



RapidSeis: Rapid Portlet Building

Jos Koetsier

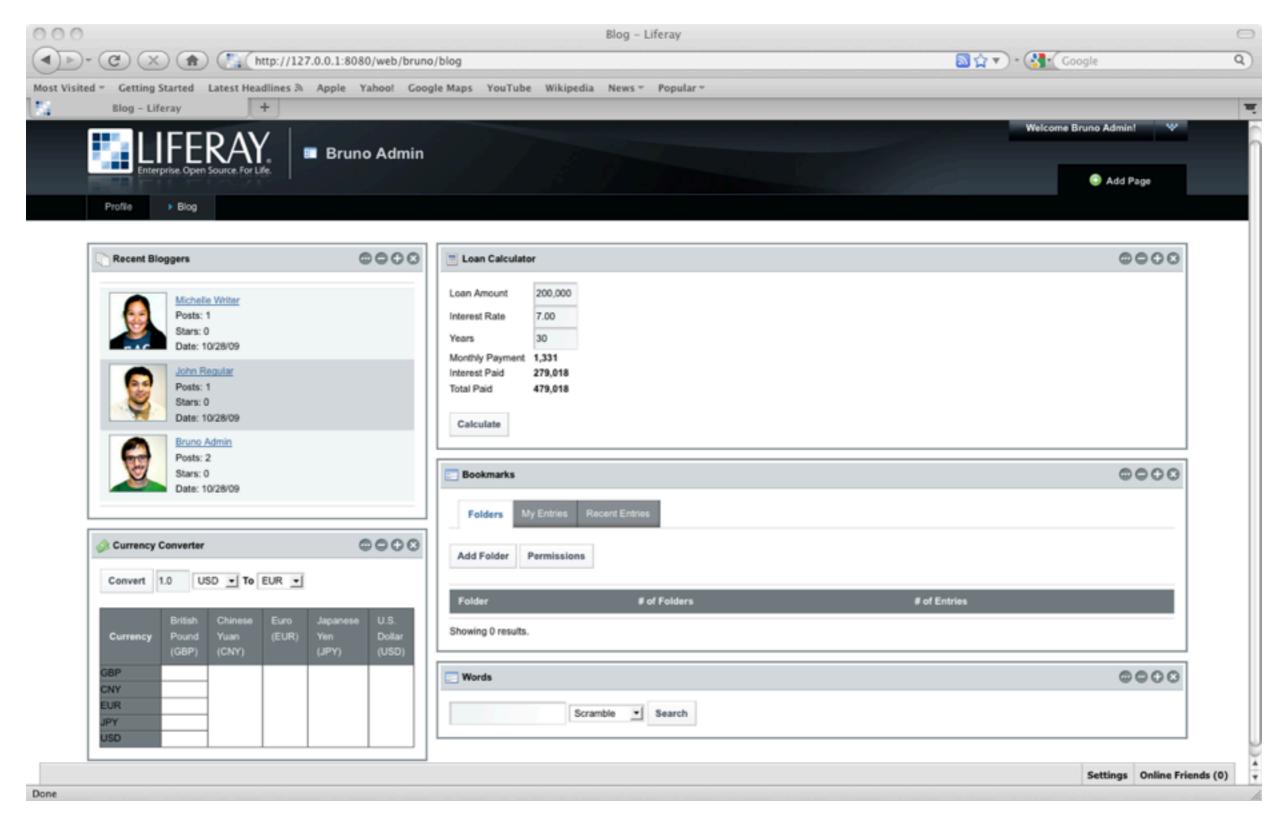


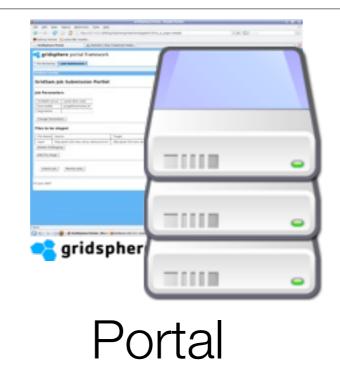


Portals and Portlets

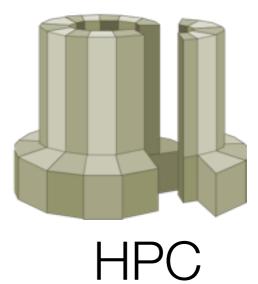
