

# *Rapid*

*giving computational science a friendly face*

Jano van Hemert and Jos Koetsier

[research.nesc.ac.uk/rapid](http://research.nesc.ac.uk/rapid)

School of  
**informatics**



 National  
e-Science  
Centre

*Efficient distributed systems*

*Applied computational models*

**Computer Science Research**

**Interdisciplinary Applications**

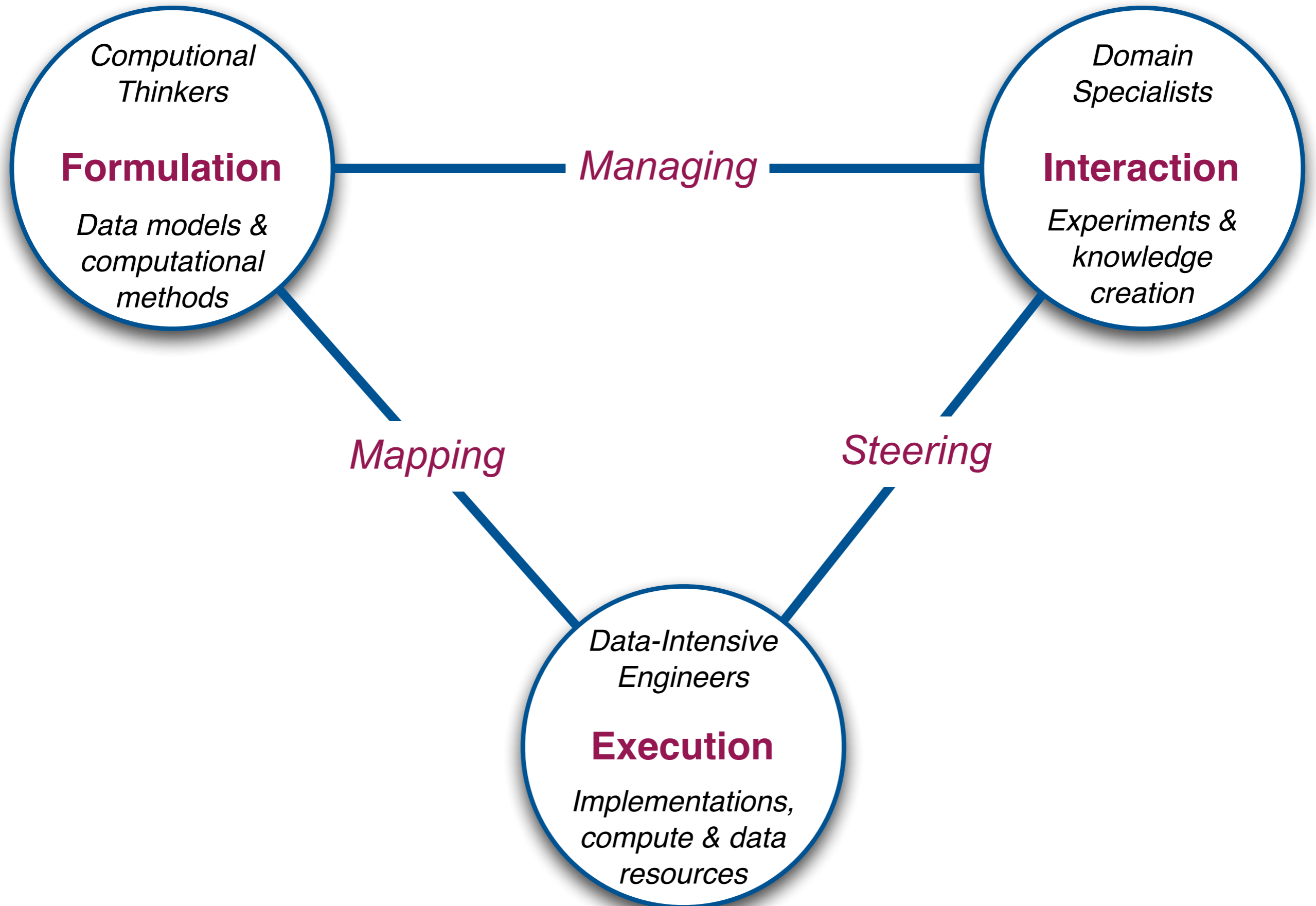
*Effective algorithms*

*Data-intensive computing*

*Collaborative environments*

*Intuitive interfaces*





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## Inbox (1 unread)

**Koye Somefun** **RE: op linked in** Sep 15 [take action](#)

Action Items: [Invitations \(3\)](#), [See all messages »](#)

## Network Updates

[See more updates »](#)

What are you working on now?

