# AHE Exercise 2: Running an Application on the NGS with the AHE Client

**Aims and Objectives**

- Launch the sort application with the AHE GUI client
- Launch the sort application with the AHE command line client
- Manually specify input and output files for an application

**Introduction**

The AHE clients allow you to launch and monitor applications on remote grid resources. In this exercise we will launch the sort application on NGS machines using both the AHE GUI and command line clients. The sort application takes a configuration file which specifies the job input and output files. The input file contained a list of words and the output file contains a sorted list of words.

After completing this section you will be familiar with launching applications using the AHE clients.

**Stage 1: Getting the Application Input Files**

1 The examples in this exercise will use the sort application installed on the NGS machines to sort a list of words. To run this application you will need to download a set of configuration and data files (sortapp-input.tgz), which can be obtained from:

http://www.realitygrid.org/AHE/training/courseinfo.html#ex2

Save the files onto your desktop.

2 Open a command prompt, change the directory to the desktop and type:

**tar zxvf sortapp-input.tgz**

The expanded directory will contain two files: config.txt is a configuration file for the sort application specifying the input file that the application will read the list of words to sort, and the output file that it will write the sorted list of words to. input.txt is the list of words that will be read in and sorted.

**Stage 2: Running an Application with the GUI Client**

1 Open the AHE GUI Client as detailed in Exercise 1.

2 Double-click on **Prepare a new job**.

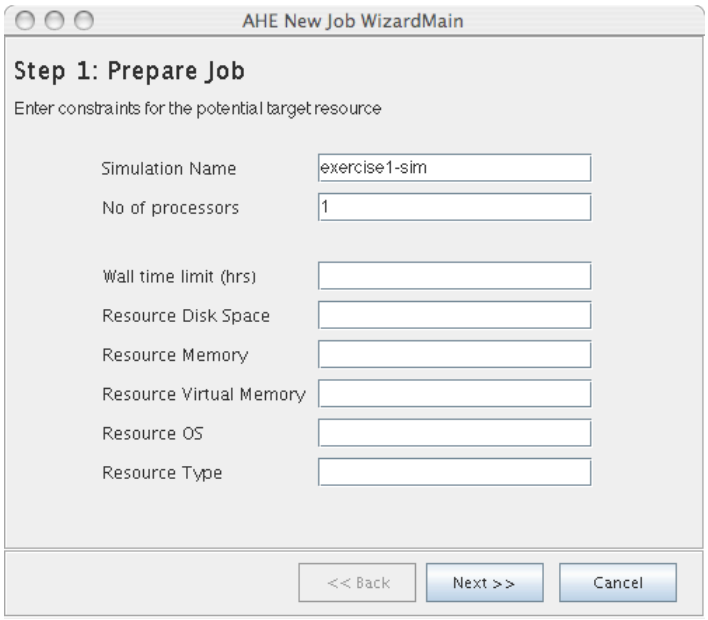
3 From the **Select an application to run** drop down list, choose **sort** then click on the button **Find Job Factories**. After a short time you will see a Sort factory endpoint appear in the box beneath.

4 Click on the sort factory endpoint to select it (it should turn blue), then click **Launch Wizard**.

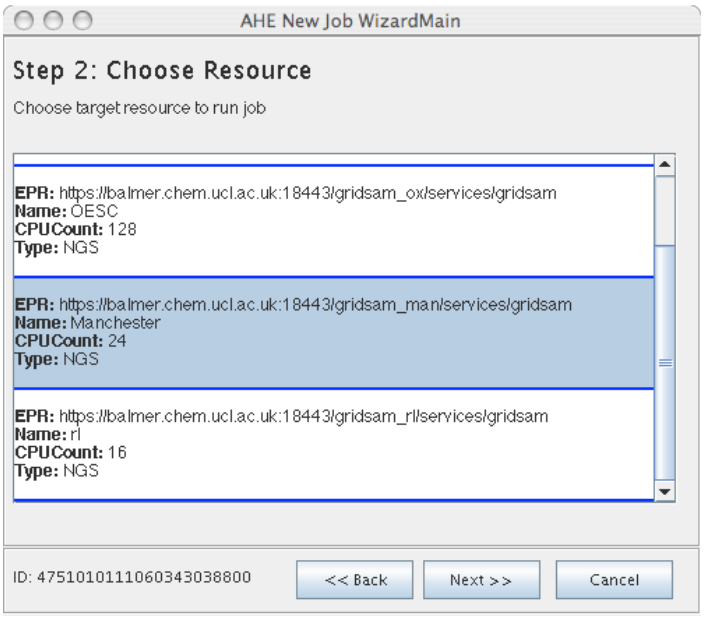
5 The AHE job launching wizard will open. Enter a name for the job, for example example-job1 (this name is used to give the user a convenient way to refer to the job in future).

