Extreme Computing

bullx cluster suite

PBS Professional Guide



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Extreme Computing

bullx cluster suite PBS Professional Guide

Software

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Preface

Note

The Bull Support Web site may be consulted for product information, documentation, downloads, updates and service offers:

http://support.bull.com

PBS Professional from Altair Engineering is used to run batch jobs.

Bibliography

The following guides are available on the PBS Professional CD-ROM:

- PBS Professional Installation and Upgrade Guide
- PBS Professional Administrator's Guide
- PBS Professional User's Guide

The following guides are available on the bullx cluster suite Documentation CD-ROM:

- bullx cluster suite Installation and Configuration Guide
- bullx cluster suite High Availability Guide
- bullx cluster suite Administrator's Guide

The following document is distributed with the bullx cluster suite systems:

• Software Release Bulletin (SRB)



The Software Release Bulletin contains the latest information for your delivery. This should be read first. Contact your support representative for more information.

Chapter 1. PBS Professional Overview

1.1 PBS Professional

PBS Professional from **Altair Engineering** is the professional version of the Portable Batch System (PBS), a flexible resource and workload management system, originally developed to manage aerospace computing resources at NASA.

PBS is a distributed workload management system which has three primary roles:

Queuing

The collecting together of jobs or tasks to be run on a computer. Users submit tasks or jobs to the resource management system, which places them in a queue until the system is ready to run them.

Scheduling

The process of selecting which jobs to run, where and when, according to predetermined policies. Sites balance competing needs and goals on the system(s) in order to maximize the efficient use of resources (both computer time and people time).

Monitoring

The act of tracking and reserving system resources and enforcing usage policy. This covers both user-level and system-level monitoring, as well as monitoring the jobs that are being run. Tools are provided to help the human monitoring of the PBS system as well.



PBS Professional does not work with SLURM and should only be installed on clusters which do not use SLURM. If SLURM has been installed, see your System Administrator or the *SLURM Guide*.

See The PBS Professional Administrator's Guide and User's Guide for detailed information on using PBS Professional, including descriptions of some of the different configurations possible, with examples, plus descriptions of the PBS Professional Administrator commands.

1.2 PBS GridWorks Analytics

The optional **GridWorks Analytics** feature uses a parser to collect information from the PBS Professional server node (normally this is the cluster Management Node). The Application Server installed on a Login Node shows the information stored in the analytics database, either graphically or in the form of tables. These reports can be used to analyse and improve the performance of PBS Professional on the cluster, and to troubleshoot configuration problems.

Chapter 2. Installing PBS Professional

2.1 Install and Configure PBS Professional on the Management Node



- The PBS license file (altair_lic.dat) must be available as a prerequisite.
- The FLEXIm License Server has to be installed before PBS Professional is installed.
- This chapter applies only if PBS Professional was not installed on the cluster. Otherwise, please refer to Chapter 3 Upgrading to bullx cluster suite XR 5v3.1U2.

See

- Chapter 4 in the PBS Professional Installation and Upgrade Guide for more information on the installation of PBS Professional, described below.
- Chapter 2 in the PBS Professional Administrator's Guide for more information on the configuration routine for PBS Professional, described below

2.1.1 Download, Install and Start the FLEXIm License Server



This step applies to the Management Node (standard installation), or to a node which is dedicated as the FlexIm Server(s).

This section only applies to clusters which do NOT feature High Availability for the Management Node NOR redundancy for PBS Professional.

See Chapter 7, PBS Professional High Availability, in the present guide, if High Availability for the Management Node and High Availability (redundancy) for PBS Professional are in place.

- Copy all tarballs and documentation from the PBS Professional CD ROM on to the Management Node.
- 2. Uncompress and extract the files, using the command below:

tar -xvf altair_flexlm-<version>.<architecture>.tar

For example:

tar -xvf altair_flexlm-10.0.amd64_s8.tar

Run the command, below, to start the installation process.

./licsetup.sh

- 4. Respond to the questions as they appear identifying the location where the licensing package will be installed (/opt is recommended). This location is known as <install loc>.
- 5. Copy the license file, provided by Bull technical support, to the folder <install loc>/altair/security/altair_lic.dat.
- 6. Run the following commands to start the FLEXIm license server:

```
cd <install loc>/altair/security/
./altairlm.init.sh start
```

7. To install the license startup script, run the following command:

```
<install loc>/altair/security/install_altairlm.sh
```

2.1.2 Starting the installation of PBS Professional

The commands for the installation have to be carried out by the cluster Administrator logged on as root.

 Extract the package from the PBS Professional CD ROM to the directory of choice on the Management Node, using a command similar to that below.

```
cd /root/PBS
tar -xvzf PBSPro_10.2.0-RHEL5_x86_64.tar.gz
```

2. Go to the installation directory on the Management Node and run:

```
cd PBSPro_10.2.0
```

3. Start the installation process:

```
./INSTALL
```

During the PBS Professional installation routine, the Administrator will be asked to identify the following:

Execution directory

The directory into which the executable programs and libraries will be installed, for example, /opt/pbs/default (this is a symbolic link to /opt/pbs/10.2.0.93147)

Home directory

The directory into which the PBS Professional daemon configuration files and log files will be installed, for example, /var/spool/PBS.

PBS installation type

The installation type depends on the type of node that PBS Professional is being installed on:

On the Management Node: type 1

Do you want to continue?

Answer Yes.

License file location

In the example above this is /opt/altair/security/altair_lic.dat

Would you like to start?

When the Installation complete window appears, the installation program offers to start PBS Professional, enter 'n' for 'no'.

2.1.3 Initial Configuration of the Management Node

See

- Chapter 4 in the PBS Professional Installation and Upgrade Guide for more information on the installation for PBS Professional.
- Chapter 2 in the *PBS Professional Administrator's Guid*e for more information on configuring PBS Professional.



See Chapter 7 PBS Professional High Availability, in the present guide, for the pbs.conf file configuration details if High Availability is in place for PBS Professional.

1. Modify the /etc/pbs.conf file as follows:

```
PBS_EXEC=/opt/pbs/default
PBS_HOME=/var/spool/PBS
PBS_START_SERVER=1
PBS_START_MOM=0
PBS_START_SCHED=1
PBS_SERVER=basename0
PBS_SCP=/usr/bin/scp
```

2. Edit and modify the PBS limits configuration file (/opt/pbs/default/lib/init.d/limits.pbs_mom) as follows:

2.1.4 Starting PBS Professional

Run the PBS start script using a command with the following format: <path to script>/pbs start.

