



Installation

Please Note: These instructions are a rough guide, things may differ depending on how your system is configured.

Installing MR Grid can essentially be broken down into 3 stages.

- Setting up Xgrid
- Setting up Tomcat
- Setting up MR Grid

Stage 1: Setting Up Xgrid

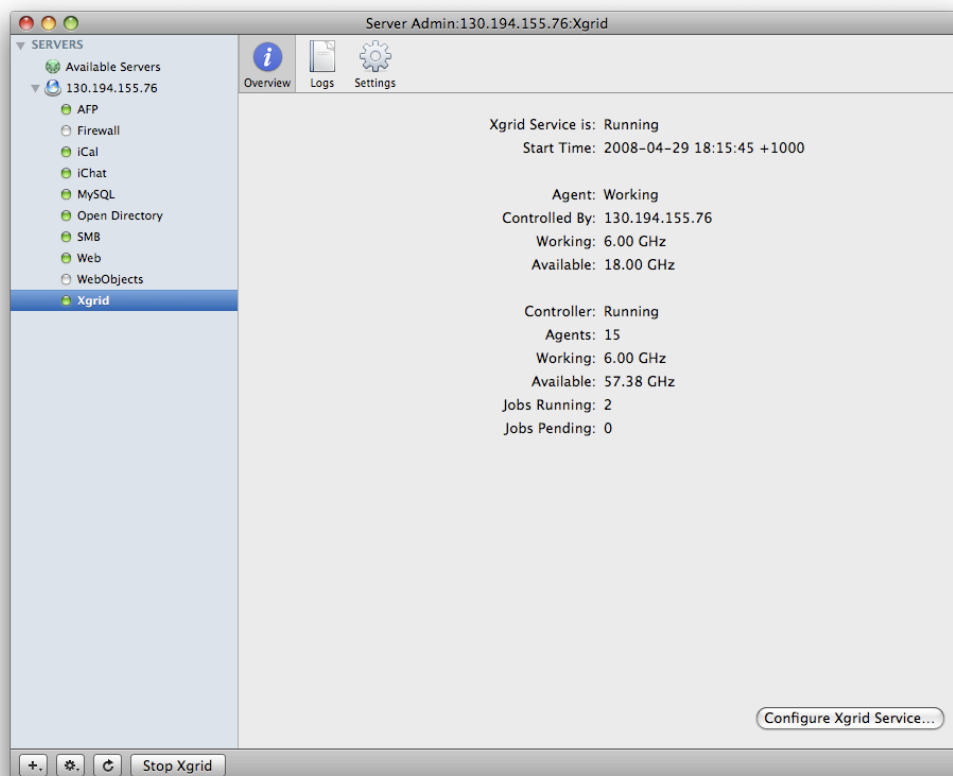
If you already have an Xgrid controller set up, then you can skip this stage.

Please Note: MR Grid has only been tested using Xgrid's "Password" authentication method. We are currently in the process of testing "Kerberos" authentication method. If you encounter any issues please email ashley.buckle@med.monash.edu.au.

