Rapid Development of Customised Web Portals for Scientific Computing

Jos Koetsier and Jano van Hemert

open middleware
infrastructure institute uk

www.omii.ac.uk

National
e-Science
Centre

Rapid

giving computational
science a friendly face

Context

Scientist

Infrastructure

Context

Scientist
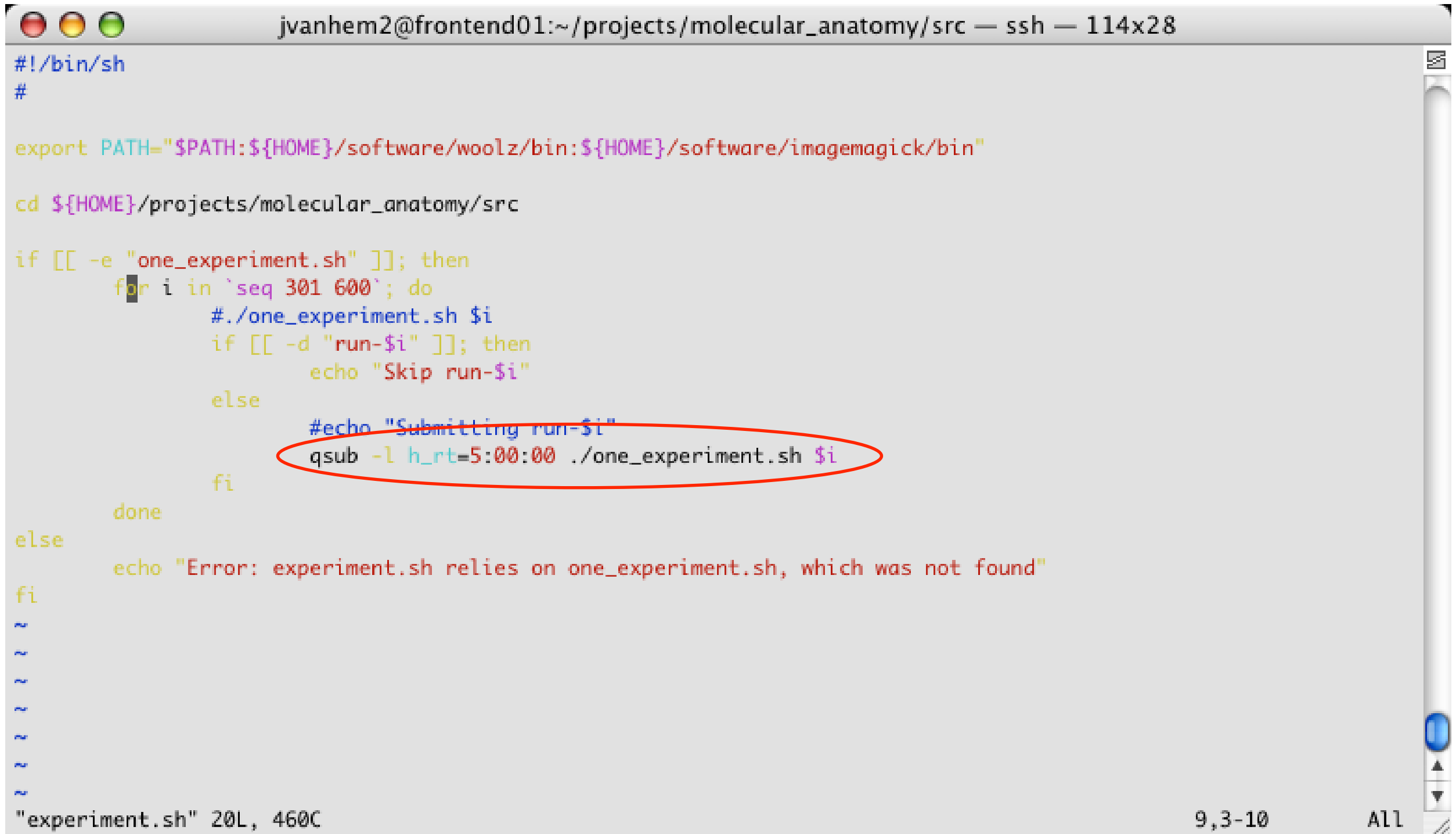
Science?

Infrastructure

Scientific Computing: The Stone Age


```sh
#!/bin/sh
#

export PATH="$PATH:${HOME}/software/woolz/bin:${HOME}/software/imagemagick/bin"

cd ${HOME}/projects/molecular_anatomy/src

if [[ -e "one_experiment.sh" ]]; then
        for i in `seq 301 600`; do
                #./one_experiment.sh $i
                if [[ -d "run-$i" ]]; then
                        echo "Skip run-$i"
                else
                        #echo "Submitting run-$i"
                        qsub -l h_rt=5:00:00 ./one_experiment.sh $i
                fi
        done
else
        echo "Error: experiment.sh relies on one_experiment.sh, which was not found"
fi
~
~
~
~
~
~
~
"experiment.sh" 20L, 460C                                                    9,3-10     All
```