For example:

```
/etc/init.d/pbs start
```

2.2 Install and Configure PBS Professional on LOGIN, COMPUTE and COMPUTEX Reference Nodes

This step describes how to install and configure PBS Professional as necessary for the Reference Nodes to be deployed.



- PBS Professional does not work with SLURM.
- PBS Professional has to be installed on the Management Node before it is installed on the COMPUTE(X)/LOGIN reference nodes.

 See - Chapter 4 in the PBS Professional Installation and Upgrade Guide for more information on the installation for PBS Professional described below.

- Chapter 3 in the *PBS Professional Administrator's Guide* for more information on the configuration routine for *PBS Professional*, described below.

2.2.1 Starting the installation of PBS Professional

The commands for the installation have to be performed by the cluster Administrator logged on as root.

 Copy and extract the package from the PBS Professional CD-ROM to the directory of choice on the COMPUTE(X) Reference Node, using a command similar to that below.

```
cd /root/PBS
tar -xvzf PBSPro_10.2.0-RHEL5_x86_64.tar.gz
```

2. Go to the installation directory on each node and run:

```
cd PBSPro_10.2.0
```

3. Start the installation process:

```
./INSTALL
```

4. Follow the installation program

During the PBS Professional installation routine, the Administrator will be asked to identify the following:

Execution directory

The directory into which the executable programs and libraries will be installed, for example, /opt/pbs/default (this is a symbolic link to /opt/pbs/10.2.0.93147)

Home directory

The directory into which the PBS Pro daemon configuration files and log files will be installed, for example, /var/spool/PBS.

PBS installation type

The installation type depends on the type of node that PBS Professional is being installed on:

- On the COMPUTE Node: type 2
- On the LOGIN Node: type 3 (this has to be a separate dedicated Login Node)

Do you want to continue?

Answer Yes.

You need to specify a hostname for the Server

Give the hostname of the node where the PBS server has been installed, normally this is the Management Node.

Would you like to start?

When the Installation complete window appears, the installation program offers to start PBS Professional, enter ' \mathbf{n} ' for ' \mathbf{no} '.

2.2.2 Initial configuration on a LOGIN or COMPUTE(X) Reference Node

See Chapter 3 in the PBS Professional Administrator's Guide for more information on configuring and starting PBS Professional.

2.2.2.1 Initial configuration on the LOGIN Reference Node

1. Modify the /etc/pbs.conf file for the node as follows:

```
PBS_EXEC=/opt/pbs/default
PBS_HOME=/var/spool/PBS
PBS_START_SERVER=0
PBS_START_MOM=0
PBS_START_SCHED=0
PBS_SERVER=<server_name>0
PBS_SCP=/usr/bin/scp
```



The Login Nodes have to be defined on the Management Node by creating a /etc/hosts.equiv file containing the Login Node names (one per line).

Note If necessary, add **/opt/pbs/default/bin** to the user's PATH.

2.2.2.2 Initial configuration on the COMPUTE(X) Reference Node

1. Modify the /etc/pbs.conf file for the node as follows:

```
PBS_EXEC=/opt/pbs/default
PBS_HOME=/var/spool/PBS
PBS_START_SERVER=0
PBS_START_MOM=1
PBS_START_SCHED=0
PBS_SERVER=<server_name>0
PBS_SCP=/usr/bin/scp
```

2. Edit and modify the PBS limits configuration file (/opt/pbs/default/lib/init.d/limits.pbs_mom) as follows:

```
if [ -f /etc/bull-infos ] ; then

MEMLOCKLIM=`ulimit -l`

NOFILESLIM=`ulimit -n`

STACKLIM=`ulimit -s`

ulimit -l 4086160

fi
```

3. Modify the initial script by removing the -s -P options from the options_to_pbs_attach line (line 177). This should appear as below:

```
vi /opt/pbs/default/lib/MPI/pbsrun.mpich2.init.in
options_to_pbs_attach="-j $PBS_JOBID"
```

4. Add the appropriate wrapper, by using the command below. For mpibull2:

/opt/pbs/default/bin/pbsrun_wrap /opt/mpi/mpibull2-<xxx>/bin/mpirun
pbsrun.mpich2



mportant At this point the Reference Nodes are ready for deployment.

5. Start PBS on the Compute Node:

```
/etc/init.d/pbs start
```

6. Run the following command on the Management Node to ensure the Compute Node is visible for the PBS server:

```
qmgr -c "create node <compute_node_name>"
```

Chapter 3. Upgrading to bullx cluster suite XR 5v3.1U2

3.1 Pre-upgrade Procedures

This chapter applies to clusters that are currently running bullx cluster suite XR 5v3.1U1 and the PBS Professional Batch Manager version 10.0. The manual operations described in this section will need to be performed for PBS Professional clusters.



• It is the customer's responsibility to back-up data and configuration files, before using the procedure described in this section. For example the PBS_HOME and PBS_EXEC directories must be saved, as well as the /etc/pbs.conf configuration file. Any site-defined configuration files that have been created must also be kept. Use the command below, to list these files.

/usr/pbs/sbin/pbs_mon -s list

- It is recommended to use the tar or cp -a command, which maintains file permissions.
- The PBS license file (altair_lic.dat) must also be kept in a safe place.

Shutdown all PBS Professional jobs

1. Use the command below to stop scheduling, so that new jobs cannot start:

```
qmgr -c set server scheduling=false
```

2. For each queue, stop the jobs that are queuing by using the command below:

```
qdisable <queue name>
```

3. Use the command below to list the jobs that are running (some of them will be listed more than once):

```
pbsnodes <hostname> | grep Jobs
```

- 4. For each job you can choose either to let it finish, to requeue it, or to kill it:
 - a. Requeue jobs with the following command:

```
qrerun <job_ID> <job_ID> ...
```

b. Use the **qdel** command to kill each job:

```
qdel <job_ID> <job_ID> ...
```

5. Stop all PBS Professional jobs that are running, and their MOM components, by running the following command on the Management Node:

```
/usr/pbs/bin/qterm -m -t immediate
```

6. Then stop the PBS Professional Server by using the command:

```
/usr/pbs/bin/qterm -s -f
```

Unwrap MPI on the COMPUTE(X) Nodes

If the PBS Professional **pbsrun_wrap** mechanism has been used with the **MPIBull2** library, then this must be unwrapped on each **COMPUTE(X)** node by using the command below:

```
pdsh -w clustername[nodelist] /usr/pbs/bin/pbsrun_unwrap pbsrun.mpich2
```

If the **pbsrun_wrap** mechanism has been used with the **MVAPICH** library, then this must be unwrapped on each **COMPUTE(X)** node by using the command below:

```
pdsh -w clustername[nodelist] /usr/pbs/bin/pbsrun unwrap pbsrun.mvapichl
```

Note

Refer to the **/opt/pbs/default/lib/MPI** directory to see which wrapping mechanism has been used for earlier versions of PBS Professional.