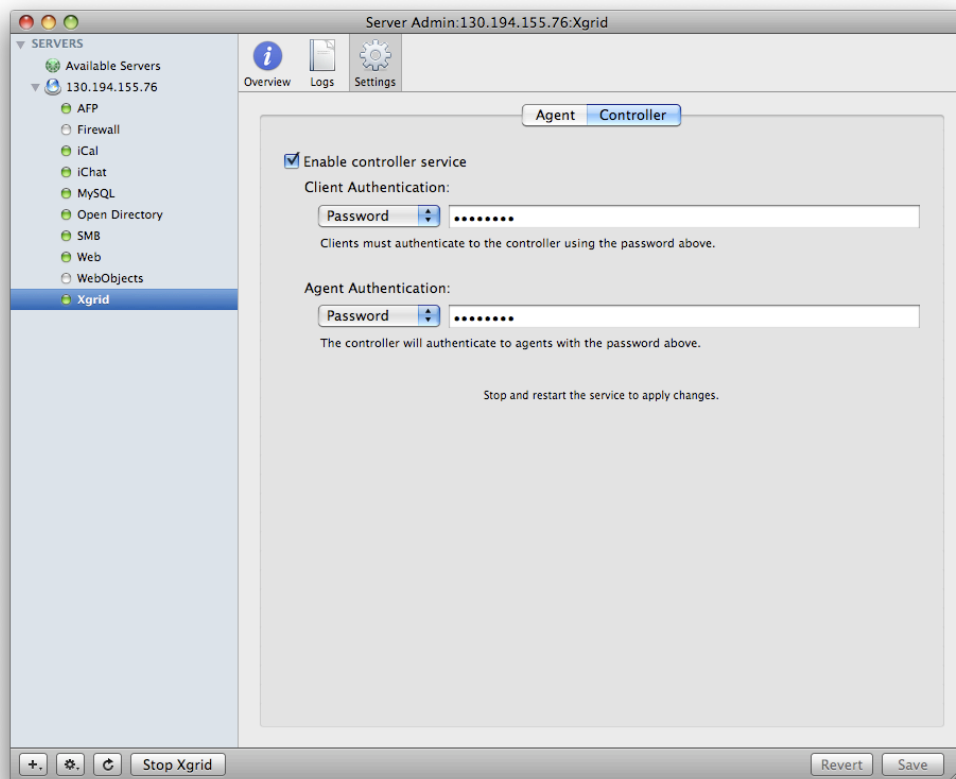
Step 1: Configure Xgrid Controller

Firstly, you need to configure Xgrid on your Mac OS X Server using Server Admin tools. Open "Server Admin", and select the Xgrid service for the server.

Note: These screenshots apply to Mac OS X Server 10.5.2 (aka Leopard), If you are using 10.4.x (Tiger) they may differ slightly.



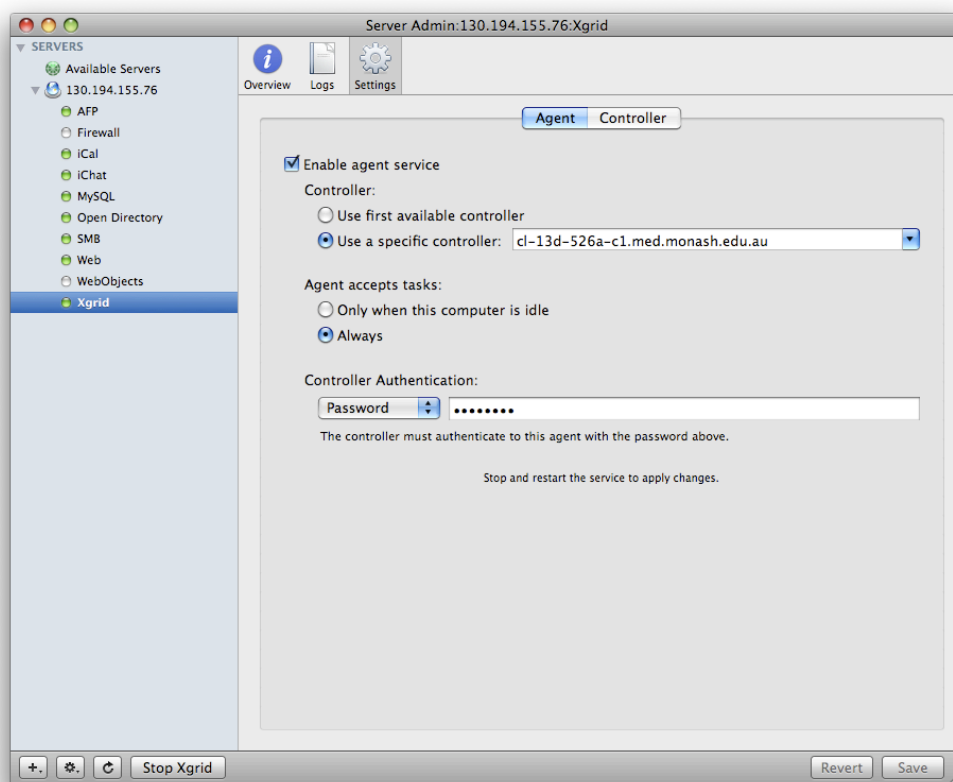
Click on the "Settings" tab. Click to view the "Controller" settings.



Select "Enable controller service" and set both "Client Authentication" and "Agent Authentication" as "Password".

Choose a password and enter it in both the client authentication and agent authentication fields. When finished click "Save".