Enter a number of processors for the job – in this case enter **1** so that the sort application is run on a single processor.

Click **Next**.

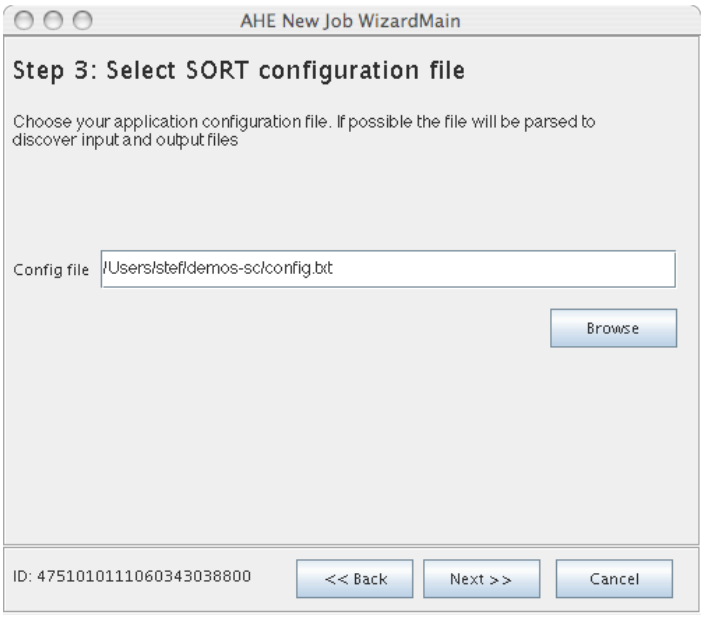



6 You are now prompted to choose an NGS machine to run the application on – for this example choose OESC (the Oxford NGS node), then click **Next**.




7 The AHE client will parse your sort job's input file to discover the data files that need to be moved from the local machine to the NGS node at Oxford, and the data that will be created at Oxford that needs to be moved back to your local machine after the job has finished.

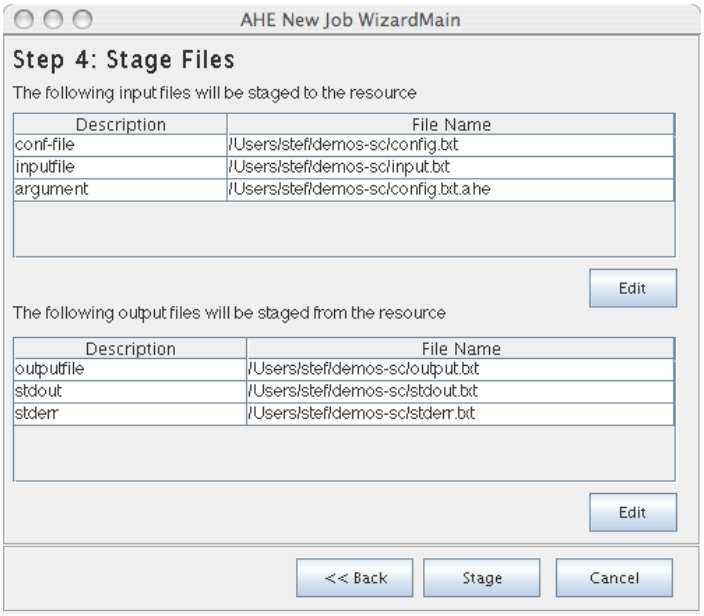
Click on the Browse button, select your sort application configuration file (**config.txt**) from the sort application input file set downloaded in stage 1. Click **Open**, then click **Next**.