3.2 Upgrade the Management Node

3.2.1 Install PBS Professional

The new PBS Professional version 10.2 packages will be installed in the **/release/** directory. Unpack and install the new version of PBS Professional using the commands below:

```
cd /release/PBSPro10.2-EM64T/
tar xvzf PBSPro_10.0.2-RHEL5_x86_64.tar.gz
cd /release/PBSPro10.2-EM64T/PBSPro_10.2.0
./INSTALL
```

During the PBS Professional installation routine, the Administrator will be asked to identify the following:

Execution directory

The directory into which the executable programs and libraries will be installed, for example, /opt/pbs/10.2.0.93147. This will be used as the new PBS_EXEC directory for PBS Professional 10.2, using a symbolic link to the /opt/pbs/default directory.

Home directory

The directory into which the PBS Professional daemon configuration files and log files will be installed, for example, /var/spool/PBS. This will be used as the new PBS_HOME directory.

PBS installation type

The installation type depends on the type of node that PBS Professional is being installed on:

On the Management Node: type 1

Do you want to continue?

Answer y for Yes.

License file location

In the example above this is /opt/altair/security/altair_lic.dat

Do you want to switch to the new version?

Answer y for Yes.

Would you like to start?

When the Installation complete window appears, the installation program offers to start PBS Professional, enter $\bf n$ for $\bf No$.

Note The PBS license file must be mirrored (in the same directory on both servers).

3.2.2 Configure PBS Professional 10

Edit the new scheduler configuration file

On the Management Node, upgrade the new bullx cluster suite XR 5v3.1U2 /opt/pbs/default/etc/pbs_sched_config file with any modifications that had been made to the previous /var/spool/PBS/sched_priv/sched_config file.

1. Identify the differences between the two versions on the scheduler configuration file by running the command below:

```
diff /opt/pbs/default/etc/pbs_sched_config
/var/spool/PBS/sched_priv/sched_config
```

2. Modify the new **/opt/pbs/default/etc/pbs_sched_config** file so that only the copyright differs, and then replace the old version by copying it across:

```
cp /opt/pbs/default/etc/pbs_sched_config
/var/spool/PBS/sched_priv/sched_config
```

3. Answer Y to the question that appears to confirm the overwriting of the /var/spool/PBS/sched_priv/sched_config file.

Upgrade Fairshare Entities and the Database

This only applies if there are some groups defined in the /var/spool/PBS/sched_priv/resource_group file.

See Section 4.16 in the PBS Professional Administrator's Guide.

Start PBS Professional version 10 on the PBS Server (Management Node)

- Edit the pbs.conf file, based on the one that has been saved. On the PBS Server (Management Node), START_MOM must be set to 0 and PBS_SCP=/usr/bin/scp must be added to the pbs.conf file.
- Edit and modify the PBS limits configuration file (/opt/pbs/default/lib/init.d/limits.pbs_mom) as follows:

```
if [ -f /etc/bull-infos ] ; then
    MEMLOCKLIM=`ulimit -l`
    NOFILESLIM=`ulimit -n`
    STACKLIM=`ulimit -s`
    ulimit -l 4086160
fi
```

3. Run the commands below on the PBS Server (Management Node) (no additional options are required):

```
/opt/pbs/default/sbin/pbs_sched
/opt/pbs/default/sbin/pbs_server
```

3.3 Upgrade PBS Professional on the Reference Node

3.3.1 Install PBS Professional version 10 on the Reference Nodes

The new PBS Professional **version 10** package is installed in the **/release/** directory. Unpack and install the new version of PBS Professional using the commands below:

```
cd /release/PBSPro10.2-EM64T/
tar xvzf PBSPro_10.2.0-RHEL5_x86_64.tar.gz
cd /release/PBSPro10.2-EM64T/PBSPro_10.2.0
./INSTALL
```

During the PBS Professional installation routine on the Reference Nodes, the Administrator will be asked to identify the following:

Execution directory

The directory into which the executable programs and libraries will be installed, for example, /opt/pbs/10.2.0.93147. This will be used as the new PBS_EXEC directory for PBS Professional 10.2, with a symbolic link to the /opt/pbs/default directory. It is recommended to switch to the new default path.

Home directory

The directory into which the PBS Professional daemon configuration files and log files will be installed, for example, /var/spool/PBS. This will be used as the new PBS_HOME directory.

PBS installation type

The installation type depends on the type of node that PBS Professional is being installed on:

- On a COMPUTE(X) Node: type 2
- On a Login Node: type 3 (this has to be a separate dedicated Login Node)

On a COMPUTE(X) reference node, the question "Do you want to continue?" will appear. Answer **y** for **Yes**.

A hostname for the Server

Give the hostname of the node where the PBS Professional server has been installed, normally this is the Management Node.

The question "Do you want to switch to the new version?" will appear.

Answer y for Yes.

The question "Would you like to start?" will appear.

When the **Installation complete** window appears, the installation program proposes starting PBS Professional, enter **n** for **No**.

3.3.2 Configure PBS Professional version 10 on the Reference Nodes

Transfer the MOM configuration information (on COMPUTE(X) Node only)

If necessary, upgrade the configuration information with the details in the /var/spool/PBS/mom_priv/config file, saved previously.

Edit the pbs.conf file

Use the **pbs.conf** file saved previously. The following line should be added to the **pbs.conf** file for the Reference Nodes:

PBS_SCP=/usr/bin/scp

Modify the start script (on COMPUTE(X) Node only)

The start script that has been modified on the Management Node must be copied to the COMPUTE(X) Reference Node, using the command below.

scp <MNGT_NODE>:/opt/pbs/default/lib/init.d/limits.pbs_mom
<REF_node>:/opt/pbs/default/lib/init.d/limits.pbs_mom

Prepare the wrapper script (on the COMPUTE(X) Node only)

Modify the **/opt/pbs/default/lib/MPI/pbsrun.mpich2.init.in** initial script by removing the **-s** and **-P** options from the **options_to_pbs_attach** line (line 177). This should appear as below:

options_to_pbs_attach="-j \$PBS_JOBID"



Deploy the Reference Nodes as described in the *Installation and Configuration Guide*.