Next Click on the "Agent" settings tab.



Select "Enable agent service", "Use a specific controller" and enter the IP address or fully qualified domain name (FQDN) of the server in the input box.

Under the "Agent accepts tasks" segment, select whichever is appropriate for how the server is used. If the server is a multicore machine that is not used a lot by other services select "Always", alternatively if the machine is often busy providing services to users select "Only when this computer is idle". Set the "Controller Authentication" to "Password" and enter a password. Then click "Save".

Click on the "Start Xgrid" button to start the Xgrid service.

Note: in these screenshots Xgrid is already running, but button is located in same location as "Stop Xgrid".

Step 2: Adding Xgrid Agents

MR Grid requires that every agent you intend to add to your Xgrid, must have a copy of Phaser installed on it.

Phaser is available either as a standalone download from <http://www.structmed.cimr.cam.ac.uk/phaser/>, or alternatively as part of the CCP4 suite available from <http://www.ccp4.ac.uk/main.html>.

CCP4 installs phaser to `"/usr/local/ccp4-version/bin/phaser"`, where "version" is the version of CCP4 suite.

Eg. `"/usr/local/ccp4-6.0.2/bin/phaser"`.

To account for this, MR Grid requires that phaser must be accessible at `"/usr/local/phaser"`.

The easiest way to achieve this is to soft link phaser to this point.

In a terminal window type:

```
ln -s location_of_phaser /usr/local/phaser
```

where `location_of_phaser` is the location phaser installs to.

Eg. `ln -s /usr/local/ccp4-6.0.2/bin/phaser /usr/local/phaser`

You should then test that the link worked by typing:

`/usr/local/phaser`

This should hopefully start running phaser with no input.

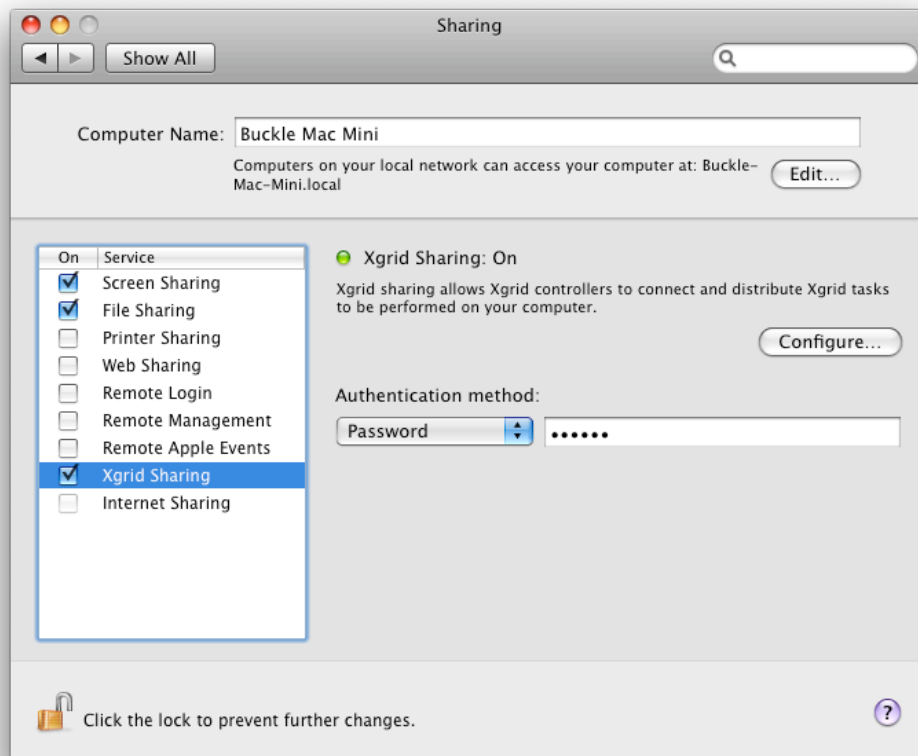
You can exit Phaser by pressing ctrl+c.

Once you've setup phaser on the agent, it is safe to be added to the Xgrid.

On the agent you plan to add to the Xgrid, open System Preferences.



