Installation

What is HUBzero?

HUBzero is a platform used to create dynamic web sites for scientific research and educational activities. With HUBzero, you can easily publish your research software and related educational materials on the web. Powerful middleware serves up interactive simulation and modeling tools via your web browser. These tools can connect you with rendering farms and powerful Grid computing resources.

Minimum System Requirements

HUBzero installations require one or more dedicated physical hosts running Debian GNU/Linux 6.0. In particular there are version specific requirements on mysql (5.1), python (2.6) and php (5.3).

Other distributions might theoretically work with some modification, although they would be totally unsupported.

A typical starter HUBzero installation might consist of a single physical server with dual 64-bit quad-core CPUs, 16 Gigabytes of RAM and a terabyte of disk.

It is possible to run HUBzero inside of a virtual machine such as ones created by VMware and VirtualBox. While fully functional there will would significant performance and resource limitations in such an environment. For demonstration or development purposes we often create VM images with less than a gigabyte of RAM and 5 gigabytes of disk. While fully functional, these virtual machines would only be suitable for a single user doing development or testing.

Target Audience

This document and the installation and maintenance of a HUBzero system has a target audience of **experienced** Linux administrators (preferably experienced with Debian GNU/Linux).

How To Get Source Code

This is optional

You'll find most of the source code within the web root of a working hub. But you can get source code for the middleware and all other parts of HUBzero by retrieving the source code packages using the debian package manager. To do so, first, update your package mechanism to pull packages from our HUBzero repository (codename 'manny' for this release). Edit your /etc/apt/sources.list and add the following line::

deb-src http://packages.hubzero.org/deb manny main contrib non-free

Then, install the hubzero archive key so that your system can verify packages from the hubzero archive. Run the following command as root:

```
wget http://packages.hubzero.org/deb/hubzero-signing-
key.asc -q -0 - | apt-key add -
```

Once the public key for http://packages.hubzero.org has been installed, you can request the hubzero source code for each package:

```
apt-get source packageName
```

where *packageName* is the desired package from the table below.

Package List

The following packages (subject to change): are available from the HUBzero repository for this release. Not all are necessarily used for any given installation.

Package Name Purpose

hubzero-app Command line tool to manage

installation/publishing of HUBzero apps

hubzero-app-workspace HUBzero App providing a lightweigth Linux

desktop, for app/tool development

hubzero-chuse HUBzero graphical front end to the user

environment manager 'use'

hubzero-cli HUBzero command line interface

hubzero-cms

hubzero-expire-sessions

hubzero-filexfer

hubzero-filexfer-xlate

hubzero-firewall hubzero-forge hubzero-icewm

hubzero-icewm-captive

hubzero-icewm-themes

hubzero-invokeapp hubzero-mailgateway hubzero-metrics hubzero-mw-client hubzero-mw-service

hubzero-mw-session hubzero-openIdap hubzero-policyrcd hubzero-python hubzero-rappture

hubzero-rappture-session hubzero-ratpoison-captive

hubzero-submit-client hubzero-submit-common hubzero-submit-condor hubzero-submit-distributor hubzero-submit-pegasus hubzero-submit-server hubzero-subversion hubzero-telequotad hubzero-textifier hubzero-texvo

hubzero-trac

hubzero-trac-mysqlauthz

hubzero-twm-captive

hubzero-use

The HUBzero Content Management System

(based on Joomla! framework)
Expires unused app/tool sessions

Transfer files between App Sessions and user's

desktop

Support daemon for the filexfer program

HUBzero firewall that protects app/tool sessions Creates project areas for tool development Linux ICE window manager configuration, used

in workspaces

Linux ICE window manager specially crafted to

support tools in a sessions

The HUBzero Linux ICE window manager

theme, used in workspaces

HUBzero application invoke script

HUBzero mail gateway

HUBzero metrics support package

HUBzero middleware - client

HUBzero middleware - execution host session

manager

HUBzero middleware - per session tools

OpenLDAP configuration package for HUBzero

HUBzero policy-rc.d for invoke-rc.d

HUBzero python API module

The Rapid APPlication infrastrucTURE toolkit

for building scientific tools

Session support packages for Rappture Linux window manager, used in app/tool

sessions

HUBzero submit client

HUBzero submit common python library HUBzero condor build for hubzero-submit HUBzero middleware submit distributor HUBzero pegasus build for hubzero-submit

HUBzero job submission server

HUBzero Subversion support package

Disk quota monitor HUBzero textifier

Helper utility to generate math fomulas for wiki

markup

HUBzero Trac support package

Plug-in for MySQL user auth in project

development areas

Linux TWM window manager, used in app/tool

sessions

Command for configuring the environment

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within a workspace

hubzero-use-apps HUBzero apps environment for 'use'

hubzero-usermap File permission mapping FUSE filesystem used

by WebDAV

hubzero-vncproxy HUBzero VNC proxy helper

hubzero-vncproxyd HUBzero VNC proxyserver

hubzero-webdav HUBzero WebDAV support package

libapache2-vncproxy HUBzero vncproxy module for apache2-mpm-

prefork

tightvnc-java Modified VNC Client that receives app/tool

sessions within a web browser

vnc4server Modified VNC Server that sends app/tool

sessions to the web browser

Linux

Install Basic Operating System

The latest version of <u>Debian GNU/Linux 6.0</u> (6.0.7 as of this writing) should be installed on each physical host used by a HUBzero installation.

To install Debian GNU/Linux, you can easily <u>obtain a copy</u>, and then follow the <u>installation</u> <u>instructions</u> for your architecture.

HUBzero has packaging support for amd64 (64bit) Intel architectures. i386 (32bit) packaging was not produced for this release due to lack of demand. Debian 7.0 is not supported at this time but will be in the next (1.2) release, scheduled for Fall 2013.