3.4 Post Installation Operations

3.4.1 If MPIBull2 is used: Set the wrappers for the MPI commands

Add the MPIBull2 wrapper by using the commands below:

pdsh -w clustername[nodelist]"cd /opt/mpi/; ln -s mpibull2-<version>
mpibull2-current"
pdsh -w clustername[nodelist] /opt/pbs/default/bin/pbsrun_wrap
/opt/mpi/mpibull2-<version>/bin/mpirun pbsrun.mpich2

3.4.2 Restart PBS Professional on all Nodes

If PBS Professional High Availability is used

If PBS Professional High Availability is used, restart PBS Professional as described in section 7.4 Starting PBS Professional High Availability on the Cluster Nodes.

If PBS Professional High Availability is NOT used

On the execution hosts, recover any jobs that were left running, by using the command below:

pdsh -w clustername[nodelist] /opt/pbs/default/sbin/pbs_mom -p

Then restart PBS Professional on all cluster nodes by using the command below:

pdsh -w clustername[nodelist] /etc/init.d/pbs restart

Note If necessary, change the user's PATH to include /opt/pbs/default.

Chapter 4. Launching an Application

PBS Professional Batch Manager is used by bullx cluster suite to run batch jobs.

4.1 Pre-requisites

- 1. The User **ssh** keys should have been dispatched so that the User can access the Compute Nodes. See the *Administrator's Guide* for details on how to do this.
- 2. To use PBS Professional with MPIBull2, the home directory of the user should include the mpd.conf file which includes the user's password details. Only the user should have read and write rights for the mpd.conf file.
- 3. If necessary add the /opt/pbs/default to the user's PATH.

4.2 Submitting a script with MPIBull2

Run the command below to see the job submission script, named test.pbs, in this example:

```
cat test.pbs
```

The script will appear, similar to that below, and can be edited if necessary.

```
#!/bin/bash
#PBS -l select=2:ncpus=3:mpiprocs=3
#PBS -l place=scatter
source /opt/mpi/mpibull2-<version>/share/setenv_mpibull2.sh
mpirun -n 6 hostname
```

4.3 Submitting a script with bullx MPI

Run the command below to see the job submission script, named **test.pbs**, in this example:

```
cat test.pbs
```

The script will appear, similar to that below, and can be edited if necessary.

```
#!/bin/bash
#PBS -1 select=2:ncpus=3:mpiprocs=3
#PBS -1 place=scatter
source /opt/mpi/bullxmpi-<version>/bin/mpivars.sh
mpirun hostname
```

4.4 Launching a job

Use the **qsub** command to launch a job with this script, as below:

```
qsub test.pbs
```

The output will be in the format:

```
466.zeus0
```

This indicates that the number of the job is 466 on machine zeus0.

4.5 Displaying the results for a job

Use the **astat** command to see the details of the jobs submitted.

```
qstat -an
```

Here it is possible to see that, as specified in the script, the job is running on 3 CPUs on two nodes, named zeus8 and zeus9.

4.6 Tracing a job

Run the **tracejob** command to see the progress for a specific job, for example 466:

```
tracejob 466
```

This will give output, similar to that below, showing all the job execution steps that have been carried out.

```
Job: 466.zeus0
10/30/2007 12:43:46 L Considering job to run
10/30/2007 12:43:46 S enqueuing into workq, state 1 hop 1 10/30/2007 12:43:46 S Job Queued at request of user@zeus0, owner =
<user_name>@zeus0, job name = test.pbs, queue = workq
10/30/2007 12:43:46 S Job Run at request of Scheduler@zeus0 on hosts
(zeus8:ncpus=3:mpiprocs=3)+(zeus9:ncpus=3:mpiprocs=3)
10/30/2007 12:43:46 S Job Modified at request of Scheduler@zeus0
10/30/2007 12:43:46 L
10/30/2007 12:43:48 S
                            Job run
                            Obit received momhop:1 serverhop:1 state:4
substate: 42
10/30/2007 12:43:48 S
                            Exit_status=0 resources_used.cpupercent=0
resources_used.cput=00:00:01 resources_used.mem=2764kb
                                resources_used.vmem=30612kb
resources_used.ncpus=6
resources_used.walltime=00:00:02
10/30/2007 12:43:48 S
                           dequeuing from workq, state 5
```

4.7 Exiting a job

If a job exits before it has completed then use the command in the format below to look at the error log:

```
cat test.pbs.e466
```

If the command issued in the job submission script ('mpirun -n 6 hostname' for example) completes successfully, run the command below:

```
cat essai.pbs.o466
```

The output will list the nodes used, for example:

```
zeus8
zeus8
zeus8
zeus9
zeus9
```

Chapter 5. Administrating PBS Professional

This chapter describes some specific details which apply to Bull Extreme Computing clusters.

5.1 Pre-requisites

 SLURM should not run on the same clusters as PBS Professional. If necessary deactivate SLURM by running the following command on the Management Node and on all the Compute Nodes:

```
chkconfig -- level 345 slurm off.
```

 The root user, administrator, should have direct access to all the Compute Nodes from the Management Node, and vice versa, without having to use a password. ssh is used to protect this access.

5.2 Post Installation checks

The /etc/pbs.conf file will have been created automatically during the installation of PBS PRO. This will contain the PBS_EXEC path (/opt/pbs/default) and the PBS_HOME directory (/var/spool/PBS by default).

See Chapter 2. *Installing PBS Professional* in the present guide, for more information about the installation and configuration of PBS Professional.

