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 examplejob1 (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 $\mathbf{1}$ so that the sort application is run on a single processor.

Click Next.

000	AHE New Job WizardMain			
Step 1: Prepare Job				
Enter constrair	nts for the potential target	resource		
Sin	nulation Name	exercise1-sim		
No	of processors	1		
Wa	all time limit (hrs)			
Re	source Disk Space			
Re	source Memory			
Re	source Virtual Memory			
Re	source OS			
Re	source Type			
		<< Back Next >>	Cancel	

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**.

000	AHE New Job WizardMain	
Step 2: Choose Ro Choose target resource to ro	esource un job	
EPR: https://balmer.chem.uk Name: OESC CPUCount: 128 Type: NGS	cl.ac.uk:18443/gridsam_ox/services/gridsam	
EPR: https://balmer.chem.uk Name: Manchester CPUCount: 24 Type: NGS	cl.ac.uk:18443/gridsam_man/services/gridsam =	=
EPR: https://balmer.chem.ue Name: rl CPUCount: 16 Type: NGS	cl.ac.uk:18443/gridsam_rl/services/gridsam	•
ID: 4751010111060343038	800 << Back Next >> Cancel]

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**.

AHE New Job WizardMain			
Step 3: Select SORT configuration file			
Choose your application configuration file. If possible the file will be parsed to discover input and output files			
Config file	/Users/stef/demos-sc/cor	nfig.bd	
	1	Browse	
ID: 475101	0111060343038800	<< Back Next >> Cancel	

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.

Step 4. Staye Fi	nes	
The following input files v	Will be staged to the resource	
Description	Description File Name	
conf-file	/Users/stef/demos-sc/config.b/t	
inputfile	/Users/stef/demos-sc/input.bd	
argument	/Users/stef/demos-sc/config.bd.a.he	
		Edit
The following output files	will be staged from the resource	Edit
The following output files	will be staged from the resource	Edit
The following output files	will be staged from the resource	Edit
The following output files Description outputfile	will be staged from the resource File Name /Users/stef/demos-sc/output.bd	Edit
The following output files Description outputfile stdout	will be staged from the resource File Name /Users/stef/demos-sc/output.bxt /Users/stef/demos-sc/stdout.bxt	Edit
The following output files Description outputfile stdout stdorr	will be staged from the resource File Name /Users/stef/demos-sc/output.bt /Users/stef/demos-sc/stdout.bt /Users/stef/demos-sc/stdem.bt	Edit
The following output files Description outputfile stdout stderr	s will be staged from the resource File Name /Users/stef/demos-sc/output.bit /Users/stef/demos-sc/stdout.bit /Users/stef/demos-sc/stdem.bit	Edit
The following output files Description outputfile stdout stderr	s will be staged from the resource File Name /Users/stef/demos-sc/output.bit /Users/stef/demos-sc/stdout.bit /Users/stef/demos-sc/stderr.bit	Edit
The following output files Description outputfile stdout stderr	s will be staged from the resource File Name /Users/stef/demos-sc/output.bit /Users/stef/demos-sc/stdout.bit /Users/stef/demos-sc/stderr.bit	Edit
The following output files Description outputfile stdout stderr	: will be staged from the resource File Name /Users/stef/demos-sc/output.bxt /Users/stef/demos-sc/stdout.bxt /Users/stef/demos-sc/stderr.bxt	Edit
The following output files Description outputfile stdout stderr	will be staged from the resource File Name /Users/stef/demos-sc/output.bd /Users/stef/demos-sc/stdout.bd /Users/stef/demos-sc/stdem.bd	Edit
The following output files Description outputfile stdout stderr	s will be staged from the resource File Name //Users/stef/demos-sc/output.bt //Users/stef/demos-sc/stdout.bt //Users/stef/demos-sc/stdem.bt	Edit

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.