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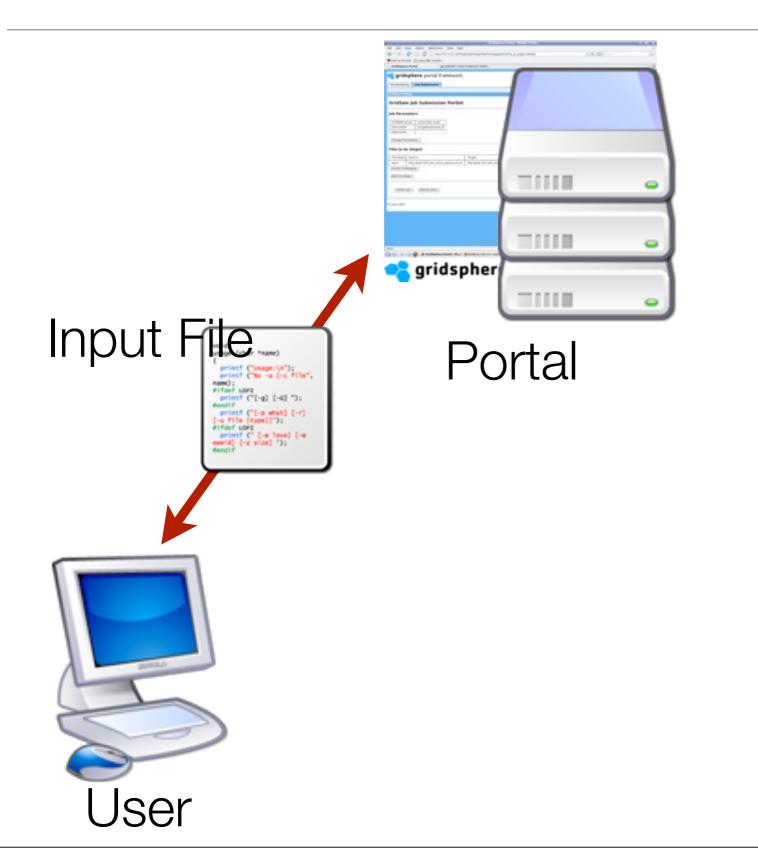
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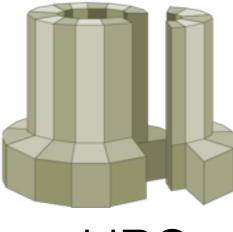