Installing Debian GNU/Linux using a a small bootable CD is the simplest method.

When the installation is complete your system will reboot into a Debian GNU/Linux system.

Don't forget to remove your installation media and/or change your server's boot media order if you changed them prior to installation.

The precise configuration (such as disk configuration, networking, etc) is dependent on how the hub is to be used and what hardware is being used. These instructions outline the simplest "hub in a box" configuration but may not be suitable for larger sites. It is expected that the hub will be managed by an experienced Linux administrator who can help scale your site to the capacity required.

Set hostname

Optional. If you didn't specify the fully qualified domain name when running setup you will need to set it here.

HUBzero expects the `hostname` command to return the fully qualified hostname for the system.

```
# hostname example.com
```

To make the change permanent you must also edit the file /etc/hostname, this be done simply with:

```
# echo "example.com" > /etc/hostname
```

Fix hosts

Now edit /etc/hosts by making sure that a line exists that looks like

```
127.0.1.1 example.com example
```

Any other lines with "127.0.1.1" should be removed.

Delete local users

HUBzero reserves all user ids from 1000 up for hub accounts. As part of the app middleware every account must map to a corresponding system account. Therefore when starting up a hub it is required to remove all accounts that have user ids 1000 or greater. On a new installation there is typically one such account that is created when you set up the hub, and this account can be removed as follows:

```
# deluser username
# rm -fr /home/username
```

If you require additional system accounts, they can be numbered between 500-999 without interfering with hub operations.

Configure Networking

Optional. If you didn't configure networking during installation you will need to do so now.

For help with networking setup try this link.

Setting up your IP address.

The IP addresses associated with any network cards you might have are read from the file **/etc/network/interfaces**. This file has documentation you can read with:

```
# man interfaces
```

A sample entry for a machine with a static address would look something like this:

```
# The loopback network interface auto lo iface lo inet loopback

# The primary network interface auto eth0 iface eth0 inet static address 192.168.1.90 gateway 192.168.1.1 netmask 255.255.255.0 network 192.168.1.0 broadcast 192.168.1.255
```

Here we've setup the IP addresss, the default gateway, and the netmask.

For a machine running DHCP the setup would look much simpler:

```
# The loopback network interface
auto lo
iface lo inet loopback

# The primary network interface - use DHCP to find our address
auto eth0
iface eth0 inet dhcp
```

(If you're using a DHCP based setup you must have a DHCP client package installed - usually one of pump or dhcp-client.)

If you make changes to this file you can cause them to take effect by running:

```
# /etc/init.d/networking restart
```

Setting up DNS

Use whatever nameserver and other options as recommended by your ISP. If you used DHCP to set up networking it is likely this has already been set.

When it comes to DNS setup Debian doesn't differ from other distributions. To cause your machine to consult with a particular server for name lookups you simply add their addresses to /etc/resolv.conf.

For example a machine which should perform lookups from the DNS server at IP address 192.168.1.10 would have a resolv.conf file looking like this:

```
nameserver 192.168.1.10
```

Configure Advanced Package Tool

Now configure the location of the HUBzero package repository by adding the following line to /etc/apt/sources.list

```
deb http://packages.hubzero.org/deb manny main
```

You will need to get and install the hubzero archive key to be able to verify packages from the hubzero archive:

```
# wget http://packages.hubzero.org/deb/hubzero-signing-
key.asc -q -0 - | apt-key add -
```

Once the public key for http://packages.hubzero.org has been install you can then upgrade the current packages to their latest releases.

```
# apt-get update
# apt-get upgrade
```

MySQL

Install

```
# apt-get install -y mysql-server
```

You will be prompted to enter a MySQL administrative password.

Configure

Default configuration works well for starters. But for optimal performance you will need a database administrator capable of tuning your database to your hardware configuration and site usage.

Mail

Install

We need to install exim4 to enable outgoing email

```
# apt-get install -y exim4
```

Configure

```
# dpkg-reconfigure exim4-config
```

Configure mail as appropriate for your site and IT infrastructure. We outline a sample standalone configuration below. The requirement is for php to be able to send mail (registration confirmation and other notices need to go out) and for exim4 to receive mail (for support ticket and forum email gateway functions to work).

This is just an example of a standalone mail configuration.

General type of mail configuration

internet site; mail is sent and received directly using SMTP

Mail name

enter the fully qualified domain name (FQDN) of the host (example.com)

IP-addresses to listen on for incoming SMTP connections

leave blank (listen for connections on all available network interfaces)

Other destinations for which mail is accepted

leave blank or (equivalently) with local hostname (all local domains will be treated identically)

Domains to relay mail for

leave blank

Machines to relay mail for

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leave blank

Keep number of DNS-queries minimal (Dial-on-Demand)

No

Delivery method for local mail

mbox format in /var/mail/

Split configuration into small files?

Yes

Test

Use a real email address below so you can see if you get the email

```
# Mail -v someone@gmail.com
```

CMS

Install

```
# apt-get install -y hubzero-cms
```

Configure

```
# hzcms install example
# a2dissite default default-ssl
# a2ensite example example-ssl
# /etc/init.d/apache2 restart
```

OpenLDAP

Install OpenLDAP

```
# apt-get install -y slapd
```

You will be prompted to enter a LDAP administrative password.

Install HUBzero LDAP support

```
# apt-get install -y hubzero-openldap
```

Some packages will ask you to configure them when you run this step. I am pretty sure you can just accept the defaults because we rewrite the configuration files during the next step anyway.

Configuring nslcd: LDAP server URI:

keep the default or enter "ldap://localhost/"

Configuring nslcd: LDAP server search base:

keep the default

Configuring libnss-Idapd

Select only "passwd", "group", "shadow"

Configure OpenLDAP Database

```
# hzldap init
# hzcms configure ldap --enable
```

To finish configuration you must manually (for now) trigger the initial synchronization of the CMS user/group tables with LDAP. Go to administrator section of your site (/administrator), go to

Site->Maintenance->LDAP and press the Export Users and Export Groups buttons in order to export all CMS users/groups. On a fresh install this would be consist solely of the user 'admin'.