**Jano...**

[Update](#)

Jano is giving a presentation for eDIKT2 9 seconds ago - [clear](#)

Today

CONNECTION UPDATES (7)

**Tom McCallum** is now connected to **Michael Dearman** 1 minute ago

**Stefano Cagnoni** is now connected to **Mirco Passeri** 12 minutes ago

**Stephan da Silva** is now connected to **Inoo Tanaka** and **Michael Bednar-Brandt** 1 hour ago

**Cecilia Di Chio** is now connected to **Florent Nollet** 1 hour ago

**Barend Mons** is now connected to **Bart Knols** 1 hour ago

[Show more...](#)

Yesterday

STATUS UPDATES (1)

**Rokesh Jankie** and the QAFE Team are all at location implementing

## People you may know



**Adrian Jackson** <sup>2nd</sup>  
Application Consultant at EPCC, The University of Edinburgh

[invite](#) | [x](#)


**Shane Threatt [LION]**  
[shane.linkedin@yahoo.com](#)  
<sup>group</sup>  
Yahoo! Talent Acquisition Team

[invite](#) | [x](#)


**Paul Fisher** <sup>2nd</sup>  
Research Associate at University of Manchester

[invite](#) | [x](#)
[See more »](#)

## My Travel


[Full view](#)

Upcoming trips

[+ADD A TRIP](#)

**Oxford, United Kingdom** (3 days) Sep 21 - Sep 23

Fly Brain Workshop

**Bratislava, Slovakia** (3 days) Oct 7 - Oct 9  
ADMIRE F2F

[View all trips](#)