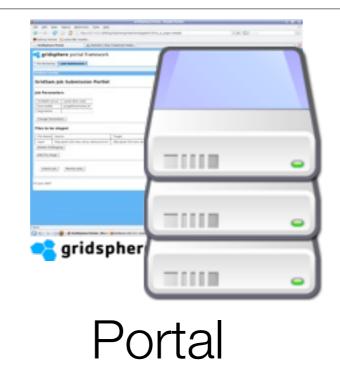




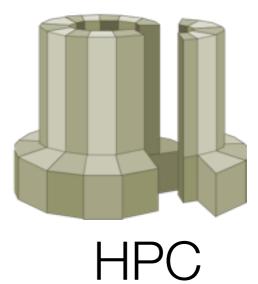


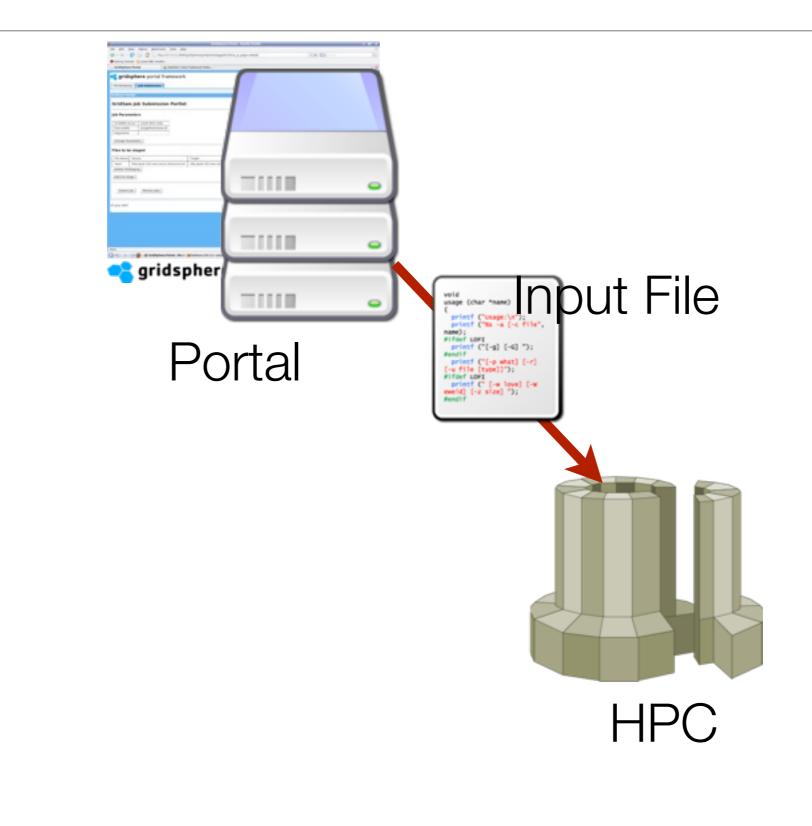