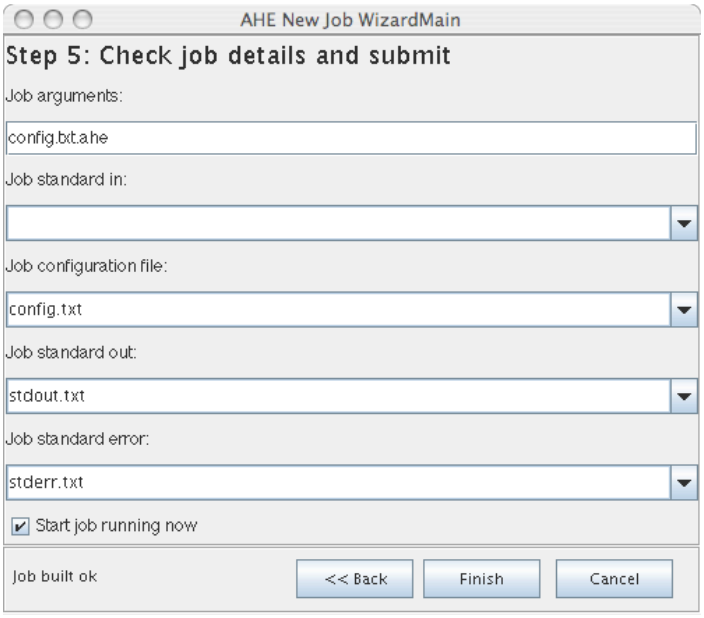

8 The AHE client will parse the config.txt file and discover the input and output files associated with the job. Clicking on the **Stage** button will move the input files over to the

AHE file staging area from where it will be moved over to the Oxford NGS machine.

Once the files have been staged click **Next**.