Portals: the ultimate solution!
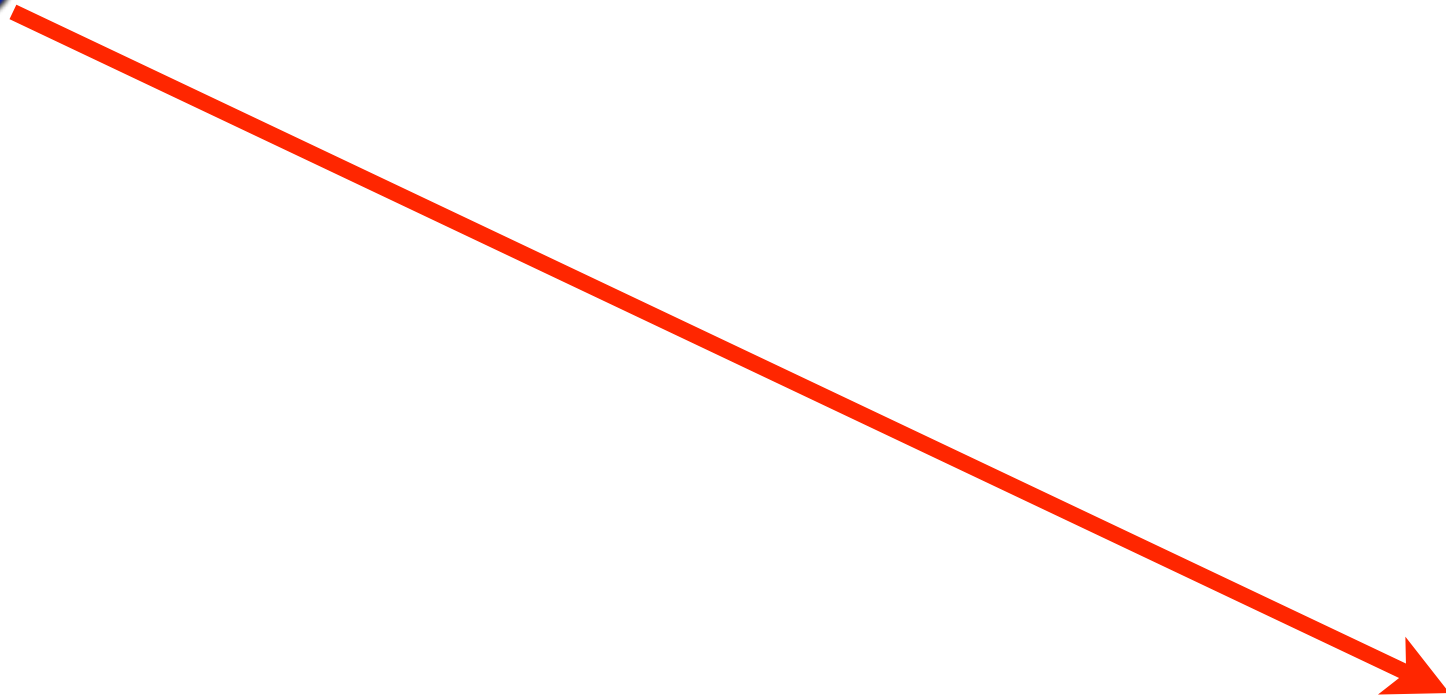
Infrastructure

Portals: the ultimate solution!

gridsphere portal framework

Infrastructure

iGoogle

*i*Google™

Advanced Search
Search Preferences
Language Tools

Google Search   I'm Feeling Lucky

New! Add social gadgets to post updates and play games with friends.   **Change theme from Classic | Add stuff »**

⊟ **Home** ▽

Weather
BBC News | UK | UK...
Google Map Search
nu.nl - Algemeen
BBC News | Scotlan...
Zementis PMML 3.2 ...

⊟ **Mail**

Gmail
.:h3w.fr:. CheckMail ...
Include gadget

Updates
Friends

⊟ **Chat**

Search, add, or invite

Jano van Hemert
Loading...

Options ▼ Add friends

BBC News | Scotland | Edinburgh, East and Fife | UK Edition

⊞ £5m plan for failed bridge bids
⊞ Row over who dispenses medicines
⊞ Case dropped in child rape trial
⊞ Airshow parking 'education' call
⊞ Famous dictionary to close office
⊞ Darth Vader voices 'scare girls'
⊞ Lost cat turns up 500 miles away
⊞ Police plea after shop ram raid

BBC News | UK | UK Edition

⊞ Benefits plan to 'make work pay'
⊞ Osborne: Brown misled MPs on cuts
⊞ Swine flu victim speaks of ordeal
⊞ Tory plans to cut 'surveillance'
⊞ Archbishop condemns bank excesses
⊞ Police stop-and-search forms cut
⊞ Bradshaw to back licence fee plan
⊞ Mis-sold mobile crackdown starts

nu.nl - Algemeen

⊞ Arrestatie wegens moord op studente van Yale
⊞ Klopjacht op gevluchte topcrimineel
⊞ Veroordeelde Schipholbrand land uitgezet
⊞ Executie uitgesteld vanwege onvindbare ader
⊞ 'Lekken was solo-actie van Tang'
⊞ 'Gehandicapten gaan er meest op achteruit'
⊞ Sarkozy weet zeker dat Iran aan atoombom werkt
⊞ Europarlement veroordeelt homofobe wet in Litouwen

Zementis PMML 3.2 Converter

Zementis PMML 3.2 Converter

Convert   Help/Feedback

PMML file (Versions 2.1, 3.0 or 3. Limit 1MB.)

Brow

Convert

Weather

EH3

12°C   Current: Mostly Cloudy
Wind: E at 11 km/h
Humidity: 72%

Wed   Thu   Fri   Sat

17° | 5°   17° | 5°   17° | 7°   20° | 6°

Google Map Search

Traffic   Map

Leith Docks
Granton   Leith
Muirhouse   A902   A901   A199
Ferry Rd
A90   Drylaw   Craigentinny
Edinburgh   Port
rphine   Newington   Duddingston
Slateford   Craigmillar
hill   Morningside

javascript:void(0);

Tuesday, 9 August 2011

myed
The University of Edinburgh

Search the University Website   Go   Your Feedback

Welcome Jano

| Today | myStuff | Teaching | Research | Admin | Finances | Services | Library | Search & Info | Help | New |

WEB Intelligence (InfoView)

WEBI

This service is available for the following:

- Legacy Student (NESI) reporting
- some Finance reports
- CMS
- MyEd
- VRS

All other business areas have been migrated to the new Business Objects Reporting service.

Launch WEBI

- Availability outside the University network

EBIS Online

Launch EBIS

- Availability outside the University network

EUCLID Staff

ⓘ EUCLID is the University online system for managing the whole student lifecycle from admissions through to graduation.

launch euclid

EUCLID availability

- EUCLID is available.

How to get started

- Apply for a EUCLID account

User support

- User Guide and FAQs
- Contact Support
- Training

HR Manager Workflow

Refresh Details

You have no outstanding notifications.