Manually create a home directory for the CMS admin user now, it will make it easier to test things later to have this already setup.

```
# mkdir -p /home/example/admin
# touch /home/example/admin/mytest
# chown -R admin.users /home/example/admin
```

Test

```
# getent passwd
```

You should see an entry for user 'admin' toward the end of the list if everything is working correctly.

ssh and sftp

Install

These packages aren't working properly. Please don't install until this message is removed. If you have installed them already please purge them using the "purge" option instead of "install"

```
# apt-get install hubzero-ssh
# apt-get install hubzero-sftp
```

Configure

These modules aren't working properly. Please don't install until this message is removed. If you have configured them already please disable them using the "--disable" option instead of "--enable"

Support for basic ssh/sftp configuration was added with hubzero-cms_20130131.1

```
# hzcms configure ssh --enable
# hzcms configure sftp --enable
```

WebDAV

Install WebDAV

```
# apt-get install -y hubzero-webdav
```

Configure WebDAV

```
# hzcms configure webdav --enable
```

Test

```
# ls -l /webdav/home/admin
mytest
```

Browse to your site's https /webdav address (e.g. https://myhub/webdav). You should get prompted for a username and password. Use the admin account. You should see a directory listing including the file "mytest".

Now test using a WebDAV client.

```
# apt-get install cadaver
# cadaver https://localhost/webdav
```

You will be prompted to accept self signed certificate (if it is still installed) and then to enter your username and password. Use the 'admin' account again to test. When you get the "dav:/webdav/>" prompt just enter "Is" and it should show the test file.

Finally clean up test case

```
# apt-get purge cadaver
```

Troubleshooting

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If the test doesn't work, check if the fuse kernel module is loaded

```
# lsmod | grep fuse
fuse 54176 0
```

If there is no output then try starting the kernel module manually

```
# modprobe fuse
```

Then try the test again

Subversion

Install

```
# apt-get install -y hubzero-subversion
```

Configure

hzcms configure subversion --enable

Trac

Install

```
# apt-get install -y hubzero-trac
```

Configure

```
# hzcms configure trac --enable
```

Forge

Install

```
# apt-get install -y hubzero-forge
```

Configure

hzcms configure forge --enable

OpenVZ

Install

HUBzero makes extensive use of OpenVZ containers so it is recommended to use the OpenVZ enabled kernel on all HUBzero servers. To install a 64 bit kernel run the command:

```
# apt-get install linux-image-2.6-openvz-amd64
```

For 32 bit kernels, run the command:

```
# apt-get install linux-image-2.6-openvz-686
```

Configure

You will need to reboot the server to activate the new kernel.

```
# reboot
```

Verify the new kernel is running (see "openvz" in the output of the command below)

For 64 bit kernels

```
# uname -a
Linux example.com 2.6.32-5-openvz-
amd64 #1 SMP Sat May 5 02:13:13 UTC 2012 x86_64 GNU/Linux
```

or for 32 bit kernels

```
# uname -a
Linux example.com 2.6.32-5-openvz-686 #1 SMP Sat May 5 02:13:13 UTC 20
12 x86_64 GNU/Linux
```

If the new kernel is running you may remove the old (non-openvz) kernel

For 64 bit kernels (the exact version number may differ on your installation)

```
# apt-get purge linux-image-2.6.32-5-amd64
```

or for 32 bit kernels (the exact version number may differ on your installation)

```
# apt-get purge linux-image-2.6.32-5-i686
```

Test

```
# vzlist
Container(s) not found
```

Or it will list the containers currently running if you check this on a running hub. The salient point being that the command doesn't issue any kind of error message.

Firewall

Install

```
# apt-get install -y hubzero-firewall
```

HUBzero requires the use of iptables to route network connections between application sessions and the external network. The scripts controlling this can also be used to manage basic firewall operations for the site. If you use manage iptables with other tools you will have to make sure the rules in these scripts are maintained. /etc/firewall_on and /etc/firewall_off turn the HUBzero firewall on and off respectively. Scripts in /etc/rc.X/ to /etc/mw/firewall_on causes the script to run at startup (these links were created for you). The firewall is enabled in all boot modes 0-6. The basic scripts installed here block all access to the host except for those ports required by HUBzero (http,https,http-alt,ldap,ssh.smtp,mysql,submit,etc).

Maxwell Service

Install

```
# apt-get install -y hubzero-mw-service
```

Configure

```
# mkvztemplate amd64 squeeze manny
```

```
# hzcms configure mw-service --enable
```

Test

This test will show a failure the first time it is run. After the first session is created additional sessions should start without error. Be sure to stop each session you start using this test (as described below).

```
# maxwell_service startvnc 1 800x600 24
```

Enter an 8 character password when prompted (e.g., "testtest")

This should result in a newly create OpenVZ session with an instance of a VNC server running inside of it. The output of the above command should look something like:

```
=====
Removing and repopulating: root etc var tmp dev
Mounting: /var/lib/vz/template/debian-5.0-amd64-maxwell home apps
=====
VE is mounted
Setting CPU units: 1000
Configure meminfo: 2000000
VE start in progress...
TIME: 0 seconds.
Waiting for container to finish booting.
/usr/lib/mw/startxvnc: Becoming nobody.
/usr/lib/mw/startxvnc: Waiting for 8-byte vncpasswd and EOF.
1+0 records in
1+0 records out
8 bytes (8 B) copied, 3.5333e-05 s, 226 kB/s
Got the vncpasswd
Adding auth for 10.51.0.1:0 and 10.51.0.1/unix:0
xauth: creating new authority file Xauthority-10.51.0.1:0
Adding IP address(es): 10.51.0.1
if-up.d/mountnfs[venet0]: waiting for interface venet0:0 before doing
NFS mounts (warning).
WARNING: Settings were not saved and will be resetted to original valu
es on next start (use --save flag)
# vzlist
     VEID
             NPROC STATUS IP_ADDR
                                       HOSTNAME
                 6 running 10.51.0.1
# openssl s_client -connect localhost:4001
```

This should report an SSL connection with a self signed certificate and output text should end with:

RFB 003.008

If you see this then you successfully connected to the VNC server running inside the newly created OpenVZ session.

