



Upgrading

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

Stage 1: Backing Up

If you do not wish to keep your existing submission data you may skip this step.

MR Grid's default data store is the "jobs" folder within the MR Grid web app. Typically this lives at the location /Library/Tomcat/webapps/MRGrid/jobs. All submission data lives within the jobs folder. Unfortunately when you choose to undeploy a web app in Tomcat manager, it deletes the MRGrid folder and everything contained within it (ie. all data in the jobs folder).

If you wish to keep the data from existing jobs, you will need to backup the contents of the jobs directory.

Open a terminal and copy the contents of the jobs folder within your MR Grid installation to somewhere outside of your MR Grid installation.

The following screenshot shows how this can easily be achieved.

Note: The screenshot assumes your Tomcat installation is at /Library/Tomcat. You will need to change accordingly.

```
Terminal — ssh — 80x24
bash-3.2$ cd /Library/Tomcat/webapps/MRGrid/jobs/
bash-3.2$ sudo mkdir -p /tmp/mrgrid/jobs
bash-3.2$ sudo cp -r * /tmp/mrgrid/jobs/
bash-3.2$
```

Line-by-line break down:

Line 1: change directory to the MR Grid data store.

Line 2: make a temporary directory to use for storing the data. -p flag builds directories on the path if they don't exist (eg. tmp/mrgrid).

Line 3: recursive copy of the everything in the current folder (*) to the temporary directory.

Stage 2: Undeploying MR Grid

Navigate to the Tomcat configuration page of your server.



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 "MRGrid" listing in the applications section of the page.

MRGrid	MRGrid	true	2	Start Stop Reload Undeploy
				Expire sessions with idle at 30 minutes

Click "Undeploy", this will completely remove the MRGrid web app.

Stage 3: Deploying MR Grid

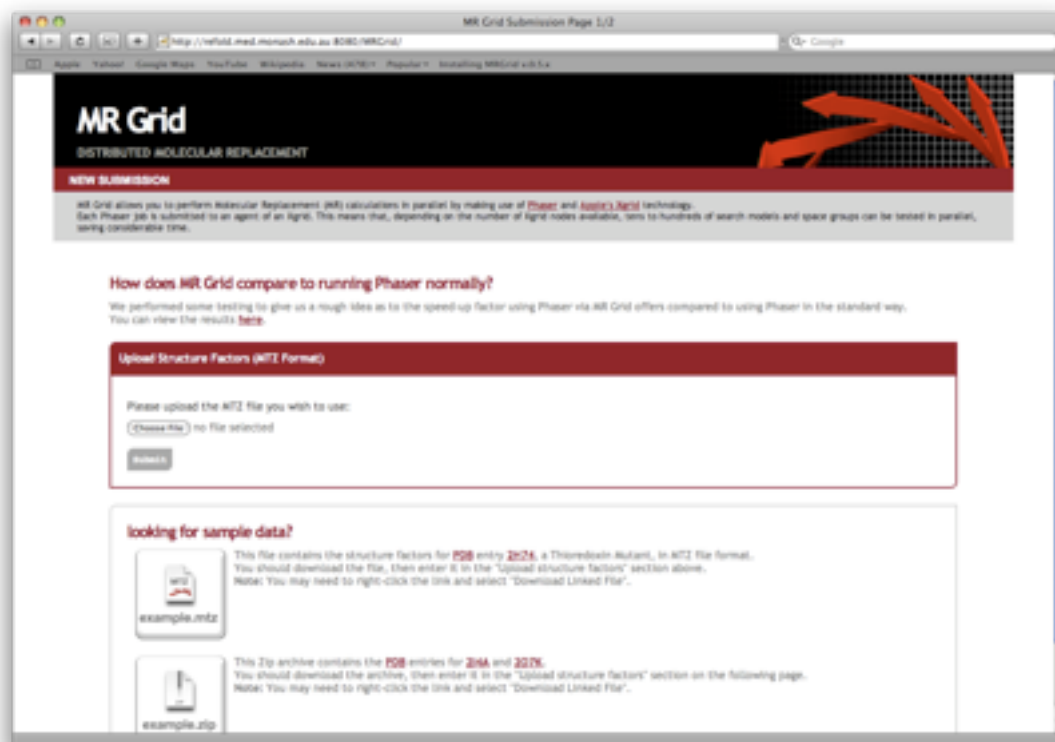
Once you've undeployed the previous version of MRGrid you can now deploy the new version. In the Tomcat Manager area, scroll down to the Deploy section.



In the "WAR file to deploy" choose the "**MRGrid.war**" file (the new version of MR Grid) and click "Deploy". Tomcat should then deploy MR Grid to the MRGrid subdirectory of your server.

You should now be able to access 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.



The new version of MR Grid is now deployed, we just need to restore the existing data.

Stage 4: Restoring Submission Data

You can restore the job data to data store by copying it back from the temporary directory.
Back in the terminal window issue the following commands:

A screenshot of a terminal window titled "Terminal — ssh — 80x24". The terminal has a blue background and white text. It shows three lines of commands entered at the "bash-3.2\$" prompt. The first line is "cd /Library/Tomcat/webapps/MRGrid/jobs/", the second line is "sudo cp -r /tmp/mrgrid/jobs/* .", and the third line is a blank prompt with a cursor. The window has standard macOS window controls (red, yellow, green buttons) in the top left corner and a scroll bar on the right side.

```
Terminal — ssh — 80x24
bash-3.2$ cd /Library/Tomcat/webapps/MRGrid/jobs/
bash-3.2$ sudo cp -r /tmp/mrgrid/jobs/* .
bash-3.2$
```

Line-by-line break down:

Line 1: change directory to the MR Grid data store.

Line 2: recursive copy of the everything in the temporary folder back to the current directory (.).

To test that the copy worked and you can access the data do an “ls” of the jobs folder, and pick one of the 8 character job IDs. We’ll use “9bd7CGqC” as an example.

Note: These IDs are randomly generated so will differ from those pictured.

Next open your browser to the MR Grid result page for that job.

Eg. <http://www.example.com:8080/MRGrid/results.jsp?id=9bd7CGqC>

You should see a page that looks something like this:

MR Grid Submission Results

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 Krig](#) technology. Each Phaser job is submitted to an agent of an MR Grid. This means that, depending on the number of MR Grid nodes available, tens to hundreds of search models and space groups can be tested in parallel, saving considerable time.

Results of Submission

Results Summary

The table below summarises the results of your MR Grid submission. You can view more details about a job, as well as the log file and any files it returned by clicking on the "View Details" link for the appropriate job. A row will appear **highlighted** if the job returned a Z Score of 7 or higher.

PDB File	Space Group	RMSD	Z Score	LLG	Run Time	
grb7_chA.pdb	P2	1.5	9.0	70.0	42 secs	View Details
grb7_chA.pdb	P2	1.1	10.4	140.0	40 secs	View Details
grb7_chA.pdb	P21	1.5	4.0	90.0	45 secs	View Details
grb7_chA.pdb	P21	1.1	4.2	95.0	47 secs	View Details

Number of Jobs: 4
Submission Run Time: 49 secs

YodPCoG-grb7-16-scaled-truncated.mtz-grb7_chA.pdb_P2_1.5

Job Summary:

Job name: YodPCoG-grb7-16-scaled-truncated.mtz-grb7_chA.pdb_P2_1.5
Input MTZ: grb7-16-scaled-truncated.mtz
Input PDB: grb7_chA.pdb
Space Group: P2
Status: Finished

If so, everything should now be setup correctly.