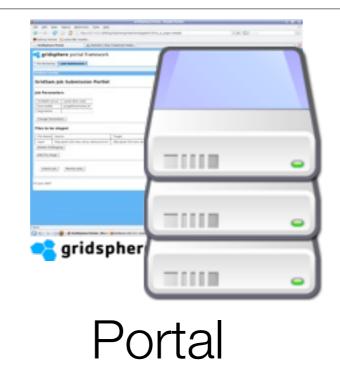




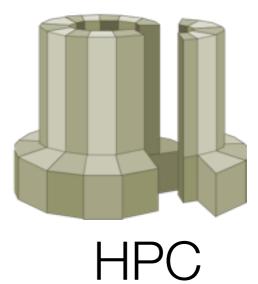


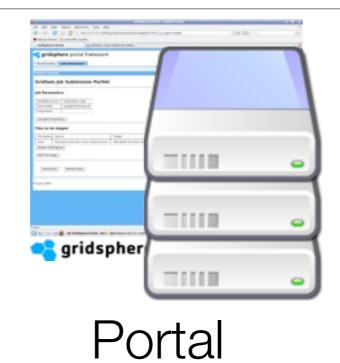


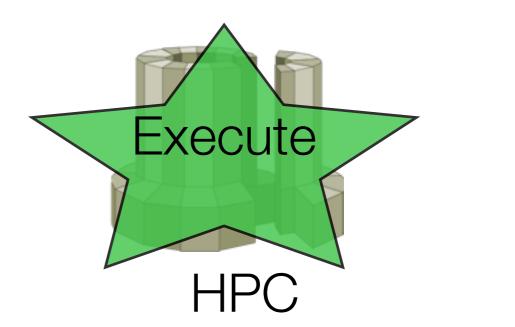




