# AHE Practical 1: Launching applications on the NGS

# **Aims and Objectives**

- Install the AHE client on your system
- · Set up a keystore containing your grid certificate
- · Configure the client with settings for UCL's AHE server
- Confirm that the client is installed and working
- · Launch the sort application with the AHE command line client
- Manually specify input and output files for an application

# Introduction

The AHE client is designed to be easily installed on an end user's machine, requiring only that they have a Java installation and an X.509 certificate for the grid which they want to access. The client package contains both GUI and command line clients which interoperate, allowing jobs launched with the GUI client to be manipulated with the command line tools and vice versa. For this short tutorial we will focus on the command line tools only.

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 the 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.

In this exercise we will install and configure the AHE client, install a certificate to allow you to access NGS resources, and check that the client is successfully installed. We will use command line clients to launch applications on the NGS.

After completing this section you should have a working installation of the AHE client and you will be familiar with launching applications using the AHE command line tools.

# Stage 1: Install and Configure the Client

- 1 For the purposes of this tutorial we will install and run the AHE client on the NeSC training cluster. Log in to your cluster node using the GSISSH applet. All files needed for the AHE practicals can be found in Comment [KW1]: Using own (real) /opt/NGSAppDev/AHE/.
- 2 The AHE client is written in Java, so a Java module will need to be loaded on the training cluster. At the command prompt type:

# module load java

3 Copy the AHE client distribution to your home directory as follows:

# cp /opt/NGSAppDev/AHE/ex1/aheclient-training.tgz ~/

4 At the command prompt unpack the AHE client by typing:

# tar zxvf aheclient-training.tgz

The client will be unpacked into your home directory.

5 Set the variable AHECLIENT\_HOME to point to do the AHE client location. To do this under Unix/Linux/MacOS X, type: export AHECLIENT\_HOME=/path to client On the training cluster type:

#### export AHECLIENT\_HOME=\$HOME/aheclient-1.0.1

Note, this will only be set for the duration that your shell session is open. To make the export survive between logins add it to your ~/.bash\_profile file.

6 Next you need to create a keystore for your client, containing your grid certificate. This will be used to authenticate you to the AHE server, and generate the proxy credentials required to access NGS resources. A script is provided to allow you to import your grid certificate in pfx format into a Java keystore for use by the AHE client. At the command prompt type:

#### cd \$AHECLIENT\_HOME cd bin ./kssetup path to certificate

where path to certificate is the full path to your grid certificate (for example /home/ahe/ nescuser00.pfx).

You will be prompted to enter the password for your pfx format certificate. Enter the password and press [**Return**]. Note: All passwords entered will be echoed back to the screen. Next, you will be prompted to enter a password for the keystore that you are setting up. This will be the password that you enter to unlock the AHE client.

You will see a message telling you that the certificate has been imported, and then you will be prompted for your keystore password again (the second password you had to enter).

Next a trusted CA root certificate for the UK e-Science authority will be imported into the keystore. Answer yes to say that you trust the certificate. You will be prompted for the keystore password a final time, enter it and then answer yes to confirm that you trust the root CA certificate of the NeSC training team.

7 Now that the keystore has been generated you can proceed to configure the AHE client.

(If this was not done in the tarball config file, alter the file aheclient.properties with the following:

uk.ac.ucl.chem.ccs.aheclient.ahedavserver=http://chemd237.chem.ucl.ac.uk\:8000/filestage/ uk.ac.ucl.chem.ccs.aheclient.jobregepr=https://chemd237.chem.ucl.ac.uk\:9443/ahe/AppWSResource uk.ac.ucl.chem.ccs.aheclient.jobfactoryepr=https://chemd237.chem.ucl.ac.uk\:9443/ahe/AppServerRegistry DBI

uk.ac.ucl.chem.ccs.aheclient.ahedavuser=training

uk.ac.ucl.chem.ccs.aheclient.ahedavpasswd=training

- this is the same as setting the endpoints using the AHE GUI client)

8. You now need to create and upload a proxy certificate using the training certificate and the MyProxy command. Users with a training certificate – your myproxy has already been uploaded and you will be told your username and password for it.

To let the AHE know where you stored your proxy certificate, edit the aheclient.properties file:

uk.ac.ucl.chem.ccs.aheclient.myproxy-un=<your\_proxy\_username>

There is no need to fill in the password – it will prompt you for it when you run a job, and this avoids storing it in clear text in the configuration file.

# Stage 5: 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 AHECLIENT\_HOME variable to be set automatically in stage 1, then you will need to export this variable again.
- 2 At the terminal type: cd \$AHECLIENT\_HOME/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. 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 ex1-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 ex1-sortjob -config \$HOME/sortapp-input/config.txt -RM Manchester -n 1

Make sure you give the full path to the sort application configuration file. 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 6: 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 5 type:

# ./ahe-monitor –s ex1-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. 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 in your home directory and download the output to there. To do this type:

# mkdir \$HOME/output-dir ./ahe-getoutput -s ex1-sortjob -I \$HOME/output-dir

# **Further Work**

# Try performing these further tasks with the AHE clients:

- Copy the further-input.tgz file from /opt/NGSAppDev/AHE/ex1/further-input.tgz to your home directory. 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.
- Familiarise yourself with the AHE client manual: <u>http://www.realitygrid.org/AHE/doc/AHEClientUserGuide.pdf</u>

# **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?