Done

Ridiculous portal
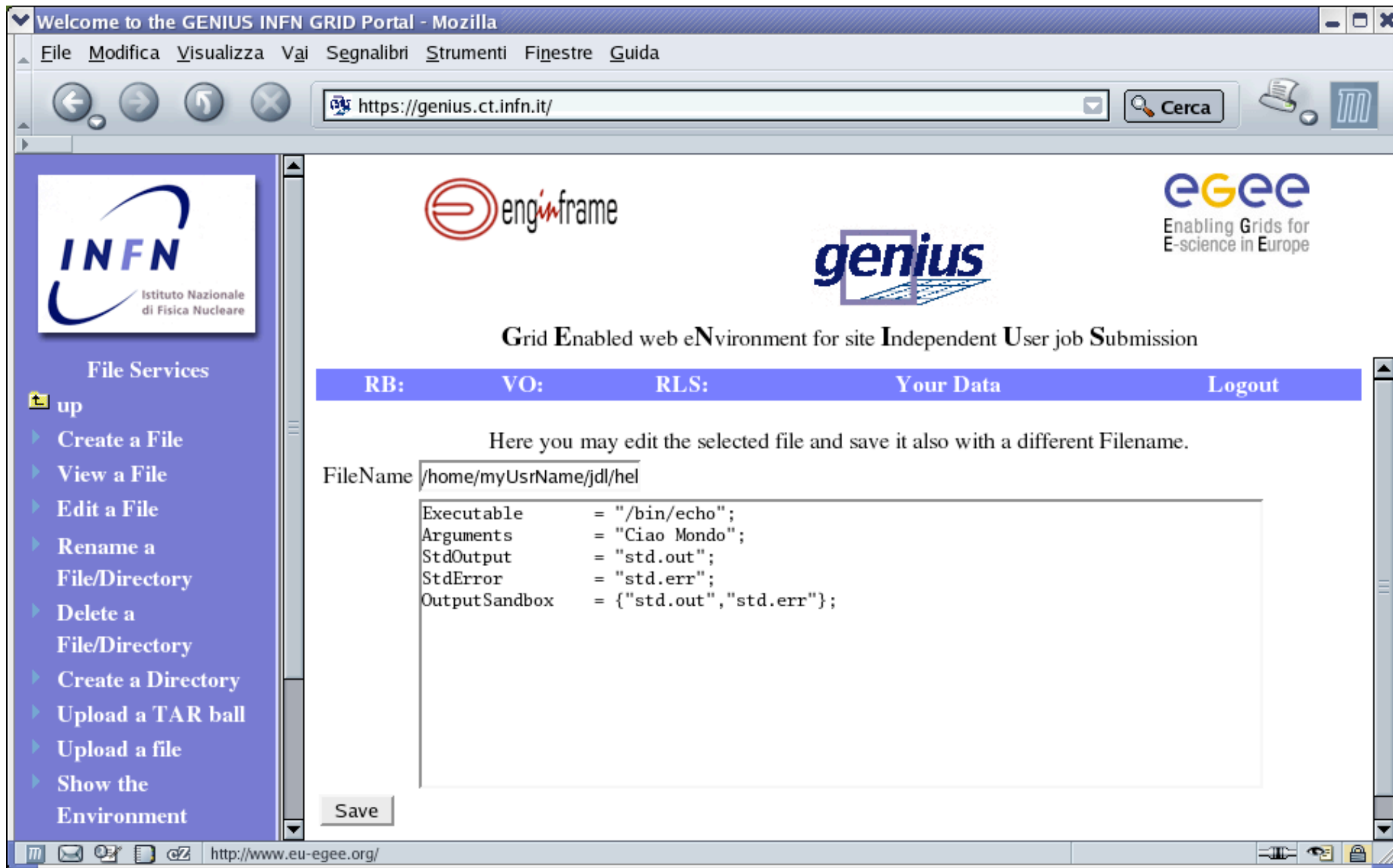
source: GENIUS portal guide

General portal

- Far too many boxes to fill in

- Arcane technical content required

- Basically a command-line / XML-editor in disguise

NGS — National Grid Service

JSDL Application Repository / Job Submission Portal (JSR-168 Compliant)

Science & Technology Facilities Council

My Grid Identity: *None*

Submit My Job

My Job : Weka "Instances" Test

Save | SaveAsNew | New

▶ Review and submit My Job (the active job) to the selected candidate host.

My Job Summary

Application Name: (Browse / Select New Application)	Weka	Edit
Application Version:	3.4.9	Edit
Job Name:	Weka "Instances" Test	Edit
Job Category:	Analysis/Stats	Edit
Selected Execute / Submission Endpoint:	ngs.rl.ac.uk:2119/lsf	Edit
Candidate Execution / Submission Endpoints:	<Candidate Hosts> Update	Edit
Executable:	/usr/ngs/WEKA_3_4_9	Edit
Standard Input File:		Edit
Standard Output File:	my_vsl_res	Edit
Standard Error File:	StdErr.txt	Edit
Working Directory:		Edit
Status (Check):	UNSUBMITTED	
JobHandle:		
Process Count:	1	Edit
Job Type:	single	Edit
Node Count:		Edit
Min Mem (MB):		Edit
Max Mem (MB):		Edit
Arguments:	weka.core.Instances soybean.arff	Edit

Left navigation:

Authenticate
Applications
Job Categories
Browse_Host
Data_Transfer
Admin
Info

My Job:
- PageLayout
- JsdlLayout

- <JobIdentification/>
  - JobName
  - JobDescription
  - JobProject
- <Application/>
  - ApplicationName
  - ApplicationVersion
  - Description
  - <Posix/>
    - Executable
    - Arguments
    - Input
    - Output
    - Error
    - Working Directory
    - Environment
    - Wall Time
- <Resources/>
  - Candidate Hosts
  - File Systems
- <DataStaging/>
  - Stage Data
- Files/Links
- <JSDL/>
- Submit/Run

Job Description: Edit

```
WEKA 3.4.9
-------------------------------------------------------
template configured by J.Churchill (HPCSG,RAL,STFC)
           updated by A.Maniopoulou  (HPCSG,RAL,STFC)
-------------------------------------------------------

This is an simple "Instances" job. Weka is a serial code.

The input files required for this example can be retrieved and staged into your home (or working) directory from
ngs.rl.ac.uk:/apps/weka/weka-3-4-9/data/soybean.arff. This template is setup to stage the example input files from this
directory. Before running this example, change and/or create the working directory on the "Active Job Profile Detail" page, then
go to the 'StageData' page and click on 'StageNow' button to copy the files into that working directory.

To now run this example job (or another  job based on this template) go to the "Submit" page and click on "Validate the RSL"
before submission. If that gives no errors, check the box next to  re-submit and then  click the "Submit active job". The status of
the job should appear in red. First it will say submitted. To update the status, click on the status wording.  When completed, go to
```