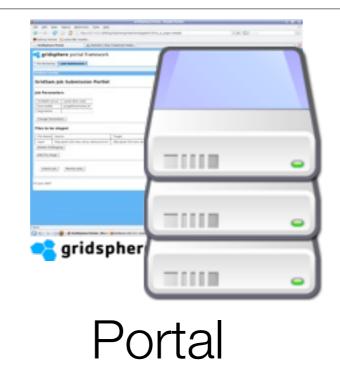




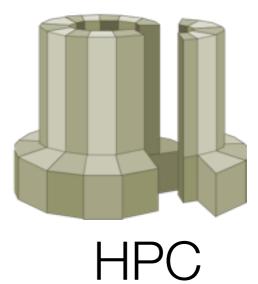


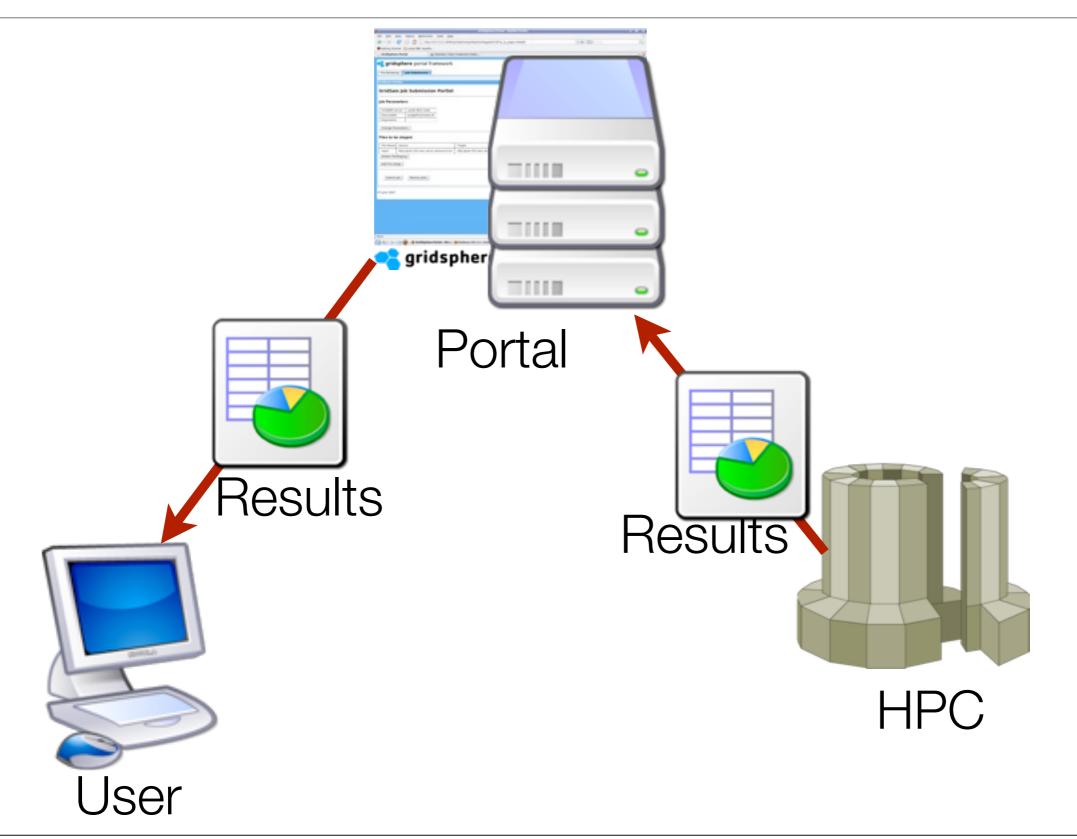