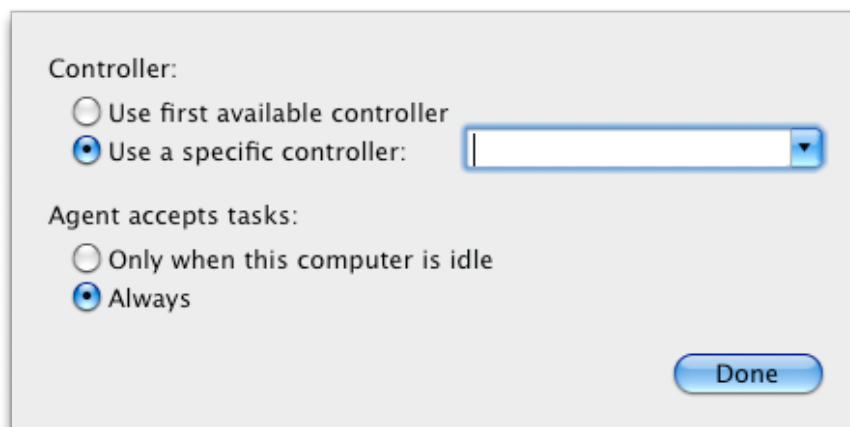
Click on the "Sharing" settings under "Internet & Network".



Click on the "Xgrid Sharing" service.

It won't let you turn it on until the service has been configured on the agent.

To configure the agent, click the "Configure" button.



Set the settings as appropriate for your Xgrid.

It is advised to "Use a specific controller" and enter the IP address or FQDN of your Xgrid controller.

Note: In the "Agent accepts tasks" section, selecting "Only when this computer is idle" means the agent will only be used if it is displaying the screensaver.

Once you have set these options, click "Done".

Then back on the Xgrid sharing screen, set Authentication Method to the method you configured it to be on the server.

Then turn the agent on (tick the checkbox next to the service).

You will need to repeat this process for all agent machines you wish to add to an Xgrid.

Stage 2: Setting Up Tomcat

If you are running tomcat 6, and already know your manager passwords, you can skip this step.

Mac OS X Server 10.5 Leopard users:

You should already have Tomcat 6 installed in `"/Library/Tomcat/"`.

You will just need to edit the tomcat users file & start or restart the server.

Mac OS X Server 10.4 Tiger users:

Unfortunately the version of Tomcat that is installed in `"/Library/Tomcat/"` is several versions old, and may not work with MR Grid, we recommend you use version 6 or above.

You can download version 6 from <http://tomcat.apache.org>. You should download the Core tar.gz file, and extract it to `"/Library/Tomcat6/"`.

You should now have Tomcat installed, but you need to configure the admin users. Open terminal & navigate to the `"conf"` folder inside your tomcat directory.

Leopard users:

```
cd /Library/Tomcat/conf
```

Tiger users:

```
cd /Library/Tomcat6/conf
```

Edit the `tomcat-users.xml` file using vim, pico, emacs or another text-editor.

```
vim tomcat-users.xml
```

Check for a user who's role includes "manager", and that the user has a password.

If the file is empty, edit it to look something like this:

```
<?xml version='1.0' encoding='utf-8'?>
<tomcat-users>
  <role rolename="tomcat"/>
  <role rolename="role1"/>
  <role rolename="manager"/>
  <role rolename="admin"/>
  <role rolename="mrgriduser"/>
  <user username="manager" password="mypass" roles="manager,tomcat,role1"/>
  <user username="admin" password="mypass" roles="admin"/>
  <user username="mrgrid" password="mrgrid_pass" roles="mrgriduser"/>
</tomcat-users>
```

If the file is not empty, you will just need to add the lines:

```
<role rolename="mrgriduser"/> and
<user username="mrgrid" password="mrgrid_pass" roles="mrgriduser"/>
```

save the file, and navigate to the bin directory of the tomcat installation.


```
cd ../bin
```

change the permissions of the shell script files to be executable.


```
chmod +x *.sh
```

next we need to start the server..
./startup.sh

hopefully the server should now be up & running.
You can test by pointing a web browser to port 8080 of your server.
Eg. <http://www.example.com:8080>
If everything worked you should see a tomcat configuration page.