5.3 Checking the status of the PBS daemons

Run the following command on the Management and Compute Node to check the status of the PBS daemons

```
/etc/init.d/pbs status
```

On the Management Node, output similar to that below, should appear:

```
pbs_server is pid xxxx
pbs_sched is pid xxxx
```

On the Compute Nodes, output similar to that below, should appear:

```
pbs\_mom is pid xxxx
```

5.4 Adding a Node to the Initial Cluster Configuration

Use the **qmgr** command, as below, to add a Compute Node to the list of Compute Nodes for a cluster:

```
/opt/pbs/default/bin/qmgr -c "create node <node_name>"
```

Use the following command to verify that the node has been created and added to the Compute Node list:

/opt/pbs/default/bin/pbsnodes -a

5.5 Useful Commands for PBS Professional

The following commands, which are in the **/opt/pbs/default/bin** directory, may be used to test that PBS Professional is up and running correctly:

pbsnodes –a Used to display the status of the nodes in cluster

qsubUsed to submit a jobqdelUsed to delete a job

qstat Used to display the job, queue and server status

tracejob Used to extract job info from the log files

See The PBS Professional Administrator's Guide and User's Guide included for detailed information on these and on other commands.

5.6 Essential Configuration Settings for bullx cluster suite

This section describes some essential configuration settings which are required to ensure that PBS Professional runs smoothly on bullx cluster suite.

5.6.1 MPIBull2 and PBS Professional for all clusters (InfiniBand and Ethernet)

To use **MPIBull2** with PBS Professional run the following commands on both the Management Node and on all the Compute Nodes:

```
cd /opt/pbs/default/bin
pbsrun_wrap /opt/mpi/mpibull2-<version>/bin/mpirun pbsrun.mpich2
```

This will give output similar to that below:

```
pbsrun_wrap: EXECUTED: "mv /opt/mpi/mpibull2-<version>/bin/mpirun
/opt/mpi/mpibull2-1.2.1-4.t/bin/mpirun.actual"
pbsrun_wrap: EXECUTED: "cp /opt/pbs/default/bin/pbsrun
/opt/pbs/default/bin/pbsrun.mpich2"
pbsrun_wrap: EXECUTED: "chmod 755 /opt/pbs/default/bin/pbsrun.mpich2"
```

pbsrun_wrap: EXECUTED: "ln -s /opt/pbs/default/bin/pbsrun.mpich2

/opt/mpi/mpibull2-<version>/bin/mpirun"

pbsrun_wrap: EXECUTED: "ln -s /opt/mpi/mpibull2<version>/bin/mpirun.actual/opt/pbs/default/lib/MPI/pbsrun.mpich2.link" pbsrun_wrap: EXECUTED: "chmod644/opt/pbs/default/lib/MPI/pbsrun.mpich2.init"

Chapter 6. Optional: GridWorks Analytics

6.1 GridWorks Analytics – DataCollector Installation

6.1.1 Installation

The Data Collector installation must be done on the Management Node.

 Check that the line, below, appears in the /etc/ssh/sshd_config file on the Management Node:

X11Forwarding yes

Note This line should **not** be commented out.

Use the command below to connect to the Management Node.

ssh -X <destination machine>

3. Execute the DataCollector Installer.

sh PBSAnalytics_DataCollector_10.2.0-RHEL5_x86_64.bin



mportant

We recommend to use all the default options for this installation:

- The license path will look like: 7788@node0
- Postgres installation and the DataStore must be on a separate Login Node (in order to avoid DataBase conflicts with the ClusterDB).
- Set this Login Node name for PostGreSQL server name (with postgres as username and password), and for the DataStore.

6.1.2 Post Installation Steps

Final installation steps, including the addition of initialization scripts for your subsystem are provided below. Once finished, you can start the PBS Data Collector.

- 1. Move \$PBSDC_INSTALL/etc/init.d/pbsdata to /etc/init.d/.
- 2. Run the commands:

ln -s /etc/init.d/pbsdata /etc/rc3.d/S84pbsdata
ln -s /etc/init.d/pbsdata /etc/rc3.d/K15pbsdata

Starting / Stopping the PBS Data Collector

service pbsdata start
service pbsdata stop

6.2 GridWorks Analytics - Portal Installation

6.2.1 Installation

The Portal installation must be done on a Login Node.

Note Do not install GridWorks Analytics Application Server on the Management Node, in order

to avoid conflicts with the ClusterDB.

 Check that the line, below, appears in the /etc/ssh/sshd_config file on the Management Node:

X11Forwarding yes

Note This line should **not** be commented out.

Use the command below to connect to the Management Node, then to the Login Node.

```
ssh -X <destination machine>
```

3. Execute the PBS Portals Installer, and select Manual Installation.

```
sh PBSPortal_10.2.0-RHEL5_x86_64.bin
```

The PBS Portals installer will extract all files to your desired location.

Note You will need to open up a Terminal Emulator and change directory to your selected PBS Portals installation directory. You will also need to run all commands as the super user.

6.2.2 PBS Portals Database Installation

The installation process has included the necessary Postgres RPMs for your platform. You can find the provided RPMs inside **\$PORTAL_INSTALL/ManualInstallation/postgres**. Install the RPMs manually using the **rpm** command. The following RPMs are provided:

- postgresql-libs-8.3.3-1
- postgresql-8.3.3-1
- postgresql-server-8.3.3-1

Please install the RPMs in this order. For instance:

```
# rpm -iv postgresql-libs-8.3.3-1PGDG.rhel5.x86_64.rpm
# rpm -iv postgresql-8.3.3-1PGDG.rhel5.x86_64.rpm
# rpm -iv postgresql-server-8.3.3-1PGDG.rhel5.x86_64.rpm
```

If necessary, edit /var/lib/pgsql/data/postgresql.conf to fit the environment:

```
datestyle = 'iso, dmy'
changed to:
datestyle = 'iso, mdy'
```

Then start the postgres services as follows:

```
# chkconfig --add postgresql
# /etc/init.d/postgresql initdb
# /etc/init.d/postgresql start
```

6.2.2.1 Database Setup

You will need to create a database for use with PBS Portals and update that database with the Altair-provided Database Schema. Below are steps to configure Postgres from the command-line:

```
su - postgres -c "createdb hwewebportal"
su - postgres -c "psql hwewebportal <
$PORTAL_INSTALL/ManualInstallation/postgres/DBSchema.sql"
```

6.2.2.2 Database Access

Host-Based Authentication

You will need to configure Postgres to allow external connections using Host-Based Authentication. This is useful not only for monitoring and managing your PBS Portals database remotely via the Postgres Administration tool, but also required for some Portal Components (for example PBS Analytics and the PBS Data Collector) to communicate directly with the database. This is achieved by modifying the **Postgres pg_hba.conf** file, located at

/var/lib/pgsql/data/pg_hba.conf. Below is an example of how you would add an allowable host to your database:

```
host hwewebportal postgres 127.0.0.1/32 trust
```

Password-based Authentication

Using password-based authentication will only allow connections from specified clients and users. PostgreSQL database passwords are separate from operating system user passwords. The password for each database user is stored in the **pg_authid** system catalog. Passwords can be managed with the SQL commands CREATE USER and ALTER USER.