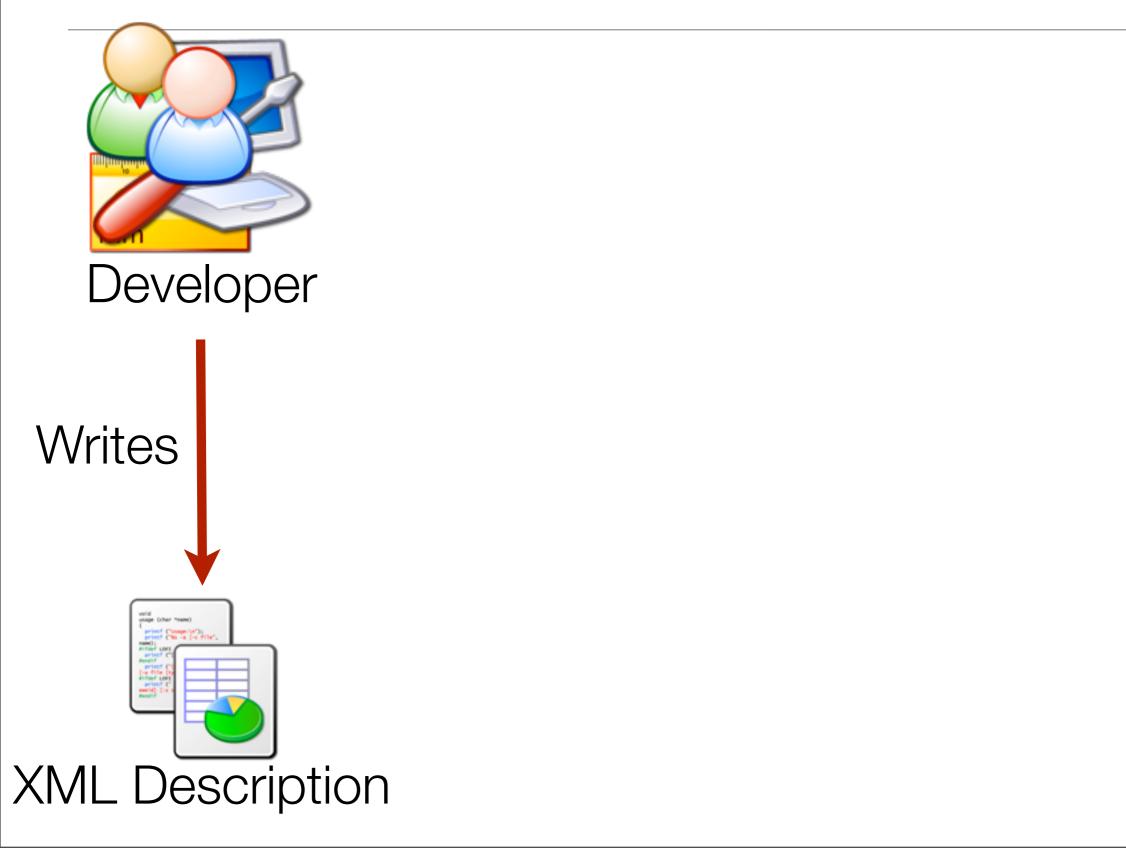
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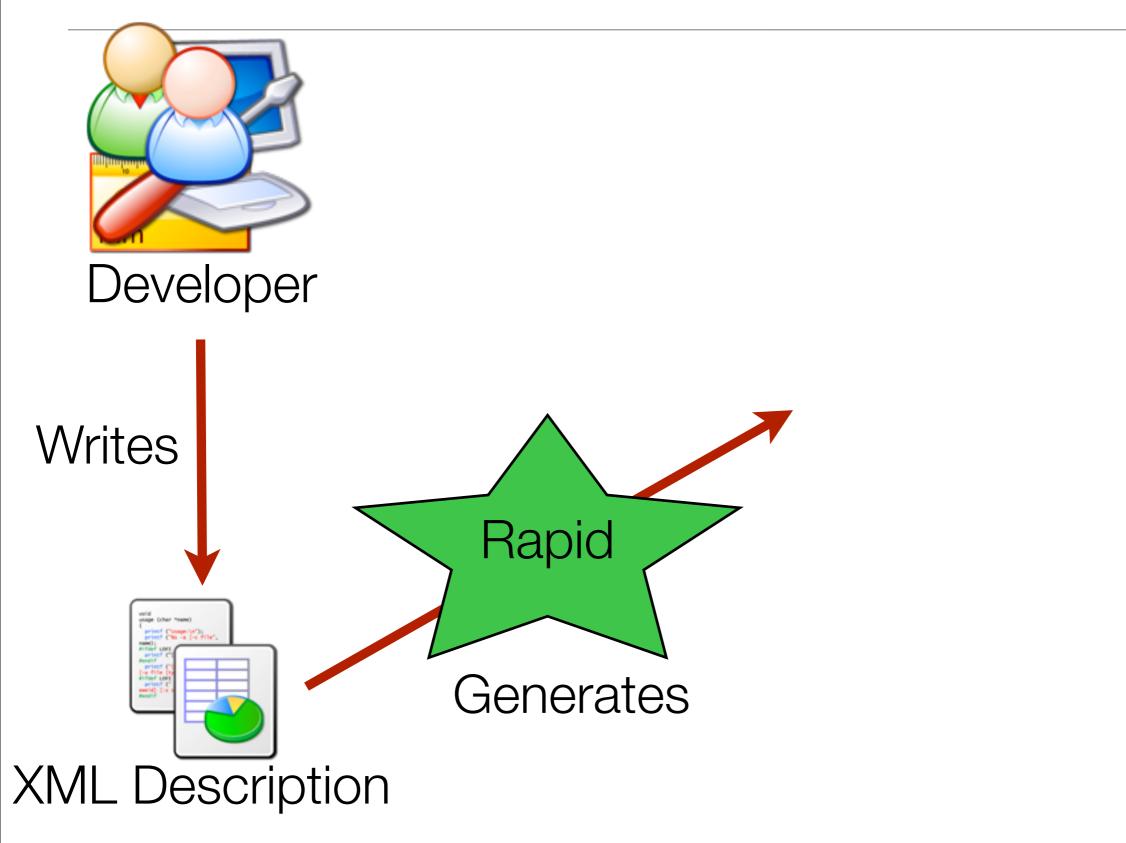