Environment Variables (None): Edit

File Systems: Edit

File System Name	MountPoint	Type
WORKINGDIR		normal
USRNGS	/usr/ngs	normal

Tuesday, 9 August 2011

Specific portal

The problems with hiring a developer

The problems with hiring a developer

Developer

The problems with hiring a developer

Developer

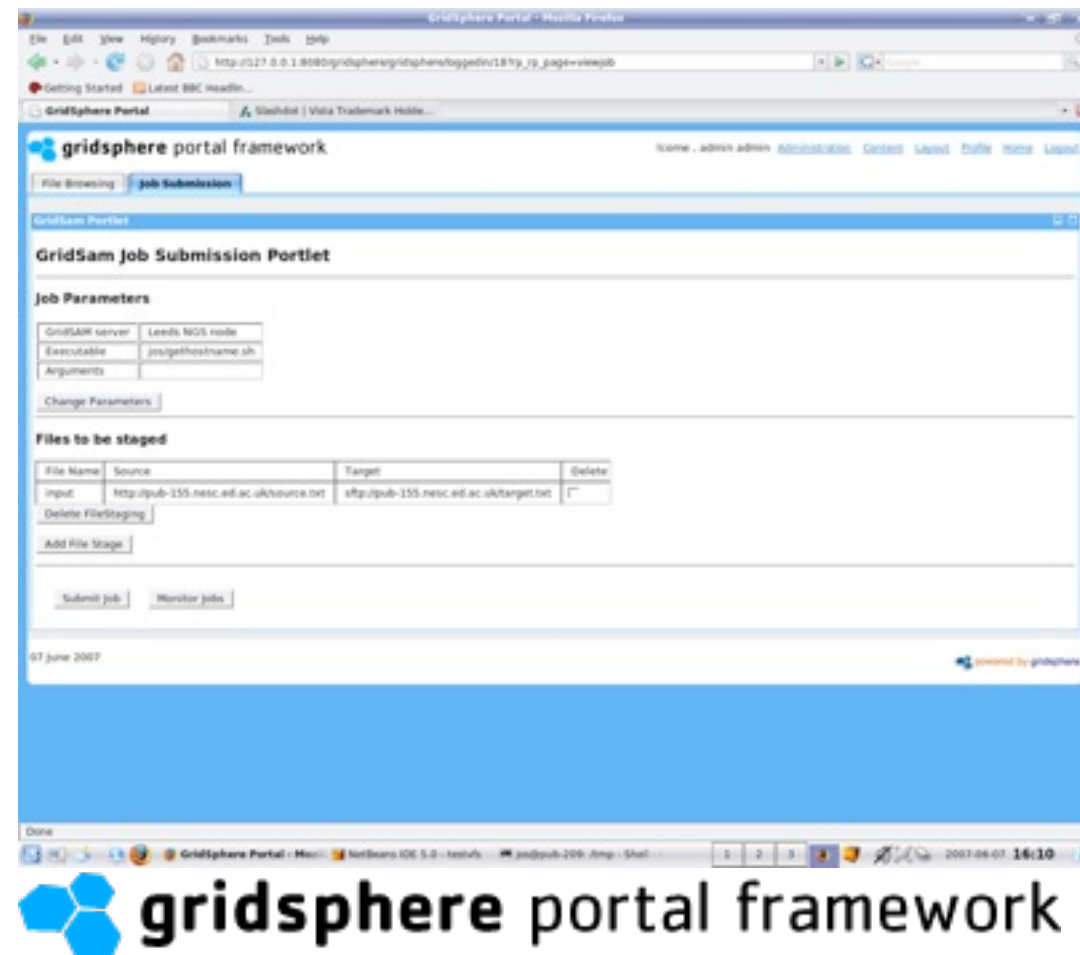# The problems with hiring a developer