OOO AHE N	ew Job Wizard	Main	
Step 5: Check job detail	s and subi	nit	
Job arguments:			
config.bxt.ahe			
Job standard in:			
Job configuration file:			
config.txt			
Job standard out:			
stdout.txt			
Job standard error:			
stderr.txt			
🖌 Start job running now			
Job built ok	<< Back	Finish	Cancel

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.

000	Арр	lication Hosting Environment G	raphical Clie	nt
File Help				
	Current Jobs 🛛 🗙	ex1		
	Job Details			Operations
	Job Start Time	2006-12-10T11:22:08+00:00		Update Job
View current jobs	Resource ID	48211110111060343079529		
	Job Type	sort		Terminate Job
	Status	GRIDSAM ACTIVE		
	Machine	Manchester		Destroy Job
Drenare a new job	CPUs Requested	1		
Prepare a new job	Configuration File	config.b/t		Delete staged files when destroying job
	Job Arguments	config.bd.a.he		Status Polling
	Job Stdout	stdout.brt		Set the polling interval
	Job Stdern	stderr.bd		
Settings	Job Stdin			0 10 20 30
	Resource Endpoint	https://chemd237.chem.ucl.ac.uk:94	43/ahe/App	Share Share Delline
			•	Every 0.0 mins Start Polling
	Job Output			
Manage certificates	GridSAM Status	Staged Files		
Ŷ	GridSAM state i	s: staging-in -10711:22:08:00:00		_
	Description:	staging files		
	GridSAM state i	s: staged-in		
	Description:	-10711:22:26+00:00 3 files staged in		
	GridSAM state i	s: active		=
	Time: 2006-12 Description:	-10T11:22:30+00:00 submitting globus job		
				•
·				Unlocker

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.

	Ap	plication I	Hosting Environment Graphical C	lient	
ine i neip	Current Jobs	(ex1]			
	Job Details			Operations	
	Job Start Time	2006-12-	10T11:21:48Z	Lindato Joh	
View current jobs	Resource ID	4821111	0111060343079529		
	Job Type	sort		Terminate Job	
	Status	GRIDSA	M DONE		
	Machine	Manches	ster	Destroy Job	
	CPUs Requested	1			
Prepare a new job	Configuration File	config.bd		🖌 Delete staged files when destroying jo	
	Job Arguments	config ht	ahe		
	Job Stdout	stdout br		Status Polling	
	Job Stdorr	etderr tyt		Set the polling interval	
Settinas	Job Stden	beach dec		Ų———	
~	Job Stain	none	1007 - how of a 100440 hold a	0 10 20	
_	Hesource Endpoil	nt nttps://cn	emd237.cnem.uci.ac.uk:9443/ane/App	Every 0.0 mins Start Polling	
]	
	Job Output	V au u			
vlanage certificates	GPICSAM Status	Staged	Files	Plin Langelow	
	Download F v outp	ut.bd	http://chemd237.chem.ucl.ac.uk:800/	Difilestage/48211110111060343079529/ou	
	✓ stdo	ut.bct	http://chemd237.chem.ucl.ac.uk:800	D/filestage/48211110111060343079529/sto	
	✓ stder	r.bd	http://chemd237.chem.ucl.ac.uk:800	D/filestage/48211110111060343079529/stc	
	confi	j.bd http://chemd237.chem.ucl.ac.uk:8000/filestage/48211110111060343079		D/filestage/48211110111060343079529/co	
	inpu	.DCC	http://chemd237.chem.ucl.ac.uk:800	U/Tiesta.ge/48211110111060343079529/Inp	
	confi	.bit g.bit.a.he	http://chemd237.chem.ucl.ac.uk:800i http://chemd237.chem.ucl.ac.uk:800i	DKilestage/4821111011106034307952 DKilestage/4821111011106034307952	
	•		II.		
				Local Dir Download	
				Unio	

- 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 –I 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 <u>further-input.tgz</u> file from <u>http://www.realitygrid.org/AHE/training/courseinfo.html#ex2</u> 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?