Apache Tomcat



The Apache Software Foundation
<http://www.apache.org/>

Administration

[Status](#)
[Tomcat Manager](#)

Documentation

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Miscellaneous

[Servlets Examples](#)
[JSP Examples](#)
[Sun's Java Server Pages Site](#)
[Sun's Servlet Site](#)

If you're seeing this page via a web browser, it means you've setup Tomcat successfully. Congratulations!

As you may have guessed by now, this is the default Tomcat home page. It can be found on the local filesystem at:

`$CATALINA_HOME/webapps/ROOT/index.html`

where "\$CATALINA_HOME" is the root of the Tomcat installation directory. If you're seeing this page, and you don't think you should be, then either you're either a user who has arrived at new installation of Tomcat, or you're an administrator who hasn't got his/her setup quite right. Providing the latter is the case, please refer to the [Tomcat Documentation](#) for more detailed setup and administration information than is found in the INSTALL file.

NOTE: For security reasons, using the administration webapp is restricted to users with role "admin". The manager webapp is restricted to users with role "manager". Users are defined in `$CATALINA_HOME/conf/tomcat-users.xml`.


Included with this release are a host of sample Servlets and JSPs (with associated source code), extensive documentation, and an introductory guide to developing web applications.

Tomcat mailing lists are available at the Tomcat project web site:

- users@tomcat.apache.org for general questions related to configuring and using Tomcat
- dev@tomcat.apache.org for developers working on Tomcat

Thanks for using Tomcat!

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TOMCAT

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Stage 3: Setting Up MR Grid

Step 1: Configuration Files

MR Grid needs to be configured before it can be used.
Create directory called "mrconfig" on the root of the server's hard drive.
In a terminal:
mkdir /mrconfig

Inside the mrconfig directory you require 3 files:

server_config.xml - defines the server's datastore (where input & output files are to be placed).
xgrid_definitions.xml - defines Xgrids available to be used by MR Grid.
ruby_phaser.rb - a Ruby script used to drive Phaser.

You will need to edit the **server_config.xml** to set the data_store attribute.

This should to "tomcat_root/webapps/MRGrid/jobs", where "tomcat_root" is location tomcat is installed to (Eg. /Library/Tomcat/ or /Library/Tomcat6/).

An example **server_config.xml** file:

```
<server_config>
  <data_store>/Library/Tomcat/webapps/MRGrid/jobs</data_store>
</server_config>
```

Next you should define your Xgrids in the xgrid_defintions.xml.

For each grid you wish to define you should have a block of xml similar to the following:

```

<grid>
  <display_name>my Xgrid</display_name>
  <host>123.123.123.123</host>
  <auth_method>password</auth_method>
  <password>my_password</password>
  <grid_id>0</grid_id>
  <available>true</available>
</grid>

```

Explanation of tags:

display_name - A unique name you wish to use to refer to the grid

host - IP address or FQDN of the Xgrid host.

auth_method - authentication method of the Xgrid, as set in stage 1

password - password required to access the grid, as set in stage 1

grid_id - If your controller has multiple Xgrids on it, set this appropriately, otherwise leave as 0 (zero).

available - boolean trigger that sets whether the grid appears on the web page. Set to false if you plan on doing maintenance, etc.


The `ruby_phaser.rb` should be fine to run as is, although you may tweak the "nice" level that jobs run at by editing line 46 of the file.

Eg. `nice -n 10`


The default value is 0 (zero).

Step 2: Deploying MR Grid

Navigate to the Tomcat configuration page of your server.



Apache Tomcat



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<http://www.apache.org/>

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Thanks for using Tomcat!

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TOMCAT

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Click on the "Tomcat Manager" link, and login as manager, using the password you defined in the `tomcat-users.xml`.

Once logged in, scroll down until you see the "Deploy" section of the page.