Clean up

```
# maxwell_service stopvnc 1
```

Which should give output similar to:

```
Killing 6 processes in veid 1 with signal 1
Killing 7 processes in veid 1 with signal 2
Killing 5 processes in veid 1 with signal 15
Got signal 9
Stopping VE ...
VE was stopped
========== begin /etc/vz/conf/1.umount ==============
Unmounting /var/lib/vz/root/1/usr
Unmounting /var/lib/vz/root/1/home
Unmounting /var/lib/vz/root/1/apps
Unmounting /var/lib/vz/root/1/.root
Removing /var/lib/vz/root/1 :root etc var tmp dev/shm dev
Removing /var/lib/vz/private/1: apps bin emul home lib lib32 lib64 mnt
opt proc sbin sys usr .root
========== end /etc/vz/conf/1.umount =============
VE is unmounted
```

Maxwell Client

Install

```
# apt-get install -y hubzero-mw-client
```

Configure

```
# hzcms configure mw-client --enable
```

Test

```
# su www-data
$ ssh -i /etc/mw-client/maxwell.key root@localhost ls
The authenticity of host 'localhost (127.0.0.1)' can't be established.
RSA key fingerprint is e5:3c:7d:41:71:0b:0f:2a:0c:0e:bb:15:4d:e7:2f:08
.
Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added 'localhost' (RSA) to the list of known host
s.
list of files
$ exit
#
```

vncproxy

Install

```
# apt-get install -y hubzero-vncproxy
```

Configure

```
# hzcms configure vncproxy --enable
```

telequotad

install

```
# apt-get install -y hubzero-telequotad
```

Configure

In order for filesystems quotas to work they must be enabled when they are mounted. Determine which filesystem contains your home directories and add "quota" to the mount option of the corresponding entry in the /etc/fstab file. Only the filesystem with /home on it matters to telequotad.

If quotas weren't already in affect, the run something like the following (depending on your filesystem configuration) to start up the quota system.

```
# mount -oremount /
# /etc/init.d/quota restart
```

Test

```
# repquota -a
```

Should show disk usage for all users.

Workspace

Install

```
# apt-get install hubzero-app
# apt-get install hubzero-app-workspace
# hubzero-
app install --publish /usr/share/hubzero/apps/workspace-1.3.hza
```

Test

You should then be able to log in to the site and see the "Workspace" tool in the tool list and launch it in your browser.

Metrics

Install

```
# apt-get install -y hubzero-metrics
```

Configure

hzcms configure metrics --enable

Rappture

Install

```
# apt-get install hubzero-rappture
```

Configure

Rappture is used from inside a container and needs several other packages installed to allow use of all its features. This process has been simplified by using the hubzero-rappture-session with only contains the dependencies needed to pull in these other packages.

```
# chroot /var/lib/vz/template/debian-6.0-amd64-maxwell
# apt-get update
# apt-get upgrade
# apt-get install hubzero-rappture-session
# exit
```

A workspace may need to be opened and closed a few times before the changes to the session template appear in a workspace.

Test

A user must setup their runtime environment in order to use the Rappture toolkit. Run the following command before attempting to run any Rappture tests.

```
use rappture
```

Rappture comes with several demostration scripts that can effectively test many parts of the package. These demonstrations must be copied to a user's home directory within a workspace before running.

```
$ mkdir examples
$ cp -r /apps/share/rappture/examples/* examples/.
$ cd examples
$ ./demo.bash
```

A window should open on the workspace showing that part of the demonstration. Close that window to see the next demonstration. Some demonstrations may need something inputted to work properly (such as the graphing calculator).

Filexfer

Install

```
# apt-get install -y hubzero-filexfer-xlate
```

Configure

hzcms configure filexfer --enable

Submit

Introduction

The submit command provides a means for HUB end users to execute applications on remote resources. The end user is not required to have knowledge of remote job submission mechanics. Jobs can be submitted to traditional queued batch systems including PBS and Condor or executed directly on remote resources.

Installation

```
# apt-get install hubzero-submit-pegasus
# apt-get install hubzero-submit-condor
# apt-get install hubzero-submit-common
# apt-get install hubzero-submit-distributor
# apt-get install hubzero-submit-server
# hzcms configure submit-server --enable
# /etc/init.d/submit-server start
```

At completion of the apt-get install commands several files will be located in the directory /opt/submit. Excluding python files the directory listing should like the following:

Configuration

submit provides a mechanism to execute jobs on machines outside the HUB domain. To accomplish this feat some configuration is required on the HUB and some additional software must be installed and configured on hosts in remote domains. Before attempting to configure submit it is necessary to obtain access to the target remote domain(s). The premise is that a single account on the remote domain will serve as an execution launch point for all HUB end users. It is further assumes that access to this account can be made by direct ssh login or using an ssh tunnel (port forwarding).

Having attained account access to one or more remote domains it is possible to proceed with submit configuration. To get started the ssh public generated by the installation should be transferred to the remote domain host(s).