Example:

```
CREATE USER foo WITH PASSWORD \secret'
```

By default, if no password has been set up, the stored password is null and password authentication will always fail for that user. By default, PBS Analytics configures all connections to be used by user **postgres**. Upon installation of PostgresSQL, the default password for user **postgres** is **postgres**. If you wish to change this password, execute the following command as user root:

```
su - postgres -c "psql -c \"ALTER USER postgres WITH UNENCRYPTED
PASSWORD 'postgres'\";"
```

To enable password-based authentication, modify the **Postgres pg_hba.conf** file, located at /var/lib/pgsql/data/pg_hba.conf. You will also need to specify the IP address of the host machine in this list. Below is an example of how you would add an allowable host to your database:

```
host hwewebportal postgres 127.0.0.1/32 password host hwewebportal postgres <host IP address>/32 password
```

Note

If migrating from GWA 10.0 or PBS Analytics 10.1, you will need to change the password in **\$PBS_DATA_COLLECTOR/analytics/parser/config/DBConnection.properties** and set it to the current password of the postgres user.

6.2.2.3 Listening Interface

By default, Postgres is configured to listen to 'localhost' which may or may not be the hostname or interface you would like the Postgres database to be listening on. Update the **postgresql.conf** file located at **/var/lib/pgsql/data/** with the below example to ensure proper interface listening.

```
Change (if applicable):
#listen_address = 'localhost'
to:
listen address = '*'
```

After making all changes, restart Postgres:

```
/etc/init.d/postgresql stop
/etc/init.d/postgresql start
```

6.2.3 Install the PBS Portal Application Server

PBS Portals uses the **JBoss** Application Server. You will need to make a few modifications to some of the existing configuration files in order to properly configure the application server, as well as connect with the PBS Portals database.

6.2.3.1 Database Connection

Check, and if necessary, modify the existing **\$PORTAL_INSTALL/thirdparty/jboss-4.2.1.GA/server/default/deploy/postgres-ds.xml** file:

- 1. Update the connection-url with the correct IP address of your Postgres server.
- 2. Update the **user-name** with the correct credentials for your Postgres server.
- 3. Update the **password** with the correct credentials for your Postgres server.

6.2.3.2 Analytical Datastore Database Connection

Check, and if necessary, modify the existing \$PORTAL_INSTALL/analyticsds/gwaolapdatasources.xml file:

1. Update the **<DataSourceInfo>** element with the correct IP address of your Postgres server.

- 2. Update the <DataSourceInfo> element's jdbcUser with the correct credentials for your Postgres server.
- 3. Update the **<DataSourceInfo>** element's **jdbcPassword** with the correct credentials for your Postgres server.

So the <DataSourceInfo> block should look like:

```
<DataSourceInfo>Provider=mondrian;Jdbc=jdbc:postgresql://127.0.0.1:543
2/hwewebportal;jdbcUser=postgres;jdbcPassword=postgres;JdbcDrivers=org
.postgresql.Driver</DataSourceInfo>
```

6.2.3.3 Server Configuration

JBoss provides a few general server parameters which can be modified via the server.xml file, located at \$PORTAL_INSTALL/thirdparty/jboss-4.2.1.GA/server/default/deploy/jboss-web.deployer/server.xml

The XML element 'Connector' contains the most basic of HTTP server information. The default port is 8080. The default address is 0.0.0.0. The address can be left as-is since JBoss will allow access to the host machine by DNS name or IP by specifying 0.0.0.0. You have the option to specify an IP address or hostname to narrow down accessibility of the server.

Update the **port** and **address** attributes to reflect your desired listening port and server IP address.

Licensing Configuration

PBS Portals will need to be made aware of your Altair License Manager. The instructions for providing this information are discussed below:

- 1. Change directory to \$PORTAL_INSTALL/thirdparty/jboss-4.2.1.GA/bin.
- 2. Update and save the following lines within **run.sh**. An example of a valid <port@hostname> is <u>7788@localhost</u>.

```
#ALTAIR LICENSING
ALTAIR_LM_LICENSE_FILE=<port@hostname>
export ALTAIR_LM_LICENSE_FILE
```

Server Administrator

You will need to define at least one administrator for your PBS Portals installation. Below are steps to add, update, and delete administrators.

- 1. Open \$PORTAL_INSTALL/awpconfig/PBSPortal/awpConfig.xml.
- 2. Scroll down until you find the following section:

```
<CustomConfig>
<BusinessAdministratorUserNames>
</BusinessAdministratorUserNames>
</CustomConfig>
```

Inside of the <BusinessAdministratorUserNames> block, place the following for each
user name you would like to be considered an Administrator of your PBS Portals
Installation:

Authentication Mechanisms

The various authentication mechanisms are stored and configured within individual files. Modifying any one of these files and saving them as **login-config.xml** will enable it as the preferred authentication mechanism upon server restart.

Properties Authentication

This authentication type consists of two Java Properties formatted text files for username to password (users.properties) and username to roles (roles.properties) mapping. The names of the properties files may be overridden by the usersProperties and rolesProperties options.

- Change directory to: \$PORTAL_INSTALL/thirdparty/jboss-4.2.1.GA/server/default/conf/
- 2. Update the list of users in the props/awp-users.properties file and the user roles in the props/awp-roles.properties files.

```
Examples:
```

```
awp-user: username=password
awp-role: username=webportalUser, username=webportalAdmin
```

3. Rename the file ./proplogin-config.xml to ./login-config.xml.

See For more information on properly setting up JBoss property files, please consult http://www.jboss.org/community/wiki/UsersRolesLoginModule.