# Scientific Computing: The Stone Age

```
jvanhem2@frontend01:~/projects/molecular_anatomy/src — ssh — 114x28
#!/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!

A screenshot of a web browser displaying the GridSphere Portal. The browser window title is "GridSphere Portal - Mozilla Firefox". The address bar shows "http://127.0.0.1:8080/gridSphere/gridSphereLoggedIn/187hp\_rp\_page=viewjob". The page content includes a navigation menu with "File Browsing" and "Job Submission" tabs. The main content area is titled "GridSam Portlet" and "GridSam Job Submission Portlet". It contains a "Job Parameters" section with a table:

GridSAM server	Leeds NGS node
Executable	jos/gethostname.sh
Arguments	

Below this is a "Change Parameters" button. The "Files to be staged" section contains a table:

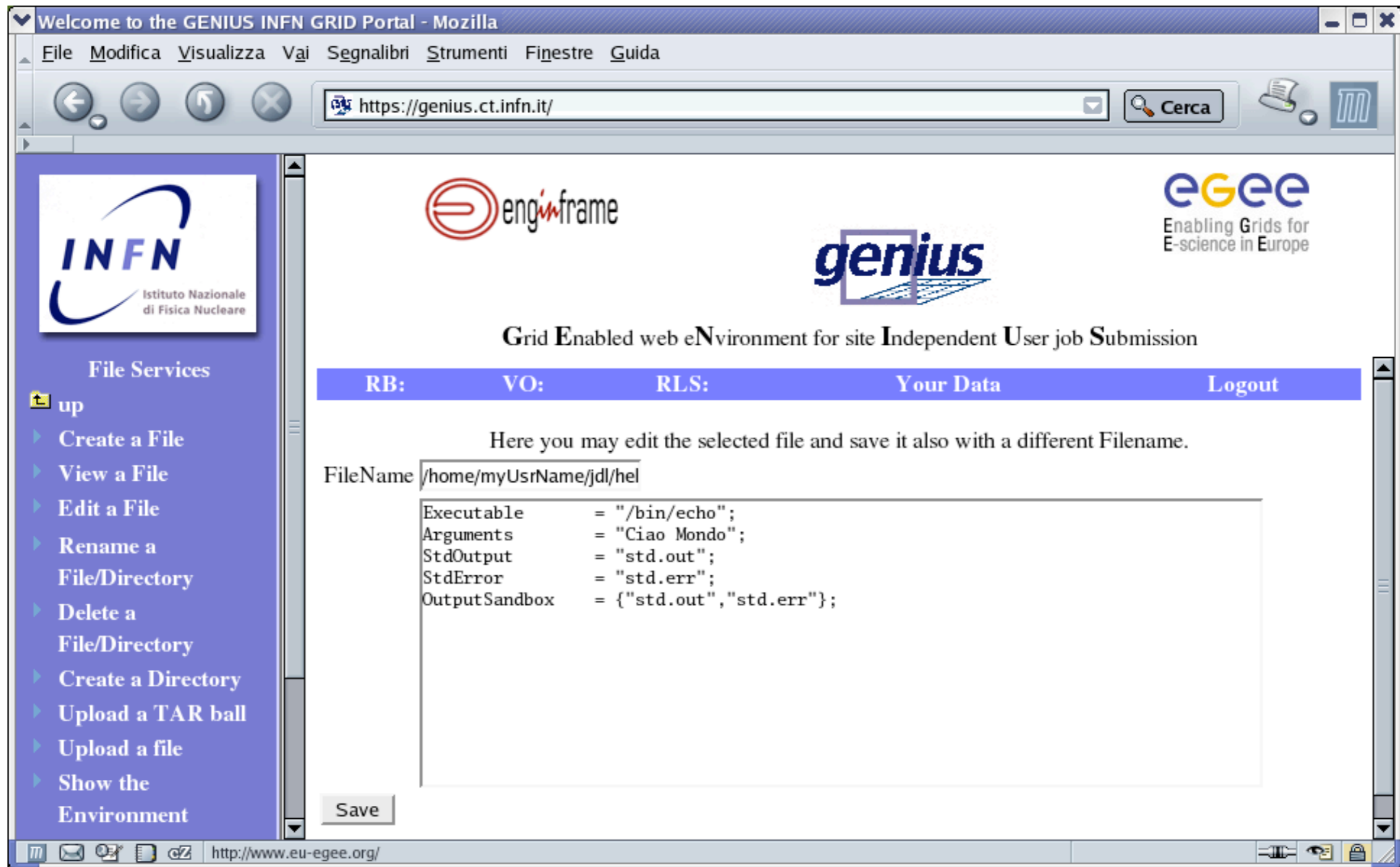
File Name	Source	Target	Delete
input	http://pub-155.nesc.ed.ac.uk/source.txt	sftp://pub-155.nesc.ed.ac.uk/target.txt	<input type="checkbox"/>

Below this table are "Delete FileStaging" and "Add File Stage" buttons. At the bottom of the portlet are "Submit job" and "Monitor jobs" buttons. The footer of the page shows "07 June 2007" and "powered by gridsphere". The browser's taskbar at the bottom shows "GridSphere Portal - Mozill", "NetBeans IDE 5.0 - testvls", and "jos@pub-209: /tmp - Shell".

 **gridsphere portal framework**



# Ridiculous portal



*source: GENIUS portal guide*

My Grid Identity: None

[Help / Get Started](#) | [Logout](#)