Deploy

Deploy directory or WAR file located on server

Context Path (optional):

XML Configuration file URL:

WAR or Directory URL:

Deploy

WAR file to deploy

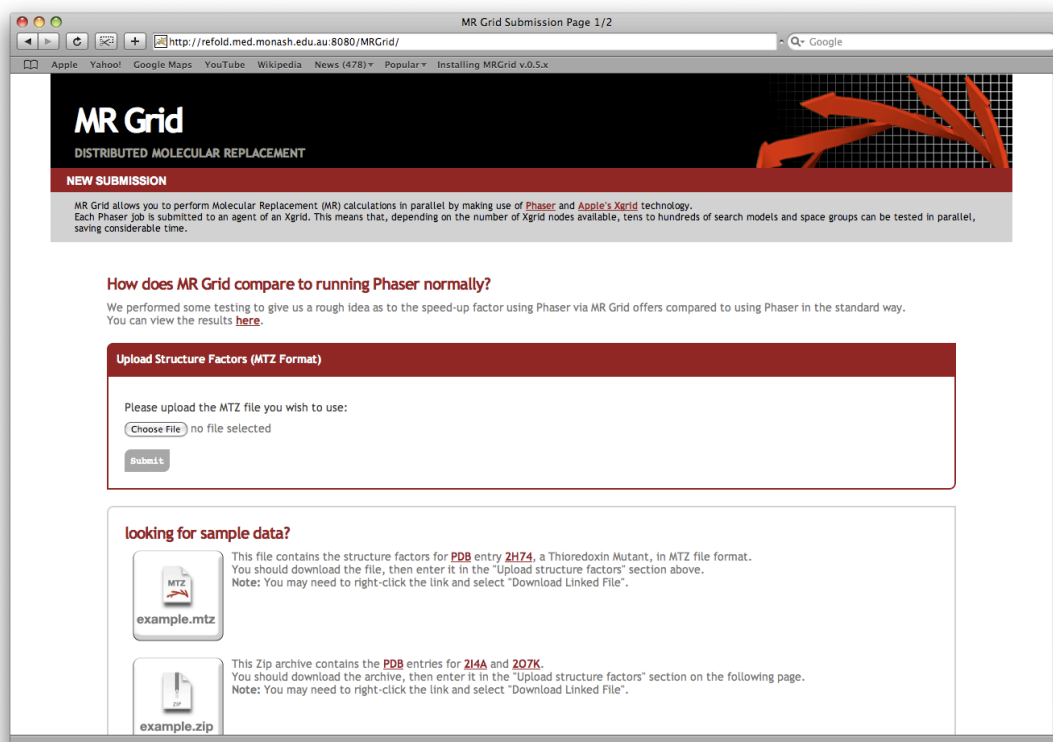
Select WAR file to upload no file selected

Deploy

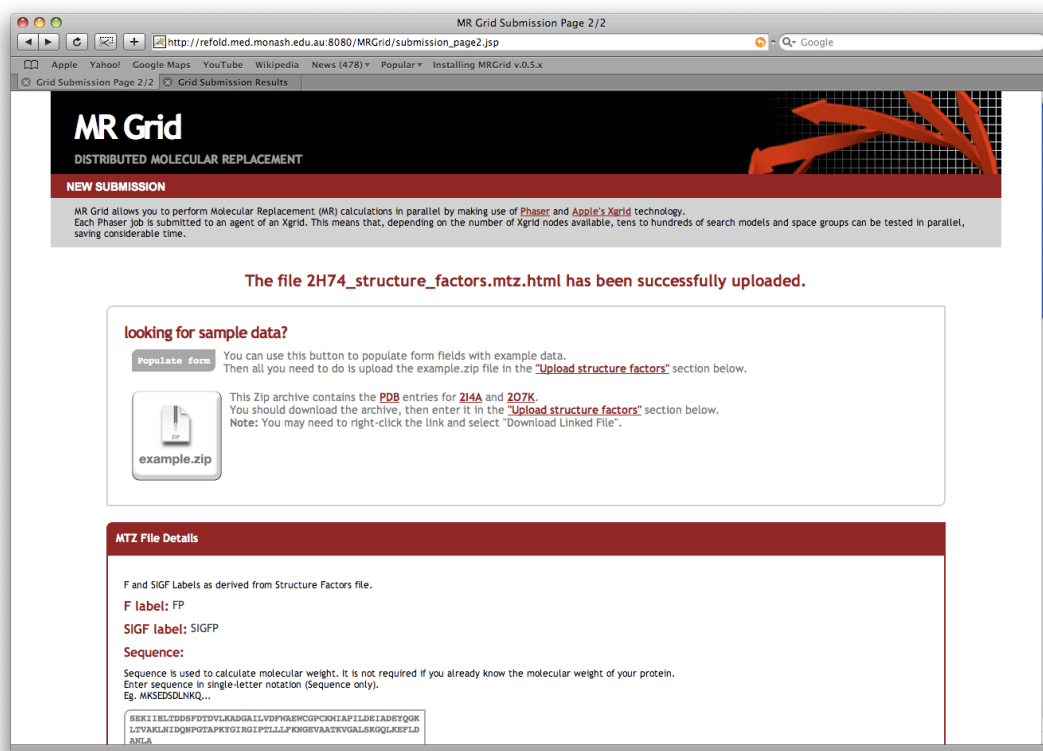
In the "WAR file to deploy" choose the "**MRGrid.war**" file and click "Deploy".
 Tomcat should then deploy MR Grid to the MRGrid subdirectory of your server.
 Eg. <http://www.example.com:8080/MRGrid/>