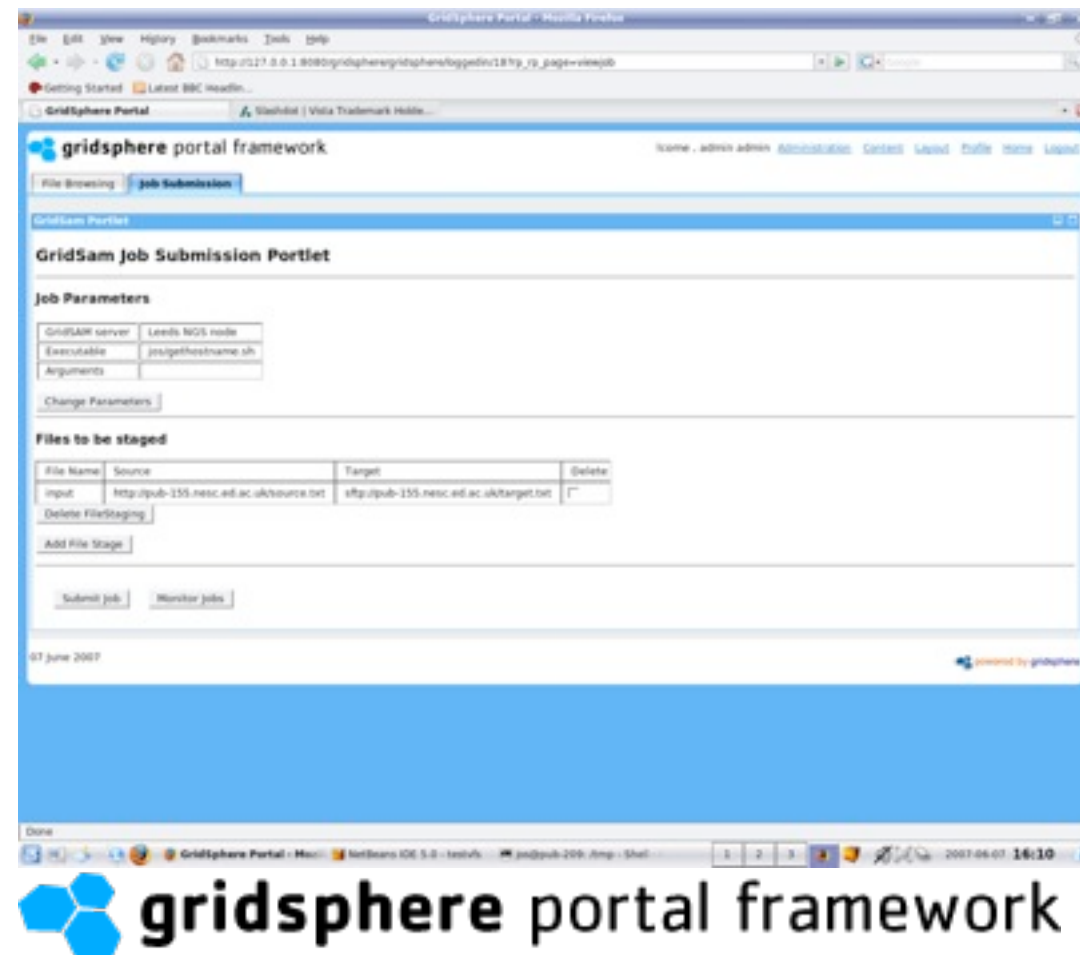Developer

The problems with hiring a developer

Developer

gridsphere portal framework

The problems with hiring a developer

The problems with hiring a developer

The Rapid Solution - Portlet Development

Developer

The Rapid Solution - Portlet Development

Developer

Writes

XML Description
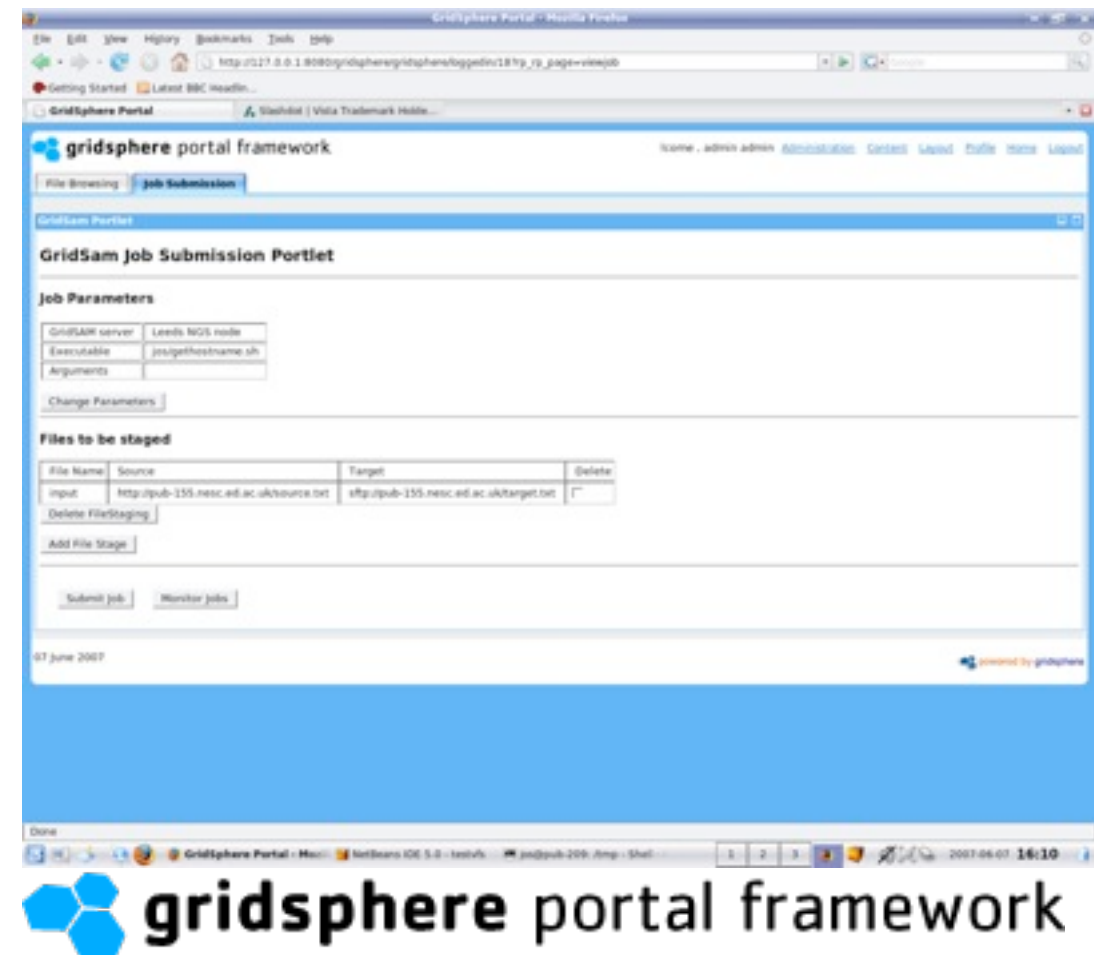
The Rapid Solution - Portlet Development