9 Review the details of your sort job and click the **Finish** button to launch the job.

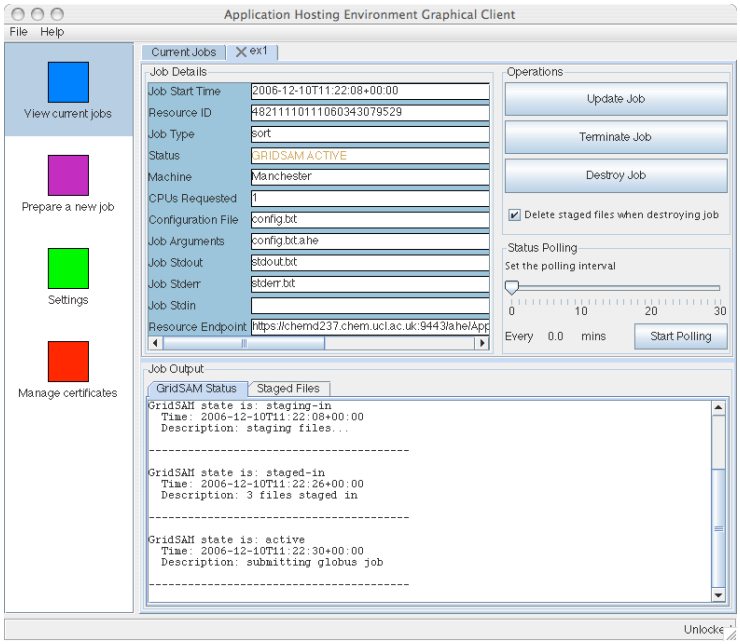



**Stage 3: Monitoring an Application with the GUI client**

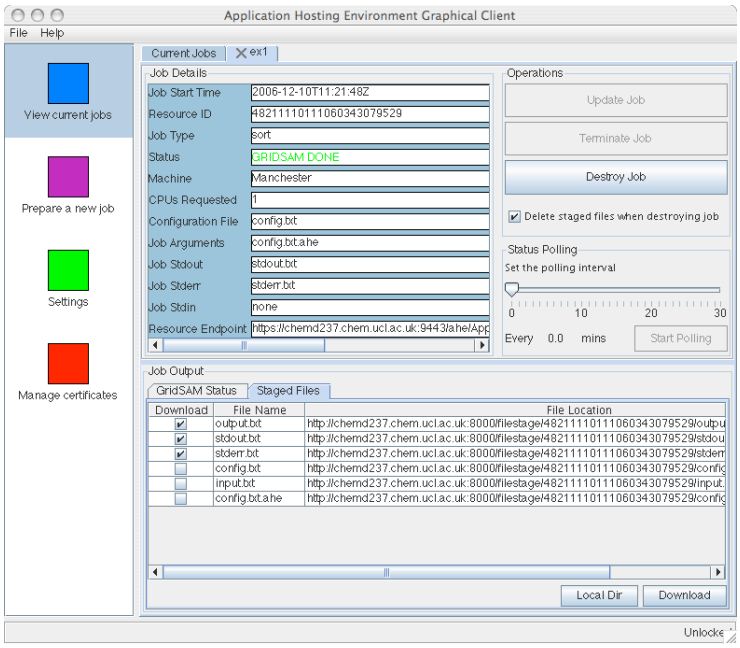
1 To check on the status of your job once launched, double-click on **View current jobs**.

You will see the job that you have just launched at the top of the list. Double-click on the job entry to open its monitoring window.

2 To check up on the status of a job, click on the **Update Job** button. This will poll the AHE server and update the status of the job.




3 When the job has finished (signalled by a status of GRIDSAM DONE) you the output files will be left on the AHE file staging server for you to download. To do so, click on the **Staged Files** tab under job output. Here you will see all of the output that has been generated.




4 Click on the **Local Dir** button. This allows you to change the directory where the output files will be saved (by default they will be saved to the same directory as the input files). Create a new output directory on your desktop and choose **Open**.

5 Click on the **Download** button. The output files will be saved to the directory specified in step 4. Browse to this folder and check the output of the sort job.

### Stage 4: Running an Application with the Command Line Client

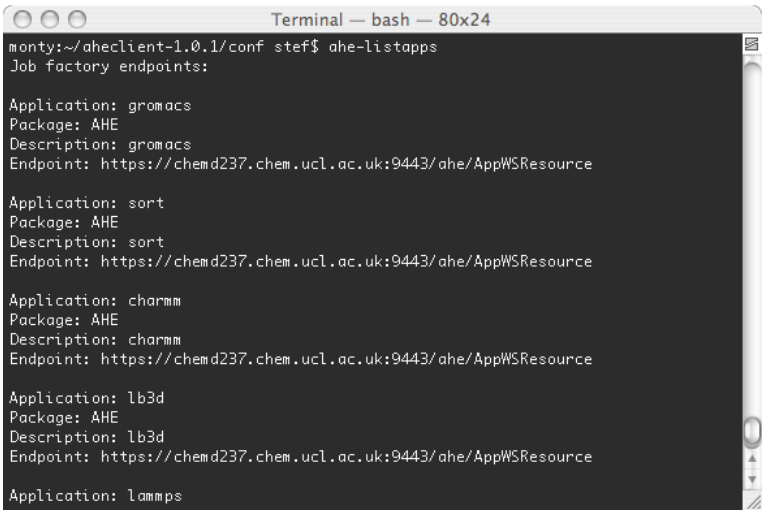
1 Open a terminal and change to the directory where you have installed the AHE client. If you didn't set the AHECLEINT_HOME variable to be set automatically in exercise 1, then you will need to export this variable again.

2 At the terminal type: **cd bin**

3 At the terminal type:

**ahe-listapps**

This will list all of the applications installed in the AHE, along with the factory endpoints needed to start them. From this list find the endpoint of the sort application.




4 The first step to launch an application using the AHE command line clients it to issue the ahe-prepare command. This is equivalent to the first step of the AHE GUI client wizard. In this example we will again launch the sort application. At the terminal type:

**./ahe-prepare –e https://chemd237.chem.ucl.ac.uk:9443/ahe/AppWSResource -app sort -s ex2-sortjob –RMCPUCount 1**

Note: -RMCPUCount specifies the minimum number of CPUs available on the target machine, -s specifies the name, -app specifies the application and –e specifies the factory endpoint. Type:
**ahe-prepare -help** for further details.