Everything should now be setup and ready to run.
 You can start using MR Grid by browsing to the MRGrid directory of your server.
 Eg. <http://www.example.com:8080/MRGrid/>

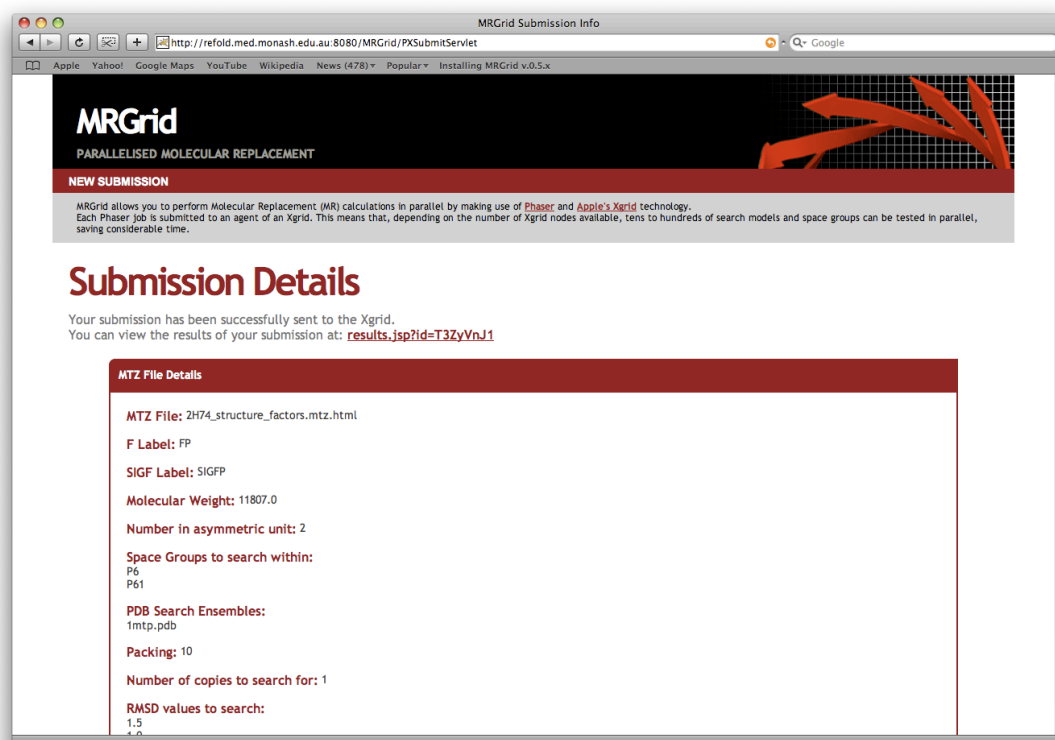
You should then login as the user **mrgrid** using the password you defined in the **tomcat-users.xml**.
 If all went well you should see the following screen.



To test that everything worked correctly you should run a new submission using the sample data provided.
 After you click "Submit" on the start page you should be taken to page 2 of the submission process.



If everything submits successfully you should see the following screen.



You can then click the results link to be taken to the results page for this submission.

MR Grid Submission Results

http://refold.med.monash.edu.au:8080/MRGrid/results.jsp?id=T3ZyVnJ1

MR Grid
DISTRIBUTED MOLECULAR REPLACEMENT

NEW SUBMISSION

MR Grid allows you to perform Molecular Replacement (MR) calculations in parallel by making use of [Phaser](#) and [Apple's Xgrid](#) technology. Each Phaser job is submitted to an agent of an Xgrid. This means that, depending on the number of Xgrid nodes available, tens to hundreds of search models and space groups can be tested in parallel, saving considerable time.