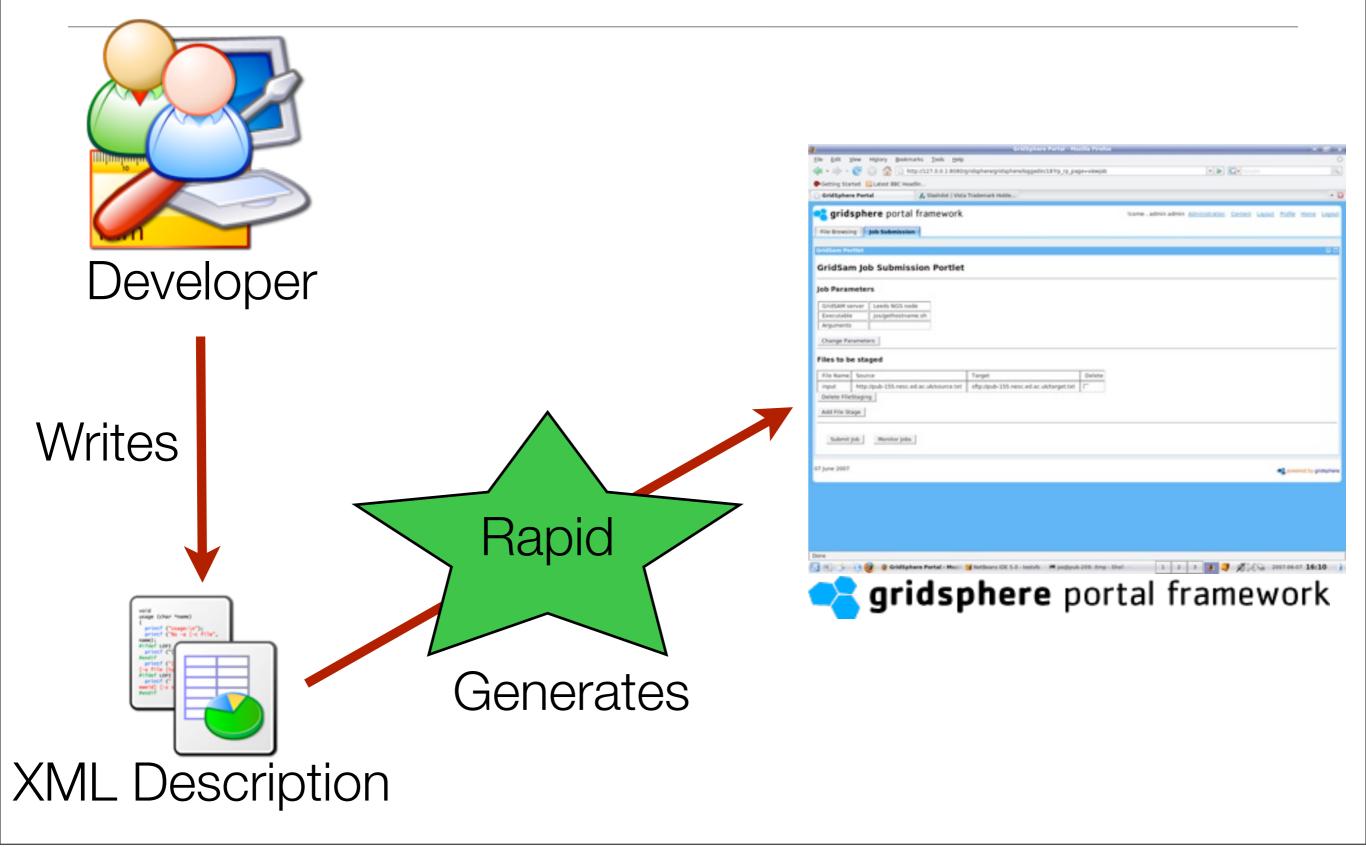
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Previous project using Rapid - ScotChem