Developer

Writes

XML Description
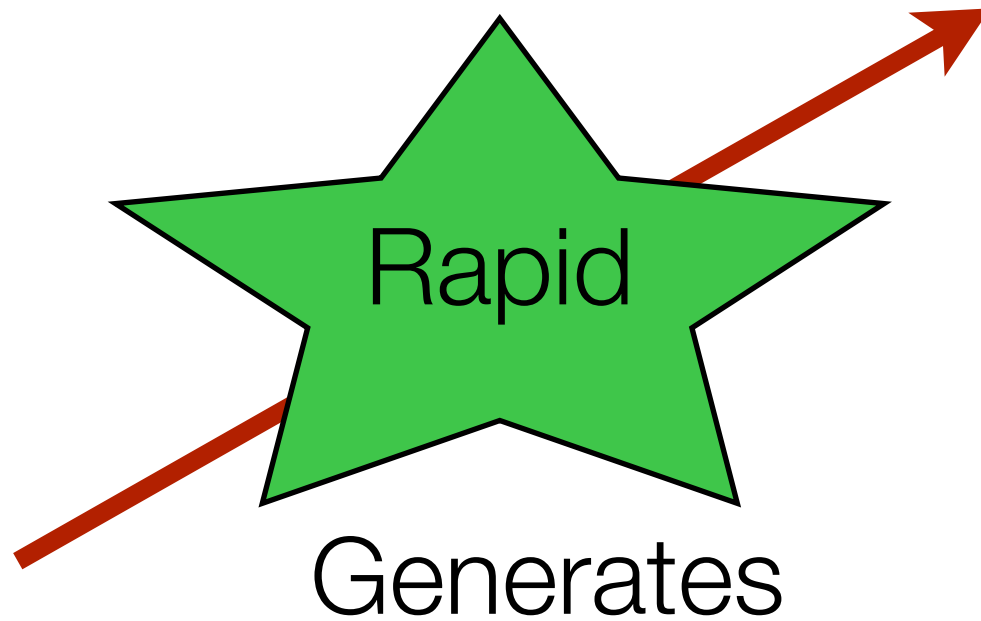
Rapid

Generates

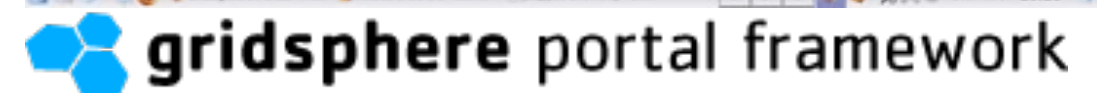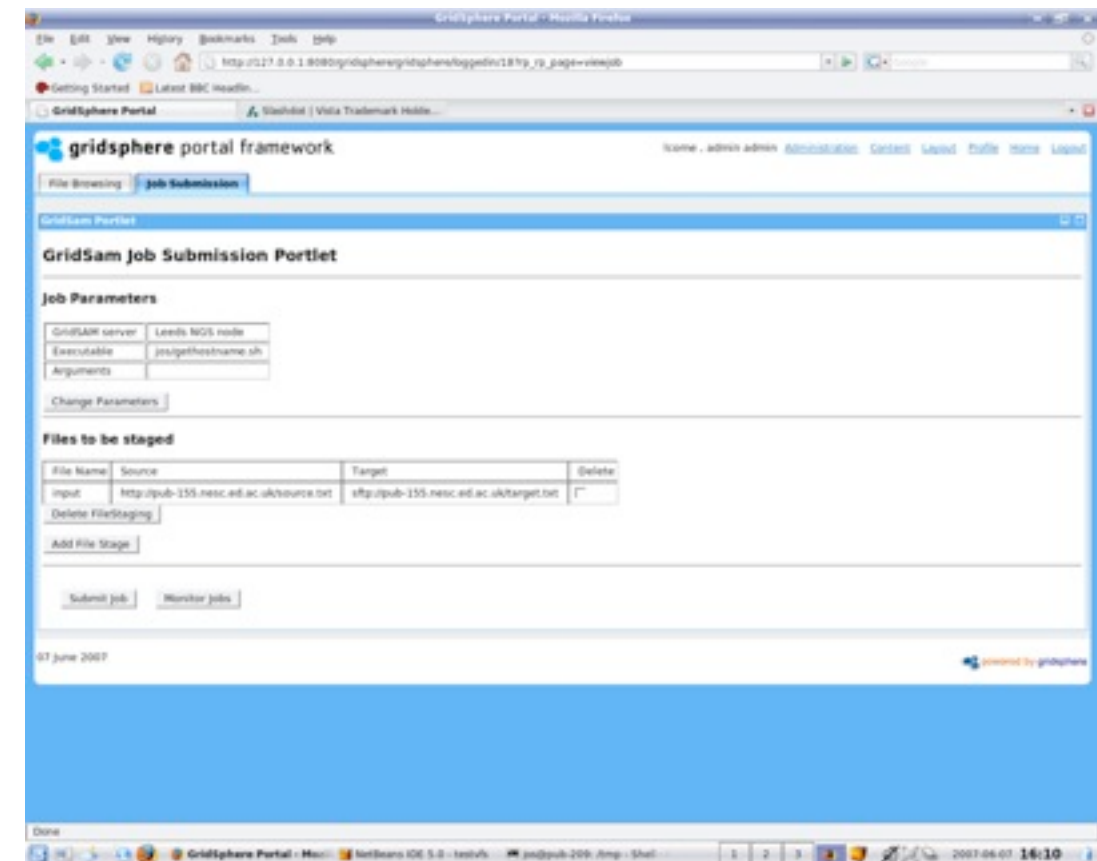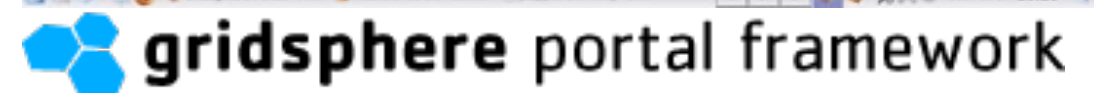# The Rapid Solution - Portlet Development

Developer

Writes

Rapid

Generates

XML Description

gridsphere portal framework

The Rapid Solution - Using the portlet

The Rapid Solution - Using the portlet

Scientist

Infrastructure

gridsphere portal framework
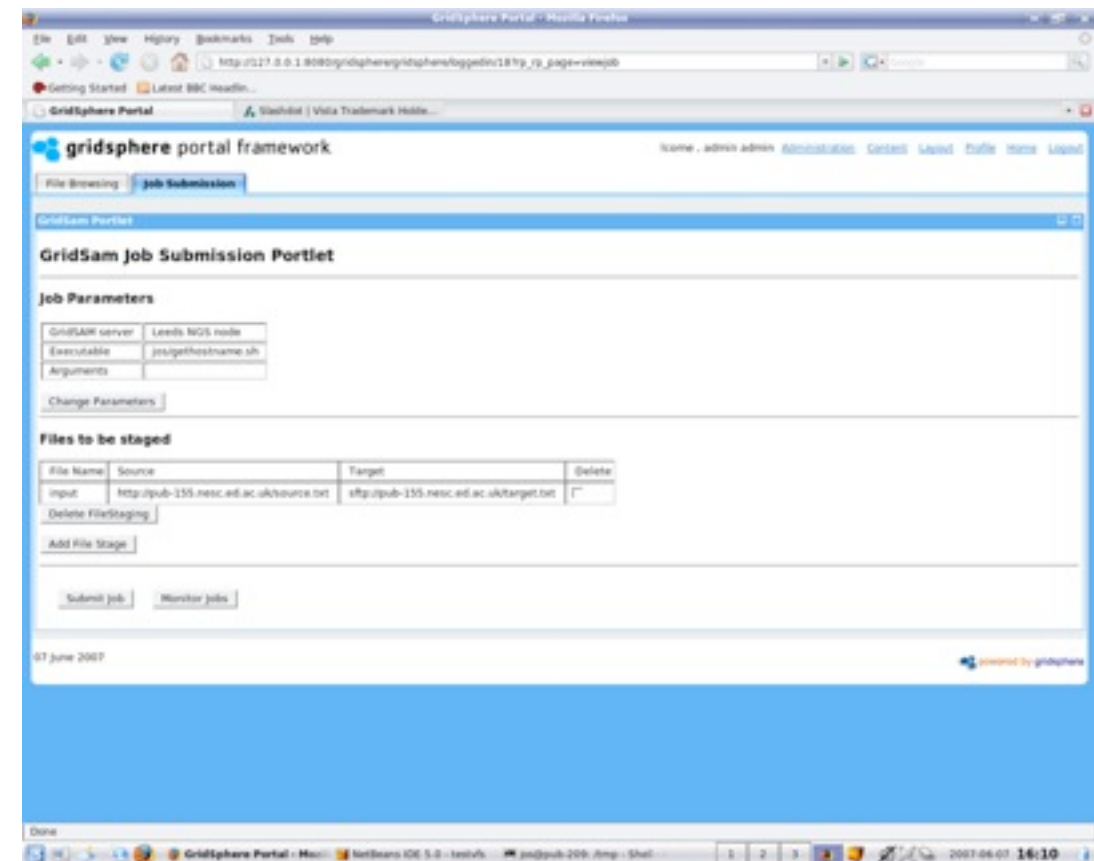
The Rapid Solution - Using the portlet