Results of Submission

Results Summary (4 Jobs)

T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.5
T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.0
T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P61_1.5
T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P61_1.0

T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.5

Job Summary:

job name: T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.5
Input MTZ: [2H74_structure_factors.mtz.html](#)
Input PDB: [1mtp.pdb](#)
Space Group: P6
Status: Running

Submission Time: Tue May 27 16:36:31 EST 2008
Start Time: Tue May 27 16:36:31 EST 2008

[show Output Log](#)

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If you see the above screen then submission works successfully. You can reload the page to get the latest data back from your Xgrid. The sample data should take a couple of minutes to complete.

MR Grid Submission Results

http://refold.med.monash.edu.au:8080/MRGrid/results.jsp?id=T3ZyVnJ1

MR Grid
DISTRIBUTED MOLECULAR REPLACEMENT

NEW SUBMISSION

MR Grid allows you to perform Molecular Replacement (MR) calculations in parallel by making use of [Phaser](#) and [Apple's Xgrid](#) technology. Each Phaser job is submitted to an agent of an Xgrid. This means that, depending on the number of Xgrid nodes available, tens to hundreds of search models and space groups can be tested in parallel, saving considerable time.

Results of Submission

Results Summary (4 Jobs)

T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.5 (Z Score: 4.2, LLG: -22.0) Run Time: 3 mins 17 secs
T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.0 (Z Score: 3.4, LLG: -372.0) Run Time: 7 mins 0 sec
T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P61_1.5 (Z Score: 3.7, LLG: -28.0) Run Time: 3 mins 1 sec
T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P61_1.0 (Z Score: 4.0, LLG: -351.0) Run Time: 7 mins 26 secs

Submission Run Time: 7 mins 29 secs

T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.5

Job Summary:

job name: T3ZyVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.5
Input MTZ: [2H74_structure_factors.mtz.html](#)
Input PDB: [1mtp.pdb](#)
Space Group: P6
Status: Finished
Z Score: 4.2
LLG: -22.0

Submission Time: Tue May 27 16:36:31 EST 2008
Start Time: Tue May 27 16:36:31 EST 2008
Stop Time: Tue May 27 16:39:48 EST 2008
Job Run Time: 3 mins 17 secs

Once it has completed scroll down to one of the jobs, and click on the “Output Files” button to expand the hidden HTML DIV.

MR Grid Submission Results

http://refold.med.monash.edu.au:8080/MRGrid/results.jsp?id=T32yVnJ1

Grid Submission Page 2/2

Grid Submission Results

T32yVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.5 (Z Score: 4.2, LLG: -22.0) Run Time: 3 mins 17 secs
T32yVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.0 (Z Score: 3.4, LLG: -372.0) Run Time: 7 mins 0 sec
T32yVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P61_1.5 (Z Score: 3.7, LLG: -28.0) Run Time: 3 mins 1 sec
T32yVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P61_1.0 (Z Score: 4.0, LLG: -351.0) Run Time: 7 mins 26 secs

Submission Run Time: 7 mins 29 secs

T32yVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.5

Job Summary:

Job name: T32yVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.5
Input MTZ: [2H74_structure_factors.mtz.html](#)
Input PDB: [1mtp.pdb](#)
Space Group: P6
Status: Finished
Z Score: 4.2
LLG: -22.0

Submission Time: Tue May 27 16:36:31 EST 2008
Start Time: Tue May 27 16:36:31 EST 2008
Stop Time: Tue May 27 16:39:48 EST 2008
Job Run Time: 3 mins 17 secs

Hide Output Files

Output Files:

Output MTZ: [1mtp.pdb_P6_1.5_result.1.mtz](#)
Output PDB: [1mtp.pdb_P6_1.5_result.1.pdb](#)
Output Sol: [1mtp.pdb_P6_1.5_result.sol](#)
Output Sum: [1mtp.pdb_P6_1.5_result.sum](#)

Show Output Log

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T32yVnJ1_2H74_structure_factors.mtz.html_1mtp.pdb_P6_1.0

You should then click to download the files. If you can download the files, then everything should be fully installed & ready to go.