HUB Configuration

The behavior of submit is controlled through a set of configuration files. The configuration files contain descriptions of the various parameters required to connect to a remote domain, exchange files, and execute simulation codes. There are separate files for defining remote sites, staged tools, multiprocessor managers, permissible environment variables, remote job monitors, and ssh tunneling. Most parameters have default values and it is not required that all

parameters be explicitly defined in the configuration files. A simple example is given for each category of configuration file.

Sites

Remote sites are defined in the file sites.dat. Each remote site is defined by a stanza indicating an access mechanism and other account and venue specific information. Defined keywords are

- [name] site name. Used as command line argument (-v/--venue) and in tools.dat (destinations)
- venues comma separated list of hostnames. If multiple hostnames are listed one site will chosen at random.
- tunnelDesignator name of tunnel defined in tunnels.dat.
- siteMonitorDesignator name of site monitor defined in monitors.dat.
- venueMechanism possible mechanisms are ssh and local.
- remoteUser login user at remote site.
- remoteBatchAccount some batch systems requirement that an account be provided in addition to user information.
- remoteBatchSystem the possible batch submission systems include CONDOR, PBS, and LSF. SCRIPT may also be specified to specify that a script will be executed directly on the remote host.
- remoteBatchQueue when remoteBatchSystem is PBS the queue name may be specified.
- remoteBatchPartition slurm parameter to define partition for remote job
- remoteBatchPartitionSize slurm parameter to define partition size, currently for BG machines.
- remoteBatchConstraints slurm parameter to define constraints for remote job
- remoteBinDirectory define directory where shell scripts related to the site should be kept.
- remoteApplicationRootDirectory define directory where application executables are located.
- remoteScratchDirectory define the top level directory where jobs should be executed.
 Each job will create a subdirectory under remoteScratchDirectory to isolated jobs from each other.
- remotePpn set the number of processors (cores) per node. The PPN is applied to PBS and LSF job description files. The user may override the value defined here from the command line.
- remoteManager site specific multi-processor manager. Refers to definition in managers.dat.
- remoteHostAttribute define host attributes. Attributes are applied to PBS description files.
- stageFiles A True/False value indicating whether or not files should be staged to remote site. If the the job submission host and remote host share a file system file staging may not be necessary. Default is True.

- passUseEnvironment A True/False value indicating whether or not the HUB 'use' environment should passed to the remote site. Default is False. True only makes sense if the remote site is within the HUB domain.
- arbitraryExecutableAllowed A True/False value indicating whether or not execution of arbitrary scripts or binaries are allowed on the remote site. Default is True. If set to False the executable must be staged or emanate from /apps.
- members a list of site names. Providing a member list gives a layer of abstraction between the user facing name and a remote destination. If multiple members are listed one will be randomly selected for each job.
- state possible values are enabled or disabled. If not explicitly set the default value is enabled.
- failoverSite specify a backup site if site is not available. Site availability is determined by site probes.
- checkProbeResult A True/False value indicating whether or not probe results should determine site availability. Default is True.
- restrictedToUsers comma separated list of user names. If the list is empty all users may garner site access. User restrictions are applied before group restrictions.
- restrictedToGroups comma separated list of group names. If the list is empty all groups may garner site access.
- logUserRemotely maintain log on remote site mapping HUB id, user to remote batch job id. If not explicitly set the default value is False.
- undeclaredSiteSelectionWeight used when no site is specified to choose between sites where selection weight > 0.
- minimumWallTime minimum walltime allowed for site or queue. Time should be expressed in minutes.
- maximumWallTime maximum walltime allowed for site or queue. Time should be expressed in minutes.
- minimumCores minimum number of cores allowed for site or queue.
- maximumCores maximum number of cores allowed for site or queue.
- pegasusTemplates pertinent pegasus templates for site, rc, and transaction files.

An example stanza is presented for a site that is accessed through ssh.

```
[cluster]
venues = cluster.campus.edu
remotePpn = 8
remoteBatchSystem = PBS
remoteBatchQueue = standby
remoteUser = yourhub
remoteManager = mpich-intel64
venueMechanism = ssh
remoteScratchDirectory = /scratch/yourhub
```

siteMonitorDesignator = clusterPBS

Tools

Staged tools are defined in the file tools.dat. Each staged tool is defined by a stanza indicating an where a tool is staged and any access restrictions. The existence of a staged tool at multiple sites can be expressed with multiple stanzas or multiple destinations within a single stanza. If the tool requires multiprocessors a manager can also be indicated. Defined keywords are

- [name] tool name. Used as command line argument to execute staged tools. Repeats are permitted to indicate staging at multiple sites.
- destinations comma separated list of destinations. Destination may exist in sites.dat or be a grid site defined by a ClassAd file.
- executablePath path to executable at remote site. The path may be given as an absolute path on the remote site or a path relative to remoteApplicationRootDirectory defined in sites.dat.
- restrictedToUsers comma separated list of user names. If the list is empty all users may garner tool access. User restrictions are applied before group restrictions.
- restrictedToGroups comma separated list of group names. If the list is empty all groups may garner tool access.
- environment comma separated list of environment variables in the form e=v.
- remoteManager tool specific multi-processor manager. Refers to definition in managers.dat. Overrides value set by site definition.
- state possible values are enabled or disabled. If not explicitly set the default value is enabled.

An example stanza is presented for a staged tool maintained in the yourhub account on a remote site.

```
[earth]
destinations = cluster
executablePath = ${HOME}/apps/planets/bin/earth.x
remoteManager = mpich-intel

[sun]
destinations = cluster
executablePath = ${HOME}/apps/stars/bin/sun.x
remoteManager = mpich-intel
```

Monitors

Remote job monitors are defined in the file monitors.dat. Each remote monitor is defined by a stanza indicating where the monitor is located and to be executed. Defined keywords are

- [name] monitor name. Used in sites.dat (siteMonitorDesignator)
- venue hostname upon which to launch monitor daemon. Typically this is a cluster headnode.
- venueMechanism monitoring job launch process. The default is ssh.
- tunnelDesignator name of tunnel defined in tunnels.dat.
- remoteUser login user at remote site.
- remoteMonitorCommand command to launch monitor daemon process.
- state possible values are enabled or disabled. If not explicitly set the default value is enabled.