Scientist

Experiment

Infrastructure

Chemistry 2 Inorganic Lab
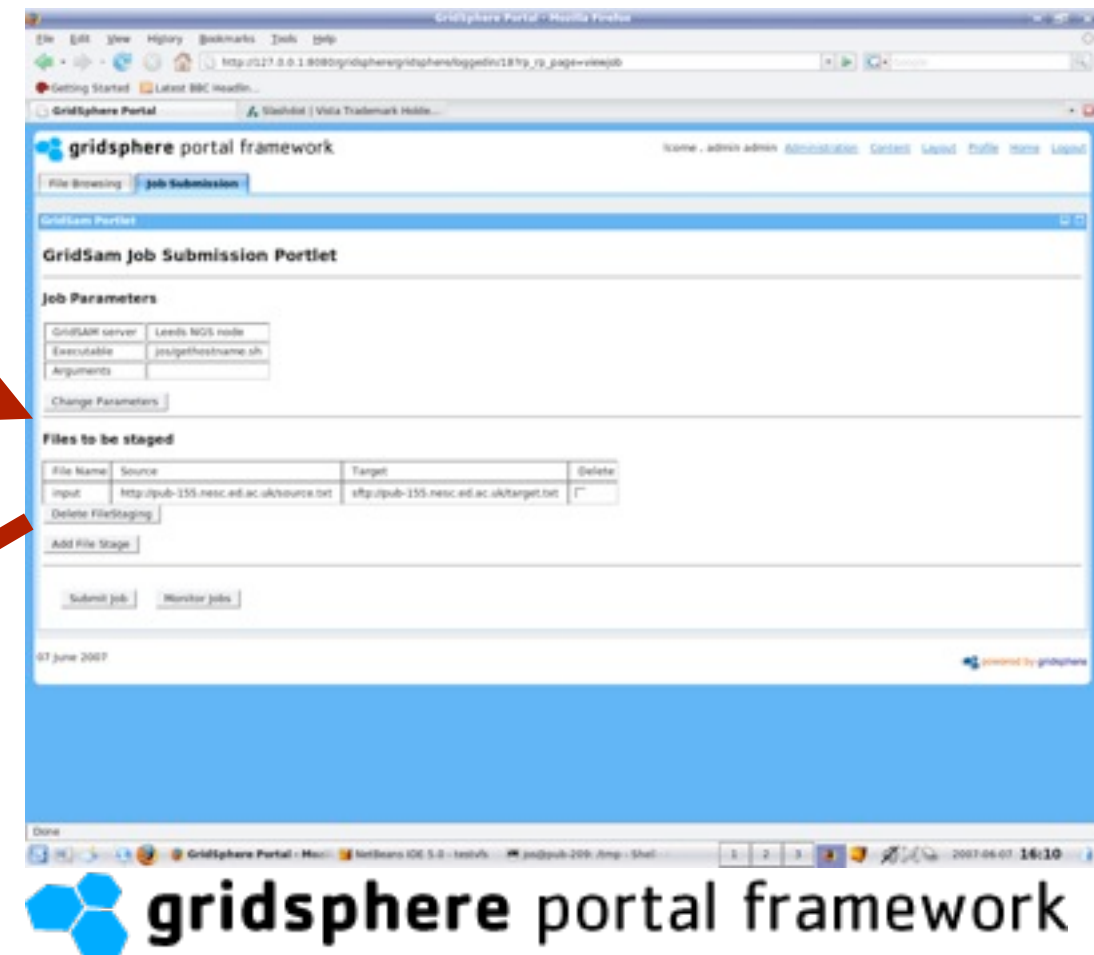
| Introduction | ▶ Ammonia | Boron Trifluoride | NH3BF3 | Sulfur Hexafluoride |

ammonia_chem2

Ammonia: Molecular Orbital (MO) Calculations

This portlet will run MO calculations on the ammonia molecule using the Gaussian 98 quantum chemistry program. All the calculations will be performed on the remote workstation 'anita-linux.chem.ed.ac.uk'.

Portlet Aims

This portlet will help you understand:

- the process of running computational chemistry calculation;
- the type of information that can be extracted from these calculations;
- the structure of a Gaussian 98 input file..

While using the portlet you should think about the chemical relevaence of the input file and the results that you see.

Portlet Structure

The portlet consists of a number pages for the various parts of the calculation:

1. setup the input file;
2. monitor the calculation;
3. view the final results.

These pages are not static web pages but are actually setting-up, running, monitoring and managing the files for the Gaussian 98 calculation. If you change things in the input file then they will affect the calculation and the results you get.

Click on the 'Next' button to load the Gaussian input file for ammonia and get started.

Next >

Done

0:04 / 0:55

Tuesday, 9 August 2011

http://193.52.21.80/jetspeed/portal/

neries portal

welcome to neries ⊗   Rapid portals improve teaching... ⊗   Windows Live Hotmail ⊗   +

neries

prototype **Seismic** **Data** **Portal**

Home   >>   WELCOME TO NERIES

WELCOME TO NERIES   MY NERIES   EVENT EXPLORER   WAVE EXP   GIVE YOUR FEEDBACK   ACCOUNT   NA4 TEST   NA5 EXPLORER   SITE MAP

Folders

RapidSeis   »

Additional Links

EMSC website   »

NERIES Project Portal   »

ORFEUS website   »

Logout

Welcome to the NERIES Portal

NERIES Seismic Data Portal
from neries

10:32   ▶   vimeo

NERIES Data Portal tools

Login to access the tools available through the NERIES Seismic Data Portal..