The ahe-prepare command will return a list of the NGS machines that are able to run the application.

5 To start the job running, at the command prompt type:

**./ahe-start –s ex2-sortjob –config /path/to/sort/config.txt -RM OESC –n 1**

Where </path/to/sort/confix.txt> is the full path to the sort configuration file that you saved earlier. Note, -s specifies the job name – this must be the same name that was set by the ahe-prepare command, -RM is the name of the machine to run the job, -n is the number of processors to run the job. Type: **ahe-start -help** for further details.

The command will stage the necessary files to the AHE file staging area and start the job running.

### Stage 5: Monitoring Jobs with the AHE Command Line Clients

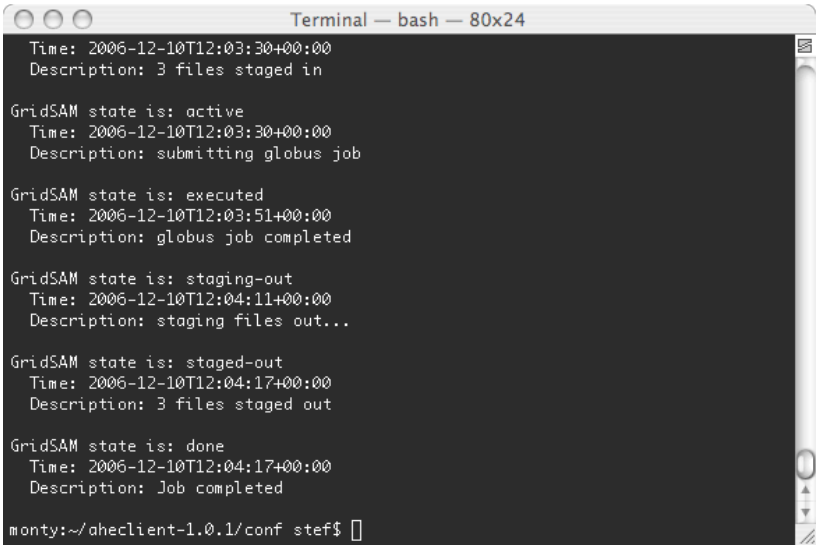
1 The ahe-list command allows you to view a list of the jobs you have previously started. At the terminal type: **ahe-list**

2 The ahe-monitor command allows you to monitor an individual job. To check the status of

the job started in stage 4 type:

**./ahe-monitor –s ex2-sortjob**

Note: the –s parameter is the name of the simulation that you set with the ahe-prepare command. The ahe-monitor command will return the status of the job.




3 Once the ahe-monitor command reports the status of the job as complete, you can retrieve the output files from the AHE file staging area. To do this type:

**./ahe-getoutput –s ex2-sortjob –l /path/to/output/dir**

The –l parameter allows you to specify the path to the directory where you would like the output to be placed. Create a new folder on the desktop and download the output to here.

## Further Work

**Try performing these further tasks with the AHE clients:**

- Use the AHE GUI client to monitor a job launched via the command line clients (Hint: you can view all of you AHE jobs by clicking on the **Update Job List** button on the View current jobs panel).
- Download the further-input.tgz file from http://www.realitygrid.org/AHE/training/courseinfo.html#ex2 This file contains a number of input files for NAMD and LAMMPS molecular dynamics applications. Try launching some of these applications on various NGS resources using the provided input files. You should specify 2-4 processors for each of the jobs. Note: the NAMD config files names end .in and can be found in the run folder. LAMMPS input files end .inp.
- As well as using parser plug-ins to automate data staging, the AHE client also allows you to specify input and output files manually, via the **Edit** button in stage 4 of the GUI client wizard. Try specifying the input and output files to the application sorf2 manually (you can

use the same files as the normal sort application).

**Discussion Points**

What data and configuration files would your application require the AHE to stage over to a grid machine in order to run a job?