# General portal

- Far too many boxes to fill in
- Arcane technical content required
- Basically a command-line / XML-editor in disguise

- [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](#)

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

- [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

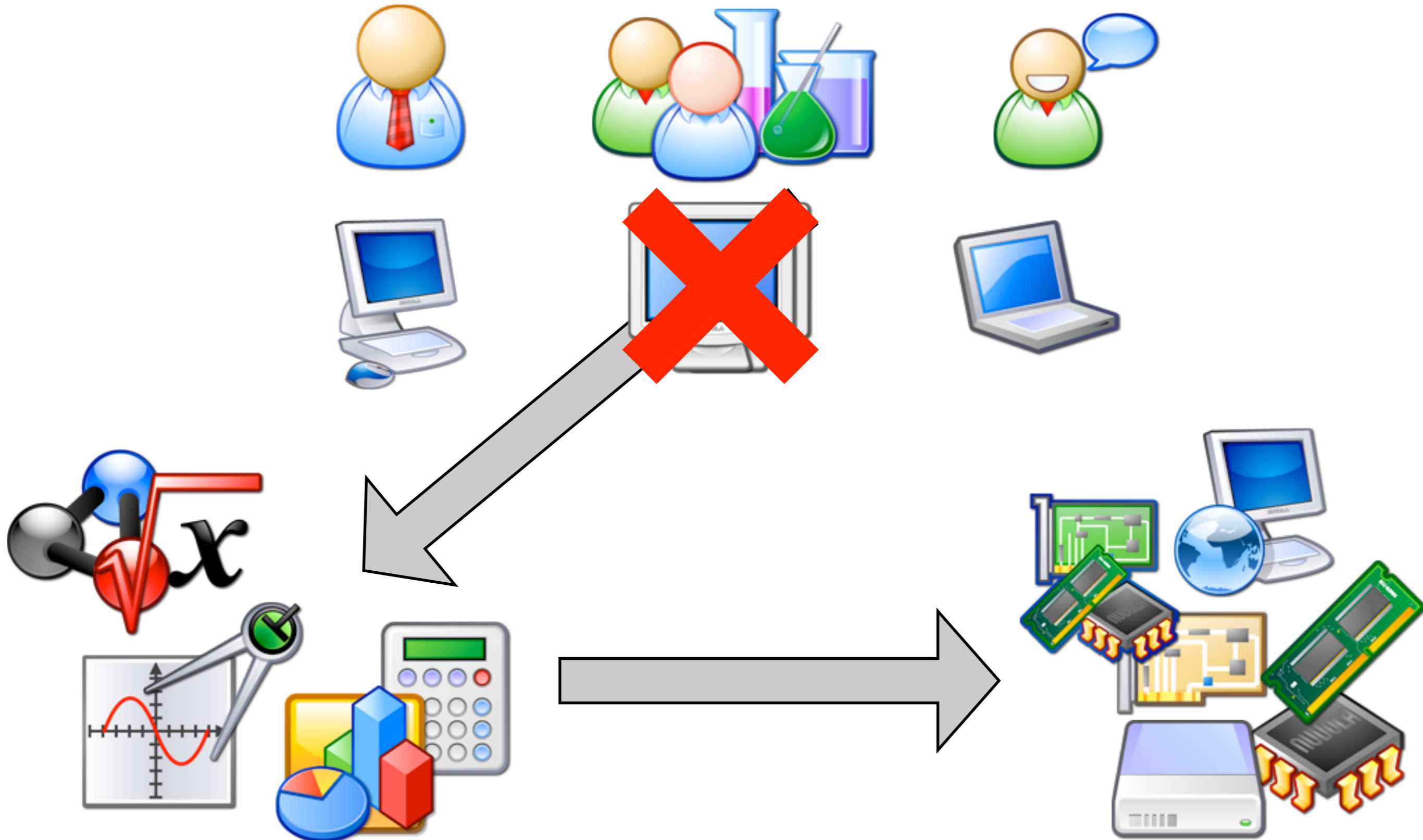
### Environment Variables (None): [Edit](#)

### File Systems: [Edit](#)

File System Name	MountPoint	Type
WORKINGDIR		normal
<b>USRNGS</b>	<b>/usr/ngs</b>	normal



# Not about one portal for all



# Task-specific portal

GridSphere Portal - Windows Internet Explorer

https://lepus.nesc.gla.ac.uk/gridsphere/gridsphere?cid=geronimo

GridSphere Portal

Nano-CMOS Portal English

GridSphere Management **Services** VP-Man Test

Atomistic Data Service **Atomistic Simulator** Aurora

Atomistic Simulator

Atomistic Simulator

Input input.inp

TIF input.tif

Demo mode

Execution Target EEE Glasgow SGE (golem.elec.gla.ac.uk)

Run Simulation

Refresh Status

- EEE Glasgow SGE (golem.elec.gla.ac.uk)
- Local Machine (lepus.nesc.gla.ac.uk)
- NGS Leeds Compute Node
- NGS Manchester Data Node
- NGS Oxford Compute Node
- NeSC (Glasgow) Condor Pool

# GridQTL

### IBD Module

Pedigree: C:\LDLA\pedigree.txt      Markers: C:\LDLA\markers.gen.txt

Traits: C:\LDLA\traits.txt      Map: C:\LDLA\map.txt

Output: simN100T100M10.zip     

Errors

Traits:  Y

Save G matrices:  Yes/No

Method:  M&G    H&HS    R