Event eXplorer   Waveform eXplorer   My N...
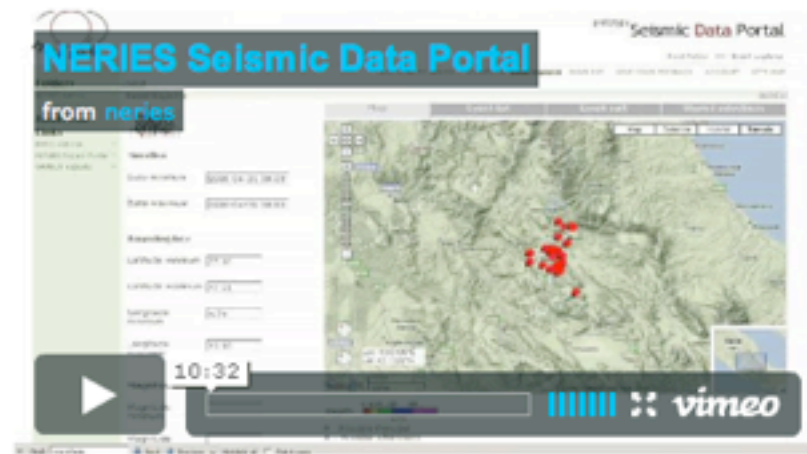
Login Portlet

Welcome aeh
Logout
Change Password

NERIES Seismic Data Portal

neries

Waveform Datasets | Latest Events | Blog NEWS | **Portal** **Blog**

Latest users' datasets composed through the **NERIES Portal**

SANTA CRUZ ISLANDS, M= 5.1, Time= 2009-10-08T14:08:3
comment: ..
published on: 2009-10-22T15:00:06
seed data - preview - sg2k - rdf metadata- quakeml

SANTA CRUZ ISLANDS, M= 5.1, Time= 2009-10-08T14:08:3
comment: ..
published on: 2009-10-22T15:53:43
seed data - preview - sg2k - rdf metadata- quakeml

SUMBAWA REGION, INDONESIA, M= 6.8, Time= 2009-11-08T19:41:4
comment: ..
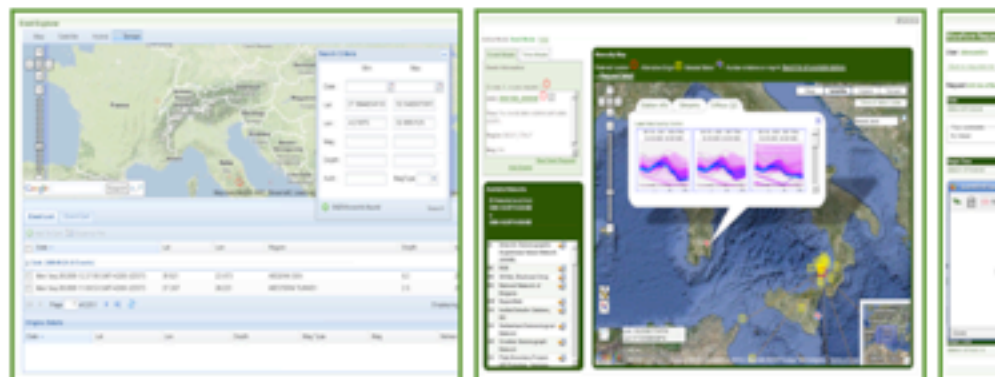published on: 2009-11-09T12:02:35
seed data - preview - sg2k - rdf metadata- quakeml

IRAQ, M= 4.2, Time= 2009-10-17T10:58:0
comment: ..
published on: 2009-10-17T11:42:07
seed data - preview - sg2k - rdf metadata- quakeml

HINDU KUSH REGION, AFGHANISTAN, M= 6.2, Time= 2009-10-22T19:51:2
comment: BS IU TU networks..
published on: 2009-10-23T11:30:25
seed data - preview - sg2k - rdf metadata- quakeml

NEAR N COAST OF PAPUA, INDONESIA, M= 6, Time=
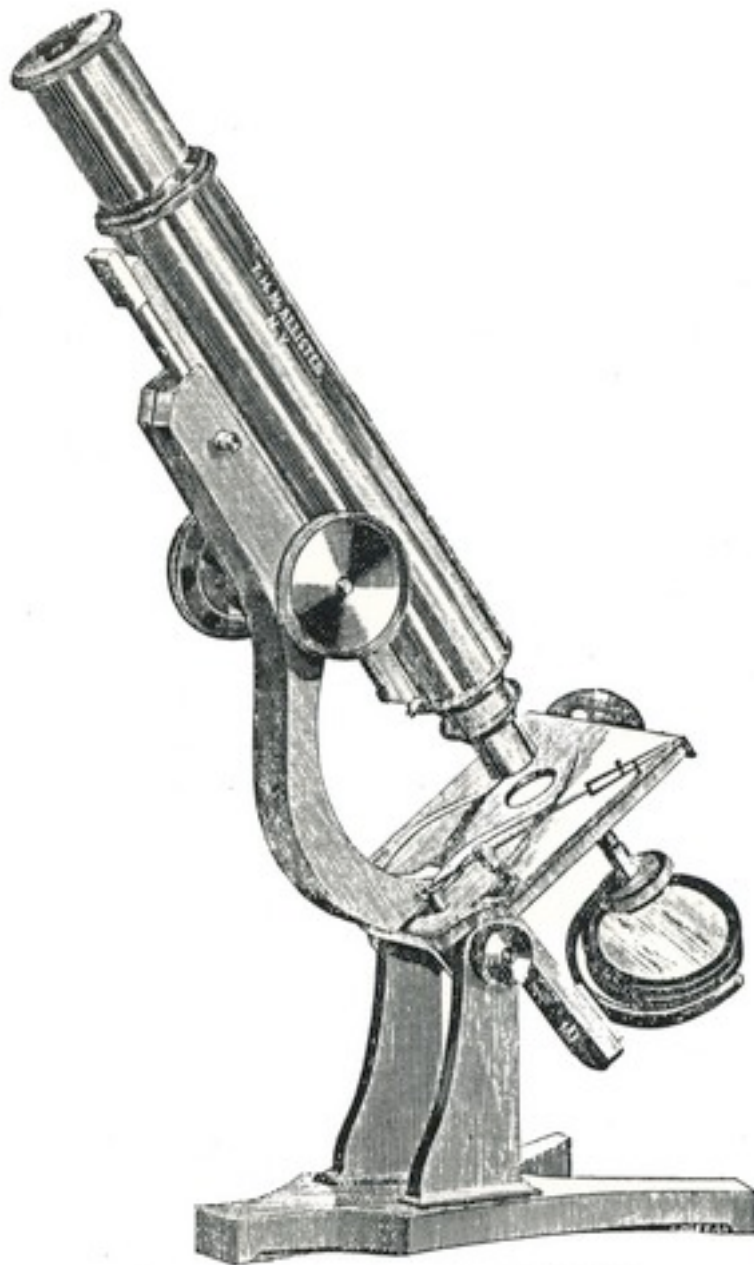
Done

Tuesday, 9 August 2011

New Use Case: Microscopy. RapidOMERO

T. H. McALLISTER'S STUDENT'S MICROSCOPE.

Obtaining Rapid

- http://research.nesc.ac.uk/rapid

  - Rapid Portlet program

  - Rapid Manual

  - Tutorials

  - Screen Casts

- https://forge.nesc.ac.uk/projects/jos/

  - Source Code (Use at Own Risk!)