6.2.4 Environment Variables

Copy:

/opt/gridworks/10.2.0/portals/thirdparty/jboss-4.2.1.GA/server/default/deploy/PBSPortal.war/WEB-INF/classes/wpResourceBundle.properties

to:

/opt/gridworks/10.2.0/portals/thirdparty/jboss-4.2.1.GA/server/default/deploy/PBSPortal.war/WEB-INF/classes/wpResourceBundle_fr.properties

2. Copy:

/opt/gridworks/10.2.0/portals/thirdparty/jboss-4.2.1.GA/server/default/deploy/PBSPortal.war/WEB-INF/classes/resourcebundle/gwpResourceBundle_en.properties to:

/opt/gridworks/10.2.0/portals/thirdparty/jboss-4.2.1.GA/server/default/deploy/PBSPortal.war/WEB-INF/classes/resourcebundle/gwpResourceBundle_fr.properties

3. Copy:

/opt/gridworks/10.2.0/portals/thirdparty/jboss-4.2.1.GA/server/default/deploy/PBSPortal.war/WEB-INF/classes/resourcebundle/pbsaResourceBundle_en.properties to:

/opt/gridworks/10.2.0/portals/thirdparty/jboss-4.2.1.GA/server/default/deploy/PBSPortal.war/WEB-INF/classes/resourcebundle/pbsaResourceBundle_fr.properties

6.2.5 Running PBS Portals

Final installation steps, including the addition of initialization scripts for your subsystem, are provided below. Once finished, you can start the PBS Analytics Application Server by starting the **PBSPortal** init script.

- 1. Move \$PORTAL_INSTALL/ManualInstallation/pbsportal to /etc/init.d/.
- 2. Run the commands:

```
ln -s /etc/init.d/pbsportal /etc/rc3.d/S84pbsportal
ln -s /etc/init.d/pbsportal /etc/rc3.d/K15pbsportal
/etc/init.d/pbsportal start
```



FlashPlayer 10 must be installed in firefox plugins (/usr/lib/mozilla/plugins/libflashplayer.so), otherwise display will not be correct.

3. To start the PBS Portal, login as "root" on the Management Node and run your browser using the following command, where <login_node> is the node where the portal has been installed:

```
firefox http://<login_node>:8080/PBSPortal/
```

6.3 GridWorks Analytics – Final checks

6.3.1 PBS Data Collector Check (on the Management node)

Verify the PBS Data Collector service is running by typing the following commands:

```
# cd /etc/init.d/
# ./pbsdata status
```

View the log file of the PBS Data Collector to verify the service is actually running and parsing data. It will only parse data contained in the accounting log directory.

Type in the following commands to verify the PBS Data Collector is parsing data:

```
# cd $PBSDC_INSTALL/analytics/parser/dist
# ls -1
```

```
total 100
-rw-rw-r-- 1 root root 90585 Nov 13 14:26 parser.jar
-rw-rw-r-- 1 root root 3535 Nov 21 01:00 parser.log
-rw-rw-r-- 1 root root 246 Nov 20 10:50 parsererror.log
#
```

6.3.2 PostgreSQL Check (on the Login Node)

Verify the PostgreSQL Service is running by typing the following commands:

```
# ps -elf | grep postgres
```

```
4 R root 879 672 0 78 0 - 320 - 08:49 pts/0 00:00:00 grep postgres 0 S postgres 16314 1 0 76 0 - 9610 - Nov18 ? 00:00:27 /usr/bin/postmaster -p 5432 -D /var/lib/pgsql/data 1 S postgres 16319 16314 0 76 0 - 2440 - Nov18 ? 00:00:00 postgres: logger process 1 S postgres 16321 16314 0 75 0 - 9643 - Nov18 ? 00:00:00 postgres: writer process 1 S postgres 16322 16314 0 75 0 - 9610 - Nov18 ? 00:00:00 postgres: wal writer process 1 S postgres 16322 16314 0 75 0 - 9610 - Nov18 ? 00:00:00 postgres: wal writer process 1 S postgres 16323 16314 0 76 0 - 9644 - Nov18 ? 00:00:07 postgres: autovacuum launcher process 1 S postgres 16324 16314 0 76 0 - 2473 - Nov18 ? 00:00:12 postgres: stats collector process 1 S postgres 16501 16314 0 76 0 - 9872 385869 Nov18 ? 00:00:38 postgres: postgres analytics 127.0.0.1(36722) idle #
```

Verify the PostgreSQL database is initialized and has data. (These commands must be executed as "root".)

The full list of tables (as shown below) will be displayed after the first successful login to the PBS Analytics Web site.

```
# whoami

root

# su - postgres -c psql
```

Welcome to psql 8.3.3, the PostgreSQL interactive terminal.

Type: \copyright for distribution terms
\h for help with SQL commands
\? for help with psql commands
\g or terminate with semicolon to execute query
\q to quit

```
postgres=# \c hwewebportal
```

You are now connected to database "hwewebportal".

hwewebportal-# \d

```
Schema
List of Name Type Owner
relations
public dashboard table postgres
public filteruserroleaccessmatrixentry table postgres
public filtervalueuserroleaccessmatrixentry table postgres
public hibernate_sequence sequence postgres
```

public preference table postgres public securityroleassignment table postgres public sharingdetails table postgres public sharingsecurity table postgres public t_gwa_host_list table postgres public t_gwa_job_attributes table postgres public t_gwa_job_attributes_jid_seq sequence postgres public t_gwa_time_by_date table postgres public tentity table postgres public tfilter table postgres public tfilter_value table postgres public tpanel table postgres public tquerypart table postgres public tquerytemplate table postgres public tquerytemplate_tquerypart table postgres public tuser table postgres public userrole table postgres public userroleassignment table postgres (22 rows)

hwewebportal-#	\ a
IIWEWEDPOI car-#	۱ч

#

Chapter 7. PBS Professional High Availability



Resource Manager High Availability varies according to the system. See the Software Release Bulletin delivered with your system for details of any limitations that may apply to your release.

7.1 Prerequisites for High Availability

Partitions

The gfs2 cluster file system allows all nodes in a cluster to access a device concurrently, via the standard file system interface. This simplifies the management of applications that run across the cluster and is essential to ensure that High Availability can function.

Each Batch Manager needs at least one partition to share their dynamic data (jobs, accounting, etc.).

See

The High Availability Guide for more information on the creation and use of different partitions for the different services/ Batch Managers.

Management Nodes

PBS Professional High Availability is only possible on a cluster which includes High Availability for the Management Node.

A Secondary Management Node for the Management Node High Availability solution is required.

See

the *High Availability Guide* for more information on configuring High Availability for the Management Nodes.

NFS Server

An NFS Server is required. This can either be on the Secondary Management Node or on a different Service Node, Login or otherwise. This NFS service will be used for the user home directories.

