

Details

Rapid can fork remote posix processes, submit compute jobs to Condor, Sun Grid Engine, PBS and, via GridSAM, to Grid infrastructures.

Rapid portlets rely on Apache Tomcat and a portal container such as Gridsphere, Liferay, Pluto or WebSphere to run.

Rapid is released and developed under an Open Source license. It is free to use.

Solutions

Rapid has provided solutions for brain imaging, chemistry, seismology, microscopy and engineering.



Want your own portal?
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Rapid is a cost-effective and efficient way of designing and delivering portal interfaces to applications that require remote compute resources

Results
This page shows the results of the selected calculation using the Jmol Applet.

This button will display the symmetry operations associated with the current molecular geometry.
Display Symmetry

These buttons display the HOMO for ammonia superimposed on the current molecular geometry. This type of display is known as a probability isosurface as it is a surface that connects points of equal probability. A smaller cutoff for the isosurface results in a larger volume enclosed. Use the buttons below to see the effect of different cutoffs.

Show HOMO (cutoff = 0.3)
Show HOMO (cutoff = 0.1)
Show HOMO (cutoff = 0.05)
Show HOMO (cutoff = 0.005)

This button will reset the view of the molecule to the original orientation.
Reset View

Output Files (right-click on the links to save):
[View Gaussian Output File](#)
[Gaussian Checkpoint File](#)
[Gaussian HOMO Cube File](#)

10 April 2009

<http://research.nesc.ac.uk/rapid/>

How Rapid Works

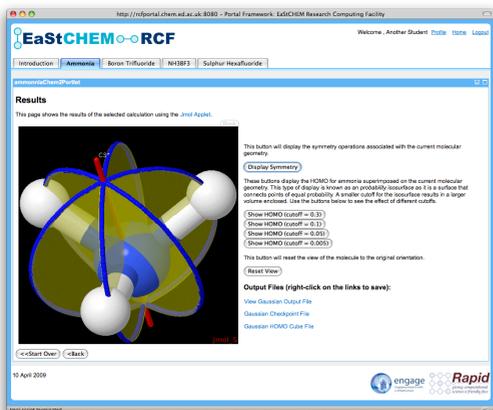


1. The portal designer specifies the user interface and logic flow of a task. This specification is created in one XML file.



2. S(he) uses Rapid to generate the portlet.

portal designer



9. These results can then be analysed by embedding web-based visualisation components.

8. returns results

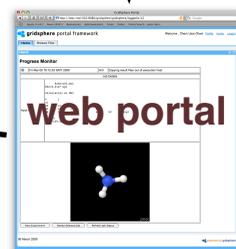
8. When the compute jobs finishes the results can be transferred to an appropriate location.



compute resources

3. The portlet is deployed into a portal container compliant with the JSR 168 industry standard.

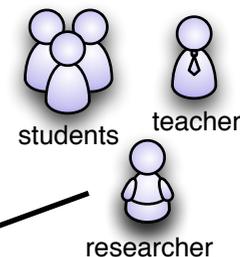
3. deploys



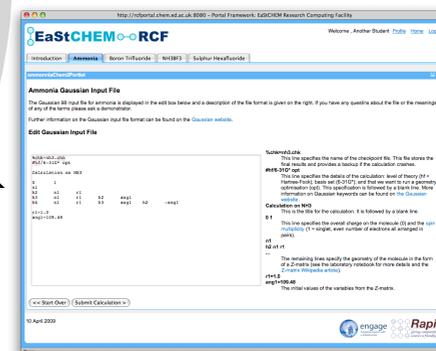
5. configures

4. Once deployed, portal users access the new portlet using a web browser to log in to the portal.

4. performs task

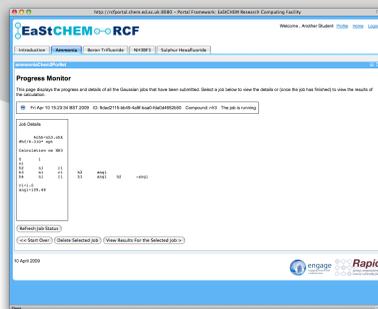


5. The user configures the task using an intuitive graphical interface with file browsers, drop-down menus, radio buttons and check boxes.



7. The portlet monitors the progress of all tasks submitted.

7. monitors



6. This transfers control to the computational task manager embedded in each Rapid portlet, which runs the appropriate compute jobs on designated compute resources.

6. runs jobs