Search Parameters:  (Every - cM | At - cM (File) | At - cM (Hand))

Markers Use:  (All | Closest | Estimate)

Demographic History: C:\LDLA\history.txt

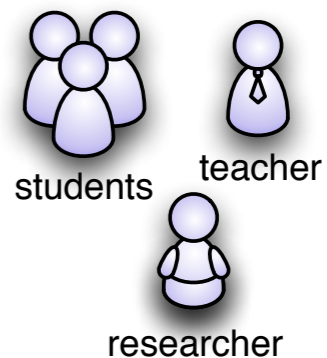
Analysis:   Display Grid Activity

**ASReml instructions panel coming soon...**

# Rapid

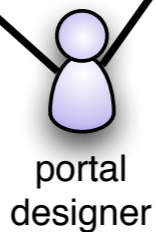
# Rapid

giving computational science a friendly face



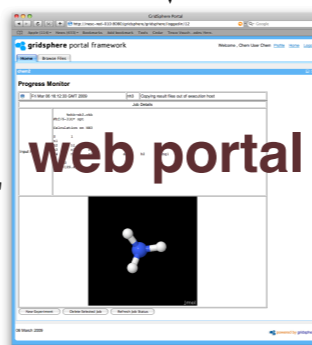
XML interface, task & resource description

1. specifies 2. uses

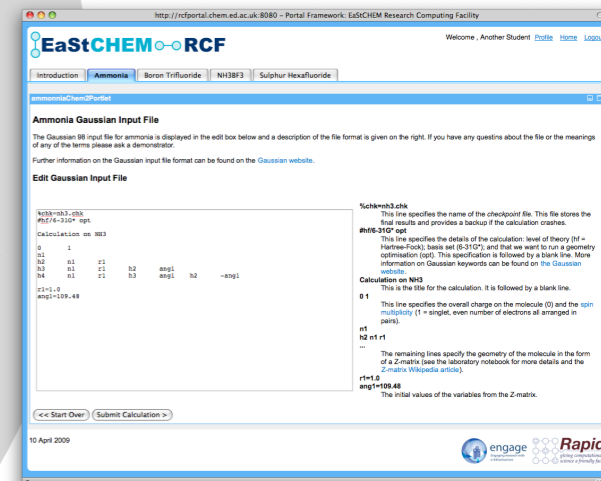


3. deploys

4. performs task

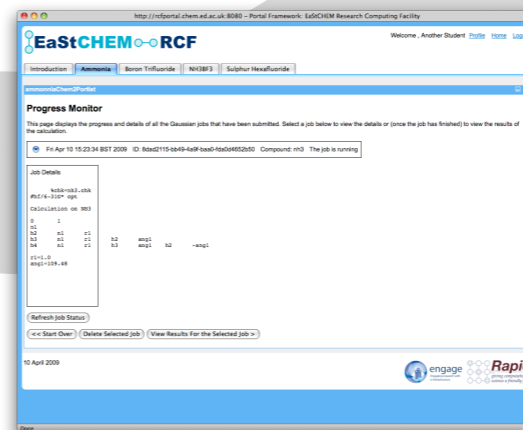


5. configures



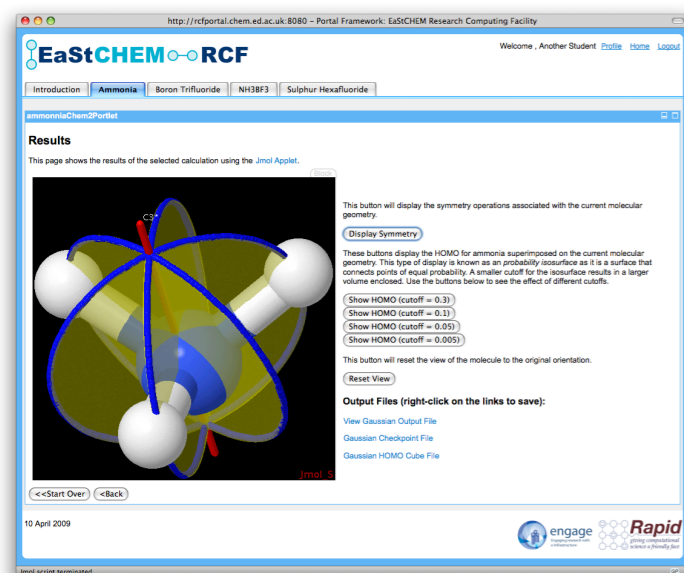
6. runs jobs

7. monitors



8. returns results

9. analyses results



# Simplicity of one XML file

Name	
<?xml version="1.0" encoding="UTF-8" ?>	
▼ rapid	
= xmlns	http://www.ne
= xmlns:x	http://www.w
▼ page	
= name	filterone
▶ datastage	
▶ datastage	
▶ posix	
x:h1	Filter an Image
▶ x:table	
x:br	
x:br	
▶ x:table	
▼ navigate	
= display	Review and Su
= nextpage	submit
▶ page	
▶ page	
▶ filesystemlist	
▶ submissionsservers	

**gridsphere portal framework**

Welcome , Jano van Hemert [Administration](#) [Content](#) [Layout](#) [Profile](#) [Home](#) [Logout](#)

**Home**

A Rapid Portlet

### Filter an Image on the NGS

**Choose Image**

<b>File System:</b>	<input type="radio"/> Portal Host <input type="radio"/> Manchester NGS Node <input type="radio"/> Oxford NGS Node <input type="radio"/> Leeds NGS Node <input type="radio"/> Pub-155-ftp <input checked="" type="radio"/> Pub-155