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Welcome Omero NH3 Fractal
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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 workstationegg.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 Nextbutton to load the Gaussian input file for ammonia and get started.
Next >

Enhancing Rapid - Andy's requirements

• Dynamic User Interface and RDF database access

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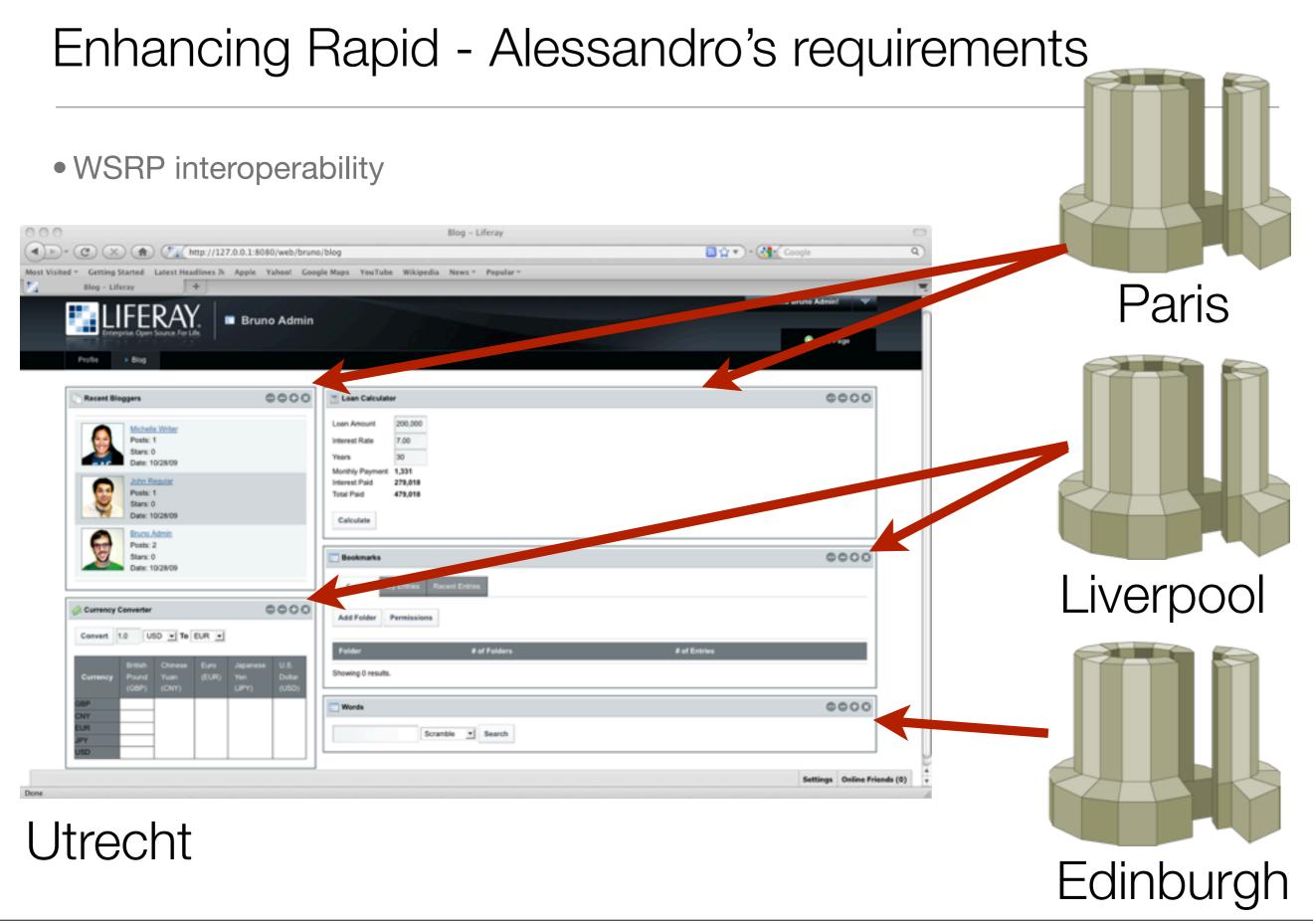
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Enhancing Rapid - Andy's requirements

• New Code Editor!

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1	php</th <th>0</th>	0
2	<pre>\$authors = array();</pre>	
3	<pre>\$news = array();</pre>	
	<pre>/* this is a long long long long long long long long</pre>	
5	<pre>\$query = "SELECT author, COUNT(id) as 'nb_news' FROM news_messages GROUP BY author";</pre>	
6	<pre>\$result = mysql query(\$query, \$DBnews);</pre>	
7	<pre>while(\$line = mysql_fetch_assoc(\$result)){</pre>	
8	<pre>\$authors[\$line["author"]] = \$line["author"];</pre>	
9	<pre>\$news[\$line["author"]] = \$line['nb_news'];</pre>	
10	}	
11		
12	<pre>\$list= sprintf("('%s')", implode("', '", \$authors));</pre>	
13		
14		
15	<pre>\$query="SELECT p.people_id, p.name, p.fname, p.status, team_name, t.leader_id=p.people_id as</pre>	
	'team_leader', w.name as 'wp_name', w.type	
16	FROM people p, teams t, wppartis wp, wps w	
17	WHERE p.people_id IN \$list AND p.org_id=t.team_id AND wp.team_id=t.team_id AND	
	wp.wp_id=w.wp_id	
18	GROUP BY p.people_id";	
19	<pre>if(isset(\$_GET["order"]) && \$_GET["order"]!="nb_news")</pre>	
20 21	<pre>\$query.=" ORDER BY ".\$_GET["order"];</pre>	
22	Specultzmuggl guory (Specal)	
23	<pre>\$result=mysql_query(\$query, \$DBkal); while(\$line = mysql_fetch_assoc(\$result)){</pre>	
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• Support for more Portal Containers

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