FLEXIm license servers

Three (3) **FLEXIm** license servers are required - one on the Primary and Secondary Management Nodes, and one on the Service Node, Login or otherwise.

See

Chapter 2 *Installing PBS Professional* in the present guide, for details on installing the **FLEXIm** license server and PBS Professional.

7.2 Hardware Architecture for PBS Professional High Availability

The cluster architecture, and the location of the **FLEXIm** license servers, varies according to the size of the cluster, as shown in the following diagrams.

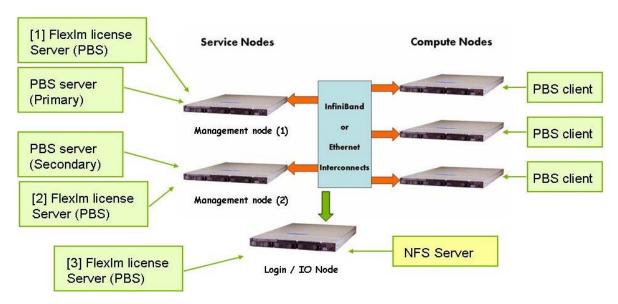


Figure 7-1. Example of the cluster Architecture for a medium-sized cluster with a **FLEXIm** license server and **NFS** Server on the same Login/IO Service Node

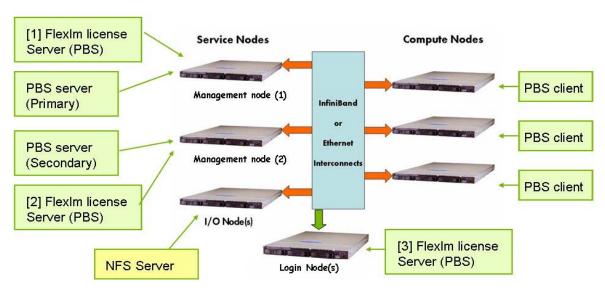


Figure 7-2. Example of a cluster architecture for a large-sized cluster with an NFS Server on a dedicated I/O Node and a FLEXIm license server on a dedicated Login Node

7.3 Configuring High Availability for PBS Professional



Before configuring High Availability for PBS Professional, the bullx cluster suite software has to be installed and correctly configured on the cluster.

- Install the FLEXIm license on each one of the nodes designated as a license server.
 Verify that the PBS license file is mirrored (in the same directory on both servers).
- Install PBS Professional on the Primary and Secondary Management Nodes and on the Reference Nodes.
- 3. Ensure that PBS Professional does not start at this point.
- 4. Edit the PBS Professional Configuration files, **pbs.conf**, for the two Management Nodes, as shown below:

Primary Management Node pbs.conf File

```
PBS_EXEC=/opt/pbs/default
PBS_HOME=/var/spool/PBS
PBS_START_SERVER=1
PBS_START_MOM=0
PBS_START_SCHED=1
PBS_SERVER=<hostname 1>
PBS_PRIMARY=<hostname 1>
PBS_SECONDARY=<hostname 2>
PBS_SCP=/usr/bin/scp
```

Secondary Management Node pbs.conf File

```
PBS_EXEC=/opt/pbs/default
PBS_HOME=/var/spool/PBS
PBS_START_SERVER=1
PBS_START_MOM=0
PBS_START_SCHED=0
PBS_SERVER=<hostname 1>
PBS_PRIMARY=<hostname 1>
PBS_SECONDARY=<hostname 2>
PBS_SCP=/usr/bin/scp
```

The /var/spool/PBS directory must be mounted on both Management Nodes with a gfs2 file system hosted on the shared storage.

5. Edit the PBS Professional Configuration file on the COMPUTE(X) Reference Nodes, as shown below:

COMPUTE(X) Reference Node pbs.conf file

```
PBS_EXEC=/opt/pbs/default
PBS_HOME=/var/spool/PBS
PBS_START_SERVER=0
PBS_START_MOM=1
PBS_START_SCHED=0
PBS_SERVER=<hostname 1>
PBS_PRIMARY=<hostname 1>
PBS_SECONDARY=<hostname 2>
PBS_SCP=/usr/bin/scp
```

Edit the PBS Professional Configuration file on the Login Reference Nodes, as shown below:

LOGIN Reference Node pbs.conf file

```
PBS_EXEC=/opt/pbs/default
PBS_HOME=/var/spool/PBS
PBS_START_SERVER=0
PBS_START_MOM=0
PBS_START_SCHED=0
PBS_SERVER=<hostname 1>
PBS_PRIMARY=<hostname 1>
PBS_SECONDARY=<hostname 2>
PBS_SCP=/usr/bin/scp
```



When starting PBS Professional in High Availability Mode it is essential that all 3 FLEXIm license servers are running.

7.4 Starting PBS Professional High Availability on the Cluster Nodes

Stop PBS Professional from being started automatically by running the command below on both the Primary and the Secondary Nodes.

```
chkconfig pbs off
```

Each Management Node must start cluster services in a predefined order.

1. Start the **HA Cluster Suite** services:

```
pdsh -w mgnt0,mgnt1 'storioha -c start'
```

2. Mount the /var/spool/PBS directory on the shared storage system:

```
pdsh -w mgnt0,mgnt1 'mount LABEL=HA_MGMT:PBS /var/spool/PBS'
```

3. Launch the PBS services on both Management Nodes:

```
ssh mgnt0 'service pbs start'
ssh mgnt1 'service pbs start'
```

4. Launch the PBS service on the Compute Nodes:

```
pdsh -w nodes[2..10] 'service pbs start'
```

7.5 Restoring PBS services High Availability following a Primary Management Node crash

The High Availability of the PBS services has to be restored following the crash of the Primary Management Node, and the Primary PBS Server is running on the Secondary Management Node. This is done as follows:

1. Restart HA Cluster Suite on the Primary Node:

storioha -c start

- 2. Wait a few seconds and then check that **HA Cluster Suite** is available by using the **clustat** command.
- 3. Mount the PBS Professional shared storage, by running the command below:

mount LABEL=HA_MGMT:PBS /var/spool/PBS

4. Launch the PBS service:

service pbs start

Glossary

PBS

Portable Batch System

GWA

GridWorks Analytic**s**

MOM

Machine Oriented Miniserver
The Job Executor is the daemon that actually places
the job into execution. This daemon, pbs_mom, is
informally called MOM.

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