

# Application Hosting Environment NAMD Tutorial

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## 1: NAMD

NAMD is a parallel molecular dynamics(MD) code used for large-scale bio-molecular simulations. More information about NAMD can be obtained at <http://www.ks.uiuc.edu/Research/namd/>

## 2: Hosting NAMD within the AHE

In this tutorial, we assume that –

- 1) the user is interested in hosting NAMD within the AHE in order to run NAMD simulations on the TeraGrid sites at NCSA and SDSC and the core National Grid Service (NGS) nodes at Leeds, Oxford, RAL and Manchester.
- 2) The AHE server has been installed and configured as per the AHE Server Installation Guide (Section 2) on the server machine in \$AHE\_LOCATION.
- 3) The AHE client has been installed as per the AHE Client User Guide (Section 1) on the client machine in \$AHECLIENT\_HOME.

### 2.1 Install NAMD on the Grid Resources

Pre-compiled NAMD executables are available on the Leeds, Oxford and RAL nodes at the following locations

- 2.1.1 Leeds node – /usr/local/Cluster-Apps/namd-2.5-intel/bin/namd2-mpi
- 2.1.2 Oxford node - /usr/local/Cluster-Apps/namd-2.5-intel/bin/namd2-mpi
- 2.1.3 RAL node - /usr/local/applications/bioinformatics/namd-2.5/Linux-i686-NGS-MPI/namd2

On the US TeraGrid Sites and NGS Manchester node, download and compile NAMD with MPI as per the instructions at <http://www.ks.uiuc.edu/Research/namd/>. Note the path to your namd executable, e.g.

- 2.1.4 TeraGrid NCSA site – /home/ac/xyz/bin/namd2-mpi
- 2.1.5 TeraGrid SDSC site – /users/xyz/bin/namd2-mpi
- 2.1.6 NGS Manchester node - /home/ngs0xyz/bin/namd2-mpi

The NAMD executable should have execute permissions according to whom it is intended will run it. For example, to allow everyone to read and execute it, the permission on the NAMD executable should be set to 0755 using the chmod command.

### 2.2 Add NAMD Application in each Grid Resource/RM's RMInfo

- 2.2.1 On the AHE server, in \$AHE\_LOCATION/config/RMInfo/RMList.xml for each <RM> element corresponding to the Grid Resources, add the <app> sub-element.

```
<ahe:app xmlns:ahe="http://www.rahwl.org/v1.0">
  <ahe:name>namd</ahe:name>
  <ahe:JSDLTemplate>config/JSDLTemplates/namd.$RMName.jsdl</ahe:JSDLTemplate>
</ahe:app>
```

Each <RM> element can have multiple <app> sub-elements for each of the applications installed on the RM

## 2.2.2 Sections of the RMList.xml file for the Grid Resources with NAMD installed would look like:

```
<ahe:RMList xmlns:ahe="http://www.rahwl.org/ApplicationHostingEnvironment/v1.0">
```

```
<!-- Entry for the NCSA node ----->
```

```
<ahe:RM>
  <ahe:commonName>NCSA</ahe:commonName>
  <ahe:app>
    <ahe:name>namd</ahe:name>
    <ahe:JSDLTemplate>config/JSDLTemplates/namd.ncsa.jsdl</ahe:JSDLTemplates>
  <ahe:app>
    ...other RM properties
</ahe:RM>
```

```
<!-- Entry for the SDSC node ----->
```

```
<ahe:RM>
  <ahe:commonName>SDSC</ahe:commonName>
  <ahe:app>
    <ahe:name>namd</ahe:name>
    <ahe:JSDLTemplate>config/JSDLTemplates/namd.sdsc.jsdl</ahe:JSDLTemplates>
  <ahe:app>
    ...other RM properties
</ahe:RM>
```

```
<!-- Entry for the Leeds node ----->
```

```
<ahe:RM>
  <ahe:commonName>leeds</ahe:commonName>
  <ahe:app>
    <ahe:name>namd</ahe:name>
    <ahe:JSDLTemplate>config/JSDLTemplates/namd.leeds.jsdl</ahe:JSDLTemplates>
  <ahe:app>
    ...other RM properties
</ahe:RM>
```

```
<!-- Entry for the Oxford node ----->
```

```
<ahe:RM>
  <ahe:commonName>oesc</ahe:commonName>
  <ahe:app>
    <ahe:name>namd</ahe:name>
    <ahe:JSDLTemplate>config/JSDLTemplates/namd.oesc.jsdl</ahe:JSDLTemplates>
  <ahe:app>
    ... other RM properties
</ahe:RM>
```

```
<!-- Entry for the RAL node ----->
```

```
<ahe:RM>
  <ahe:commonName>rl</ahe:commonName>
  <ahe:app>
    <ahe:name>namd</ahe:name>
    <ahe:JSDLTemplate>config/JSDLTemplates/namd.rl.jsdl</ahe:JSDLTemplates>
  <ahe:app>
    ... other RM properties
</ahe:RM>
```

```
<!-- Entry for the Manchester node ----->
```

```

<ahe:RM>
  <ahe:commonName>man</ahe:commonName>
  <ahe:app>
    <ahe:name>namd</ahe:name>
    <ahe:JSDLTemplate>config/JSDLTemplates/namd.man.jsdl</ahe:JSDLTemplates>
  </ahe:app>
  ... other RM properties
</ahe:RM>

</ahe:RMList>

```

## 2.3 Create NAMD JSDL Templates for each Grid Resource/RM

2.3.1 On the AHE server, for each Grid Resource, create a NAMD JSDL Template. All the JSDL Templates should be placed in \$AHE\_LOCATION/config/JSDLTemplates.