<b>Image:</b>	./.. Link badelepht.jpg <b>paint.jpg</b> unique.jpg
<b>Image Filename:</b> /home/fileuser/Images/paint.jpg	

27 November 2007

powered by gridsphere

# Taskflow-based approach

The image illustrates a taskflow-based approach through three components:

- XML Metadata:** A tree view of XML metadata for a 'rapid' portlet. The 'page' element is circled in red. The metadata includes:
  - xmlns
  - xmlns:x
  - page (circled in red)
    - name
    - datastage
    - datastage
    - posix
    - x:h1
    - x:table
    - x:br
    - x:br
    - x:table
    - navigate
      - display
      - nextpage
    - page (circled in red)
    - page
    - filesystemlist
    - submissionsservers

- Gridsphere Portal Screenshot 1:** Shows the 'Filter an Image on the NGS' portlet. The 'Choose Image' section includes a 'File System' dropdown (selected: Pub-155) and an 'Image' list (selected: paint.jpg). The 'Image Filename' is /home/fileuser/Images/paint.jpg. A red arrow points from the 'page' element in the XML to this screenshot.
- Gridsphere Portal Screenshot 2:** Shows the 'Filter Job:' portlet. The 'Filter' is 'emboss' and the 'Input Image' is '/home/fileuser/Images/paint.jpg'. The 'Submit to Host' dropdown is selected: Manchester. A red arrow points from the 'page' element in the XML to this screenshot.

# Define Compute Resources

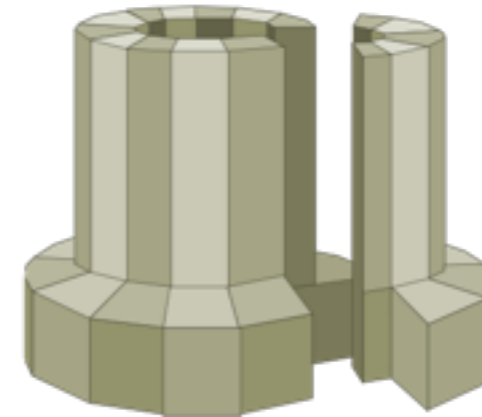
---

- Condor / Sun Grid Engine / PBS / GridSAM / Fork process