An example stanza is presented for a remote monitor tool used to report status of PBS jobs.

```
[clusterPBS]
venue = cluster.campus.edu
remoteUser = yourhub
remoteMonitorCommand = ${HOME}/SubmitMonitor/monitorPBS.py
```

Multi-processor managers

Multiprocessor managers are defined in the file managers.dat. Each manager is defined by a stanza indicating the set of commands used to execute a multiprocessor simulation run. Defined keywords are

- [name] manager name. Used in sites.dat and tools.dat.
- computationMode indicate how to use multiple processors for a single job. Recognized values are mpi, parallel, and matlabmpi. Parallel application request multiprocess have there own mechanism for inter process communication. Matlabmpi is used to enable the an Matlab implementation of MPI.
- preManagerCommands comma separated list of commands to be executed before the manager command. Typical use of pre manager commands would be to define the environment to include a particular version of MPI amd/or compiler, or setup MPD.
- managerCommand manager command commonly mpirun. It is possible to include strings that will be sustituted with values defined from the command line.

- postManagerCommands comma separated list of commands to be executed when the manager command completes. A typical use would be to terminate an MPD setup.
- mpiRankVariable define environment variable set by manager command to define process rank. Recognized values are: MPIRUN_RANK, GMPI_ID, RMS_RANK, MXMPI_ID, MSTI_RANK, PMI_RANK, and OMPI_MCA_ns_nds_vpid. If no variable is given an attempt is made to determine process rank from command line arguments.
- environment comma separated list of environment variables in the form e=v.
- moduleInitialize initialize module script for sh
- modulesUnload modules to be unloaded clearing way for replacement modules
- modulesLoad modules to load to define mpi and other libraries
- state possible values are enabled or disabled. If not explicitly set the default value is enabled.

An example stanza is presented for a typical MPI instance. The given command should be

suitable for /bin/sh execution.

```
[mpich-intel]
preManagerCommands = . ${MODULESHOME}/init/sh, module load mpich-
intel/11.1.038
managerCommand = mpirun -machinefile ${PBS_NODEFILE} -np NPROCESSORS
```

The token NPROCESSORS is replaced by an actual value at runtime.

Environment variables

Legal environment variables are listed in the file environmentwhitelist.dat. The objective is to prevent end users from setting security sensitive environment variables while allowing application specific variables to be passed to the remote site. Environment variables required to define multiprocessor execution should also be included. The permissible environment variables should be entered as a simple list - one entry per line. An example file allowing use of a variables used by openmp and mpich is presenter here.

environment variables listed here can be specified from the command line with -e/--env option. Attempts to specify other environment varia bles will be ignored and the values will not be passed to the remote s ite.

OMP_NUM_THREADS MPICH_HOME

Tunnels

In some circumstances access to clusters is restricted such that only a select list of machines is allowed to communicate with the cluster job submission node. The machines that are granted such access are sometimes referred to as gateways. In such circumstances ssh tunneling or port forwarding can be used to submit HUB jobs through the gateway machine. Tunnel definition is specified in the file tunnels.dat. Each tunnel is defined by a stanza indicating gateway host and port information. Defined keywords are

- [name] tunnel name.
- venue tunnel target host.
- venuePort tunnel target port.
- gatewayHost name of the intermediate host.
- gatewayUser login user on gatewayHost.
- localPortOffset local port offset used for forwarding. Actual port is localPortMinimum + localPortOffset

An example stanza is presented for a tunnel between the HUB and a remote venue by way of

```
[cluster]
venue = cluster.campus.edu
venuePort = 22
gatewayHost = gateway.campus.edu
gatewayUser = yourhub
localPortOffset = 1
```

Initialization Scripts and Log Files

The submit server and job monitoring server must be started as daemon processes running on the the submit host. If ssh tunneling is going to be used an addition server must be started as a daemon process. Each daemon process writes to a centralized log file facilitating error recording and debugging.

Initialize daemon scripts

Scripts for starting the server daemons are provided and installed in /etc/init.d. The default settings for when to start and terminate the scripts are adequate.

Log files

Submit processes log information to files located in the /var/log/submit directory tree. The exact location varies depending on the vintage of the installation. Each process has its own log file. The three most important log files are submit-server.log, distributor.log, and monitorJob.log.

submit.log

The submit-server.log file tracks when the submit server is started and stopped. Each connection from the submit client is logged with the command line and client ip address reported. All log entries are timestamped and reported by submit-server process ID (PID) or submit ID (ID:) once one has been assigned. Entries from all jobs are simultaneously reported and intermingled. The submit ID serves as a good search key when tracing problems. Examples of startup, job execution, and termination are given here. The job exit status and time metrics are also recorded in the MyQSL database JobLog table.