2.3.2 We follow the following convention in naming JSDL Templates – \$applicationName.\$RMName.jsdl. So for NAMD JSDL templates we have –

```

namd.ncsa.jsdl
namd.sdsc.jsdl
namd.leeds.jsdl
namd.oesc.jsdl
namd.rl.jsdl
namd.man.jsdl

```

2.3.3 The JSDL templates are included in the AHE server source distribution. The important sections are the specification of the location of the executable on the Grid Resource and environment variables that need to be set for the application to be run.

2.3.3.1 namd.ncsa.jsdl

```

...
<Executable>/home/ac/xyz/bin/namd2-mpi</Executable>

```

2.3.3.2 namd.leeds.jsdl

```

...
<Executable>/usr/local/Cluster-Apps/namd-2.5-intel/bin/namd2-mpi</Executable>
<Environment name="NGSMODULES">gm/2.0.8</Environment>
...

```

## 2.4 Re-populate the Application Server Registry

2.4.1 Destroy the old registry of Applications hosted within the AHE.

```

cd $AHE_LOCATION/scripts
./ahe_destroyAppServerRegistry.pl

```

2.4.2 Populate the registry of Applications hosted within the AHE.

```

cd $AHE_LOCATION/scripts
./ahe_createAppServerRegistry.pl

```

2.4.3 Print out the list of Applications hosted within the AHE

```

cd $AHE_LOCATION/scripts
./ahe_queryAppServerRegistry.pl

```

You should see the new application:  
Printing Application Server Registry.....

...

```

Application Type: newApp
Application Factory EPR:
https://chemd.rahwl.ac.uk:8443/ahe/AppWSResource

```

...

## 2.5 Run NAMD Simulations

From the AHE client, launch the NAMD simulation.

- 2.5.1 List all applications available within the AHE  
`$AHECLIENT_HOME/ahe-listapps`
- 2.5.2 Prepare the Application Instance/Simulation  
`$AHECLIENT_HOME/ahe-prepare -s namdsim1 -app namd`
- 2.5.3 Start the Simulation  
`$AHECLIENT_HOME/ahe-start -s namdsim1 -config /tmp/input.namd  
-RM leeds -n 2`
- 2.5.4 Monitor the Simulation  
`$AHECLIENT_HOME/ahe-monitor -s namdsim1`
- 2.5.5 Retrieve output files on completion  
`$AHECLIENT_HOME/ahe-getoutput -s namdsim1 -l .`
- 2.5.6 Destroy the Simulation  
`$AHECLIENT_HOME/ahe-destroy -s namdsim1`
- 2.5.7 List all your simulations launched via the AHE  
`$AHECLIENT_HOME/ahe-list`
- 2.5.8 Script an ensemble of simulations  
Scripts can be written using the command-line clients above to launch ensembles of simulations. For example, one could launch 10 simulations with the namd input files named input\_1.namd, input\_2.namd....input\_10.namd, by using the following perl script.

```
#!/usr/bin/perl -w
```

```
#pre-processing of input files goes here
```

```
my @RMArray = ("NCSA", "SDSC", "leeds", "oesc", "rl");  
my @CPUArray = (8,8,4,8,2);  
my $numSims = 2*@RMArray;
```

```
#assign the 10 simulations to the resources in a round-robin fashion  
for(my $i = 0;$i < $numSims;$i++){
```

```
    $idx = $i % scalar(@RMArray);
```

```
    system "$ENV{AHECLIENT_HOME}/ahe-prepare -s namdsim$i -app namd";  
    system "$ENV{AHECLIENT_HOME}/ahe-start -s namdsim$i  
        -config /tmp/input_.$i.namd  
        -RM $RMArray[$idx]  
        -n $CPUArray[$idx]";
```

```
}
```

```
#wait until all the simulation has finished and retrieve the output to local directory
```

```
for(my $i = 0;$i < $numSims;$i++){  
  while(1){  
    $status =~ `${ENV{AHECLIENT_HOME}}/ahe-monitor namdsim.$i`;  
    if(!$status =~ / files staged out/){  
      next;  
    }  
    system "${ENV{AHECLIENT_HOME}}/ahe-getoutput -s namdsim$i -l .";  
    last;  
  }  
}
```

#post-processing of output files goes here

```
exit(0);
```

### 2.5.9 Using the GUI to run a NAMD simulation

Each of the steps 2.5.1 to 2.5.7 can be performed using the AHE Graphical User Interface Client. Please refer to the instructions in the AHE Client User Guide (Section 2).