_
	User: AUTHENTICATED_USER	Job: JobProfile n	стпе		<u> </u>	ave [
Br	owse Host					
(T)	Browse Host/Port (grid data.r.ac.uk) grid-da	tarta 🕈 2811	2			
0	Browse Host/Port: , (grid data.r.ac.uk) grid-da		2			
٢	ExecuteHost: (Update) + ()					
	· • • •					
۲	Selected URI: grid-data.rl.ac.uk:2811/home/ngs	0153				
۲	Selected File: >					
۲	Selected Dir: /home/ngs0153		Update W	ORKINGDIR Va		
	Pwd: / /home/ngs0153			ORKINGDIR Va		
. 1			opuate n	OKKINGDIN Va		
U.	Make Dir In Pwd: >	Create				
٢	Staging Options: WORKINGDIR overwrite	_				
22						
ø	Name	Stage				
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	d daff.txt dafTest1 dave daveName dave.pl		755 755 644 755 755 755 755 755	3864 3864 21 3864 3864 3864 3864 3319	Aug 13 Dec 17 Dec 17 Jul 25 Nov 20 Jan 8 Aug 22	
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	d daff.txt daffest1 dave daveName dave.pl daveTestLSF 13-Dec-2006 13 56 28 dave.txt delGramLogs.sh dummy.scala ftpGUI.jar	Image: Constraint of the second sec	755 755 644 755 755 755 755 664 644 644 644 644 644	3864 3864 21 3864 3864 3864 3319 3864 10 22 5813 13028780	Aug 13 Dec 17 Dec 17 Jul 25 Nov 20 Jan 8 Aug 22 Dec 13 Dec 19 Nov 26 Feb 14	





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).

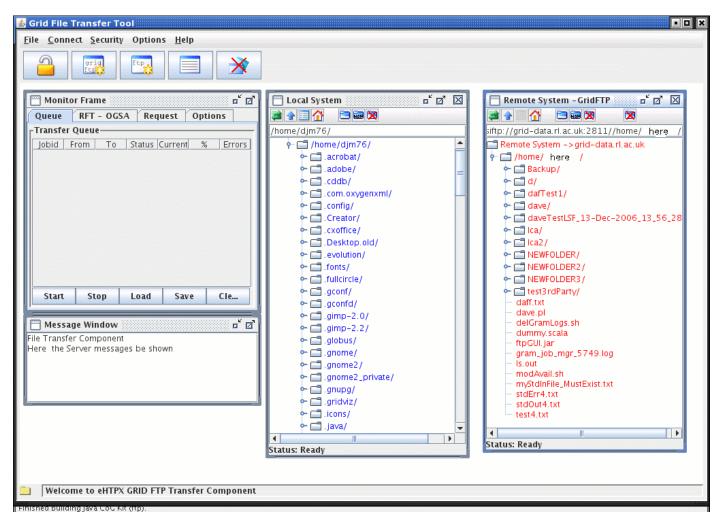
ActiveJob: Detail Candidate Hosts Description Args Env File Systems St User: AUTHENTICATED_USER ③ Active Job: stdInputExample Candidate Hosts Active Job: stdInputExample Add hosts from NGS and personal lists to this job's candidate host list + select the execute host and port > Select the Execute Host by clicking on a host name in one of the tables. Yeardidate hosts are associated with the active job and are those which may be selected to run the job.	File Systems Stage
User: AUTHENTICATED_USER ③ Active Job: stdInputExample Candidate Hosts Add hosts from NGS and personal lists to this job's candidate host list + select the execute host and port > Select the Execute Host by clicking on a host name in one of the tables. > Candidate hosts are associated with the active job and are those which may be selected to run the job.	
Candidate Hosts Add hosts from NGS and personal lists to this job's candidate host list + select the execute host and port > Select the Execute Host by clicking on a host name in one of the tables. > Candidate hosts are associated with the active job and are those which may be selected to run the job.	2.
Add hosts from NGS and personal lists to this job's candidate host list + select the execute host and port Select the Execute Host by clicking on a host name in one of the tables. Candidate hosts are associated with the active job and are those which may be selected to run the job.).
Add hosts from NGS and personal lists to this job's candidate host list + select the execute host and port Select the Execute Host by clicking on a host name in one of the tables. Candidate hosts are associated with the active job and are those which may be selected to run the job.).
 Select the Execute Host by clicking on a host name in one of the tables. Candidate hosts are associated with the active job and are those which may be selected to run the job. 	o.
Candidate hosts are associated with the active job and are those which may be selected to run the job.	
© Selected Execute Host: grid-compute.leeds.ac.uk:2119 © JobManager Port: 2119 Update Port	119 Update Port
© Selected Execute Host: grid-compute.leeds.ac.uk:2119 © JobManager Port: 2119 Update Port	Update Port
© Selected Execute Host: grid-compute.leeds.ac.uk:2119 © JobManager Port: 2119 Update Port	119 Update Port
Add NGS + Personal Hosts To Candidate List	
NGS Grid Hosts:	
grid-data.rl.ac.uk Add	
grid-data.man.ac.uk Add ►	
	te Host List
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grid-data.man.ac.uk Add > grid-compute.leeds.ac.uk Add > grid-compute.oesc.ox.ac.uk Add > monster2.phy.bris.ac.uk Add > grid.lancs.ac.uk Add > grid.compute.cpc.wmin.ac.uk Add > grid.compute.cpc.wmin.ac.uk Add >	date Hosts: X
grid-data.man.ac.uk Add > grid-compute.leeds.ac.uk Add > grid-compute.oesc.ox.ac.uk Add > monster2.phy.bris.ac.uk Add > grid.lancs.ac.uk Add > grid.compute.cpc.wmin.ac.uk Add > grid.compute.cpc.wmin.ac.uk Add >	date Hosts: X
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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







TODO / Future

- 1. 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).
- 2. Extend the interface for:-
 - a) Parameter sweep style jobs (parameter replacement in jsdl).
 - b) Data visualisation via the portal interface.
- 3. Portal is designed to be generic and not tied to any particular set of Grid technologies. Extend portal to support more Grid + Web protocols (e.g. SRB, WebDav, GridSam, WSRF).
- 4. Release the portlets for use in other projects / Grids.

Final note - 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