==========

=830

```
===========
[Sun Sep 23 12:33:28 2012] (1154) Connection to tcp://:830 from ('192.
168.224.14', 38770)
[Sun Sep 23 12:33:28 2012] 0: Server will time out in 60 seconds.
[Sun Sep 23 12:33:28 2012] 0: Cumulative job load is 0.84. (Max: 510.
00)
[Sun Sep 23 12:33:28 2012] 1670: Args are:['/usr/bin/submit', '--local
', '-p', '@@iv=-3:1.5:3', '/home/hubzero/user/hillclimb/bin/hillclimb1
.py', '--seed', '10', '--initialvalue', '@@iv', '--lowerbound', '-3',
'--upperbound', '3', '--function', 'func2', '--solutionslog', 'solutio
ns.dat', '--bestresultlog', 'best.dat']
[Sun Sep 23 12:33:28 2012] 1670: Server stopping.
[Sun Sep 23 12:33:28 2012] 1670: Server(JobExecuter) exiting(2).
===========
[Sun Sep 23 12:33:38 2012] (1154) Connection to tcp://:830 from ('192.
168.224.14', 38774)
[Sun Sep 23 12:33:38 2012] 0: Server will time out in 60 seconds.
[Sun Sep 23 12:33:38 2012] 1670: Job Status: venue=1:local status=0 cp
u=0.030000 real=0.000000 wait=0.000000
[Sun Sep 23 12:33:38 2012] 1670: Job Status: venue=2:local status=0 cp
u=0.040000 real=0.000000 wait=0.000000
[Sun Sep 23 12:33:38 2012] 1670: Job Status: venue=3:local status=0 cp
u=7.050000 real=7.000000 wait=0.000000
[Sun Sep 23 12:33:38 2012] 1670: Job Status: venue=4:local status=0 cp
u=0.080000 real=0.000000 wait=0.000000
[Sun Sep 23 12:33:38 2012] 1670: Job Status: venue=5:local status=0 cp
u=0.020000 real=1.000000 wait=0.000000
[Sun Sep 23 12:33:38 2012] 1670: Job Status: venue= status=0 cpu=10.42
8651 real=9.561828 wait=0.000000
```

[Sun Aug 26 17:28:24 2012] 0: Listening: protocol='tcp', host='', port

[Sun Aug 26 17:28:17 2012] 0: Server(10836) was terminated by a signal 2.

[Sun Sep 23 12:33:38 2012] 1670: Server(JobExecuter) exiting(0).

[Sun Aug 26 17:28:17 2012] 0: Server(Listener) exiting(130).