```
<condor name="condorlocal">
  <bin>/Users/fileuser/condor/bin</bin>
  <universe>vanilla</universe>
  <submitline>priority = 10</submitline>
  <submitline>image_size = 20</submitline>
  <filesystemname>Local File System</filesystemname>
  <condorconfig>CondorFS</condorconfig>
</condor>

<sungridengine name="sgelocal">
  <sgeroot>/home/sge/sge</sgeroot>
  <filesystemname>Local File System</filesystemname>
</sungridengine>

<fork name="forkpub-155">
  <filesystemname>Pub-155</filesystemname>
</fork>
```

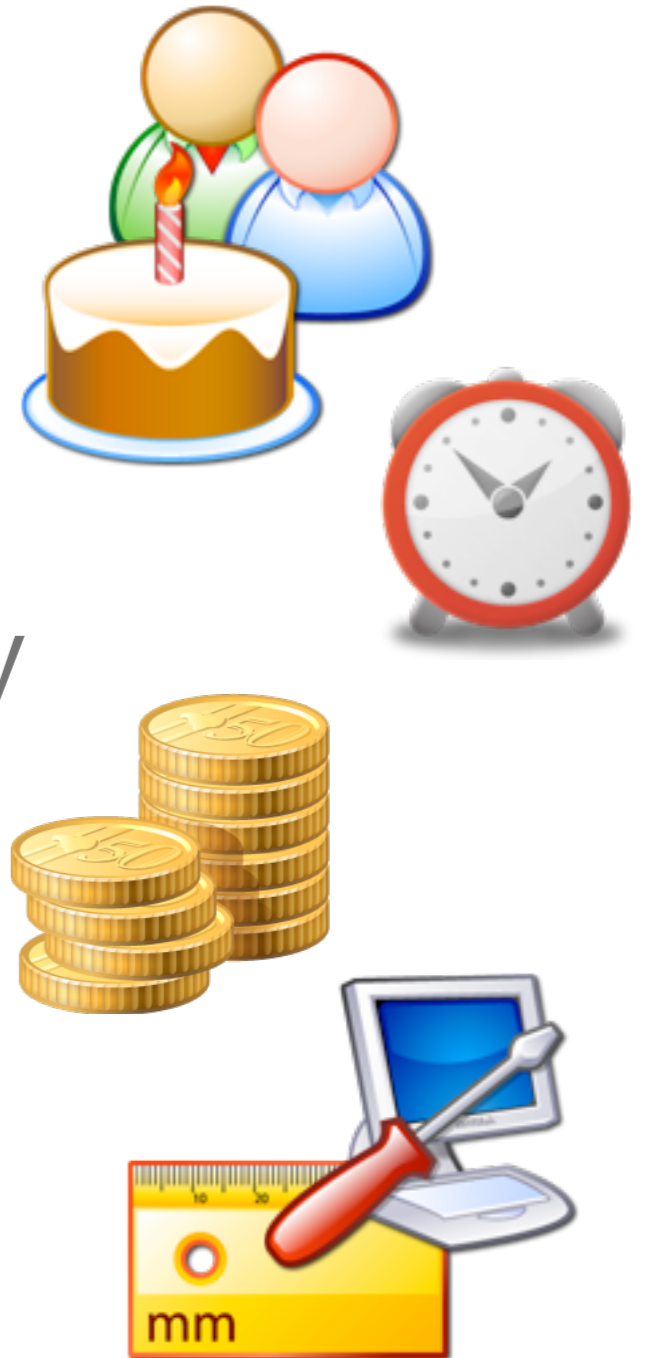




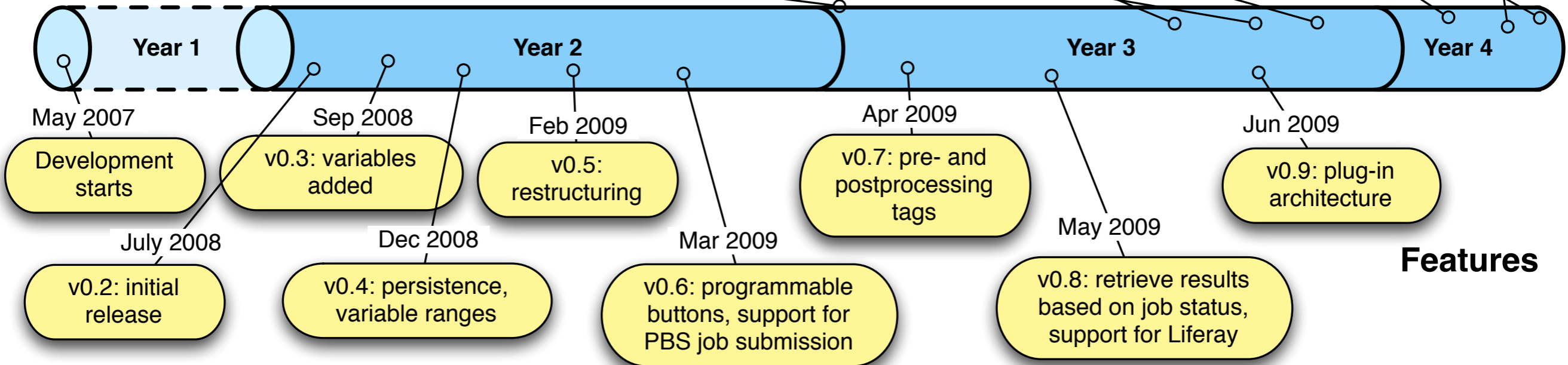
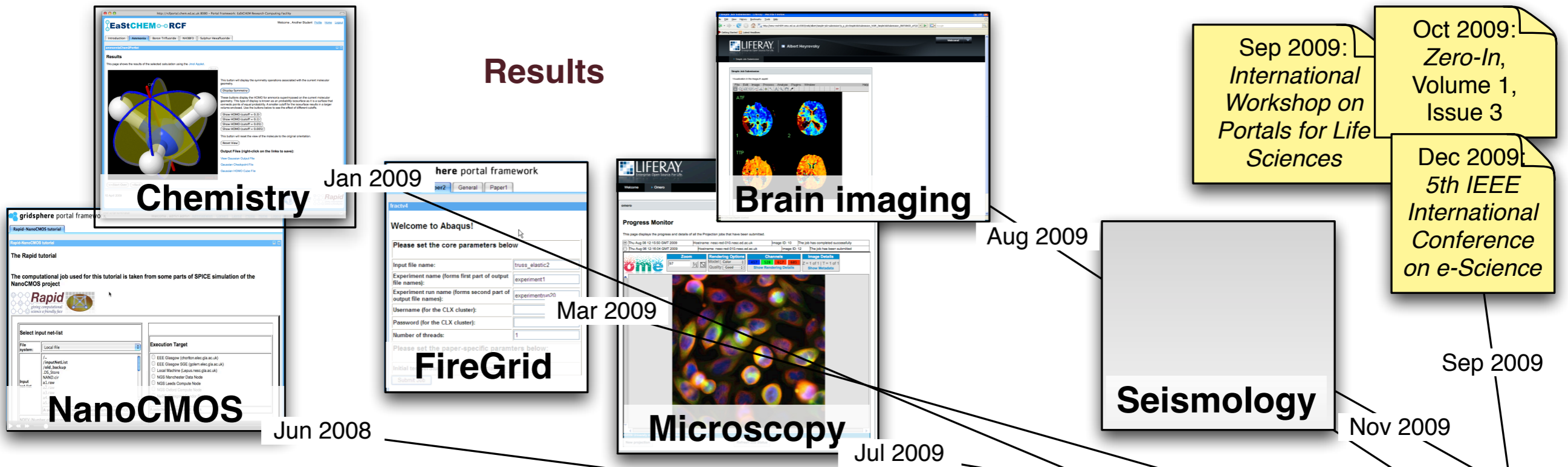
## Why choose Rapid?

---

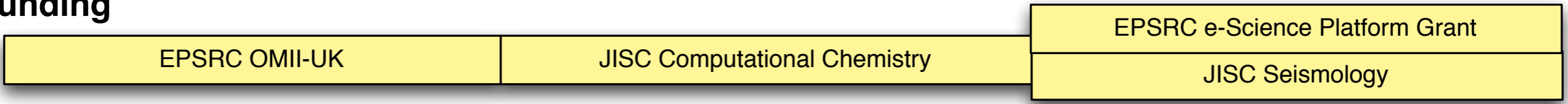
- Focuses on users' tasks
- Delivers solutions quickly
- Enables ownership by the community
- Lowers development costs
- Lowers maintenance effort



# Use Cases



**Funding**



http://hesc-red-009.nesc.ed.ac.uk:58767/web/albert

Google Search

Volume Reconstruction - Liferay

**LIFERAY** Enterprise Open Source For Life

**Albert Heyrovsky**

Welcome!

Volume Reconstruction | Image Registration | Perfusion Quantification

Volume Reconstruction

Please enter your Eddie username and password.

Username:

Password:



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 relevance 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 >

Omero liferay.com



Welcome Test Test!

Add Page

Welcome Omero NHG

omero

### Project images in OMERO

This profile projects a selected image omers, projects it and copies it back into omers

Username:	root
Password:	
Omero Host:	Omero Host at NCSU
Image ID:	1
Submit Job To:	<input checked="" type="radio"/> Condor Cluster <input type="radio"/> PBS cluster <input type="radio"/> Nexas-red-010 computer

Continue

Settings Online Friends (0)

# research.nesc.ac.uk

Jano van Hemert & Malcolm Atkinson

## Research Assistants

Jos Koetsier

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## PhD Students

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