distributor.log

The distributor.log file tracks each job as it progresses from start to finish. Details of remote site assignment, queue status, exit status, and command execution are all reported. All entries are timestamped and reported by submit ID. The submit ID serves as the key to join data reported in submit-server.log. An example for submit ID 1659 is listed here. Again the data for all jobs are intermingled.

```
[Sun Sep 23 00:04:21 2012] 0: quotaCommand = quota -w | tail -n 1
[Sun Sep 23 00:04:21 2012] 1659: command = tar vchf 00001659_01_input.
tar --exclude='*.svn*' -C /home/hubzero/user/data/sessions/3984L .__lo
cal_jobid.00001659_01 sayhiinquire.dax
[Sun Sep 23 00:04:21 2012] 1659: remoteCommand pegasus-
plan --dax ./sayhiinquire.dax
[Sun Sep 23 00:04:21 2012] 1659: workingDirectory /home/hubzero/user/d
ata/sessions/3984L
[Sun Sep 23 00:04:21 2012] 1659: command = tar vrhf 00001659_01_input.
tar --exclude='*.svn*' -C /home/hubzero/user/data/sessions/3984L/00001
659/01 00001659_01.sh
[Sun Sep 23 00:04:21 2012] 1659: command = nice -n 19 gzip 00001659_01
_input.tar
[Sun Sep 23 00:04:21 2012] 1659: command = /opt/submit/bin/receiveinpu
t.sh /home/hubzero/user/data/sessions/3984L/00001659/01 /home/hubzero/
user/data/sessions/3984L/00001659/01/.__timestamp_transferred.00001659
_01
[Sun Sep 23 00:04:21 2012] 1659: command = /opt/submit/bin/submitbatch
job.sh /home/hubzero/user/data/sessions/3984L/00001659/01 ./00001659_0
1.pegasus
[Sun Sep 23 00:04:23 2012] 1659: remoteJobId = 2012.09.23 00:04:22.996
        Submitting job(s).
2012.09.23 00:04:23.002 EDT:
                               1 job(s) submitted to cluster 946.
2012.09.23 00:04:23.007 EDT:
2012.09.23 00:04:23.012 EDT:
                               File for submitting this DAG to Condor
2012.09.23 00:04:23.017 EDT:
          : sayhi_inquire-0.dag.condor.sub
                               Log of DAGMan debugging messages
2012.09.23 00:04:23.023 EDT:
          : sayhi_inquire-0.dag.dagman.out
2012.09.23 00:04:23.028 EDT:
                               Log of Condor library output
          : sayhi_inquire-0.dag.lib.out
2012.09.23 00:04:23.033 EDT:
                               Log of Condor library error messages
```

```
: sayhi_inquire-0.dag.lib.err
2012.09.23 00:04:23.038 EDT:
                              Log of the life of condor_dagman itself
          : sayhi_inquire-0.dag.dagman.log
2012.09.23 00:04:23.044 EDT:
2012.09.23 00:04:23.049 EDT:
______
2012.09.23 00:04:23.054 EDT:
2012.09.23 00:04:23.059 EDT:
                              Your Workflow has been started and runs
 in base directory given below
2012.09.23 00:04:23.064 EDT:
2012.09.23 00:04:23.070 EDT:
                              cd /home/hubzero/user/data/sessions/398
4L/00001659/01/work/pegasus
2012.09.23 00:04:23.075 EDT:
2012.09.23 00:04:23.080 EDT:
                               *** To monitor the workflow you can run
2012.09.23 00:04:23.085 EDT:
2012.09.23 00:04:23.090 EDT:
                              pegasus-status -l /home/hubzero/user/da
ta/sessions/3984L/00001659/01/work/pegasus
2012.09.23 00:04:23.096 EDT:
2012.09.23 00:04:23.101 EDT:
                               *** To remove your workflow run ***
2012.09.23 00:04:23.106 EDT:
                              pegasus-remove /home/hubzero/user/data/
sessions/3984L/00001659/01/work/pegasus
2012.09.23 00:04:23.111 EDT:
2012.09.23 00:04:23.117 EDT:
                              Time taken to execute is 0.993 seconds
[Sun Sep 23 00:04:23 2012] 1659: confirmation: S(1):N Job
[Sun Sep 23 00:04:23 2012] 1659: status:Job N WF-DiaGrid
[Sun Sep 23 00:04:38 2012] 1659: status:DAG R WF-DiaGrid
[Sun Sep 23 00:10:42 2012] 0: quotaCommand = quota -w | tail -n 1
[Sun Sep 23 00:10:42 2012] 1660: command = tar vchf 00001660_01_input.
tar --exclude='*.svn*' -C /home/hubzero/clarksm .__local_jobid.0000166
0 01 noerror.sh
[Sun Sep 23 00:10:42 2012] 1660: remoteCommand ./noerror.sh
[Sun Sep 23 00:10:42 2012] 1660: workingDirectory /home/hubzero/clarks
[Sun Sep 23 00:10:42 2012] 1660: command = tar vrhf 00001660_01_input.
tar --exclude='*.svn*' -C /home/hubzero/clarksm/00001660/01 00001660_0
[Sun Sep 23 00:10:42 2012] 1660: command = nice -n 19 gzip 00001660_01
input.tar
[Sun Sep 23 00:10:42 2012] 1660: command = /opt/submit/bin/receiveinpu
t.sh /home/hubzero/clarksm/00001660/01 /home/hubzero/clarksm/00001660/
01/.__timestamp_transferred.00001660_01
[Sun Sep 23 00:10:42 2012] 1660: command = /opt/submit/bin/submitbatch
job.sh /home/hubzero/clarksm/00001660/01 ./00001660_01.condor
[Sun Sep 23 00:10:42 2012] 1660: remoteJobId = Submitting job(s).
1 job(s) submitted to cluster 953.
```

```
[Sun Sep 23 00:10:42 2012] 1660: confirmation: S(1):N Job
[Sun Sep 23 00:10:42 2012] 1660: status:Job N DiaGrid
[Sun Sep 23 00:11:47 2012] 1660: status:Simulation I DiaGrid
[Sun Sep 23 00:12:07 2012] 1660: Received SIGINT!
[Sun Sep 23 00:12:07 2012] 1660: waitForBatchJobs: nCompleteRemoteJobI
ndexes = 0, nIncompleteJobs = 1, abortGlobal = True
[Sun Sep 23 00:12:07 2012] 1660: command = /opt/submit/bin/killbatchjo
b.sh 953.0 CONDOR
[Sun Sep 23 00:12:07 2012] 1660: Job 953.0 marked for removal
[Sun Sep 23 00:12:07 2012] 1660: status:Simulation I DiaGrid
[Sun Sep 23 00:12:52 2012] 1660: status:Simulation D DiaGrid
[Sun Sep 23 00:12:52 2012] 1660: venue=1:localCONDOR:953.0:DiaGrid sta
tus=258 cputime=0.000000 realtime=0.000000 waittime=0.000000 ncpus=1
[Sun Sep 23 00:28:14 2012] 1659: status:DAG D WF-DiaGrid
[Sun Sep 23 00:28:14 2012] 1659: waitForBatchJobs: nCompleteRemoteJobI
ndexes = 1, nIncompleteJobs = 0, abortGlobal = False
[Sun Sep 23 00:28:14 2012] 1659: command = /opt/submit/bin/cleanupjob.
sh /home/hubzero/user/data/sessions/3984L/00001659/01
[Sun Sep 23 00:28:15 2012] 1659:
Job instance statistics
                               : /home/hubzero/user/data/sessions/3
984L/00001659/01/work/pegasus/statistics/jobs.txt
************************
********
[Sun Sep 23 00:28:15 2012] 1659: venue=1:localPEGASUS:946.0:WF-DiaGrid
status=0 cputime=1.430000 realtime=2.000000 waittime=0.000000 ncpus=1
[Sun Sep 23 00:28:15 2012] 1659: venue=2:PEGASUS:952.0:DiaGrid status=
0 cputime=0.003000 realtime=0.000000 waittime=681.000000 ncpus=1 event
=/sayhi_inquire-sayhi-1.0
[Sun Sep 23 00:28:15 2012] 1659: venue=3:PEGASUS:954.0:DiaGrid status=
0 cputime=0.003000 realtime=0.000000 waittime=631.000000 ncpus=1 event
=/sayhi_inquire-inquire-1.0
```

monitorJob.log

The monitorJob.log file tracks the invocation and termination of each remotely executed job monitor. The remote job monitors are started on demand when job are submitted to remote sites. The remote job monitors terminate when all jobs complete at a remote site and no new

activity has been initiated for a specified amount of time - typically thirty minutes. A typical report should look like:

```
[Sun Aug 26 17:29:16 2012] (1485) ***************************
[Sun Aug 26 17:29:16 2012] (1485) * distributor job monitor started *
[Sun Aug 26 17:29:16 2012] (1485) ***************************
[Sun Aug 26 17:29:16 2012] (1485) loading active jobs
[Sun Aug 26 17:29:16 2012] (1485) 15 jobs loaded from DB file
[Sun Aug 26 17:29:16 2012] (1485) 15 jobs loaded from dump file
[Sun Aug 26 17:29:16 2012] (1485) 4 jobs purged
[Sun Aug 26 17:29:16 2012] (1485) 11 monitored jobs
[Sun Aug 26 18:02:04 2012] (24250) Launching wf-diagrid
[Sun Aug 26 18:02:04 2012] (1485) 12 monitored jobs
[Sun Aug 26 18:02:15 2012] (1485) Update message received from wf-
diagrid
[Sun Aug 26 18:03:15 2012] (1485) Update message received from wf-
diagrid
[Sun Aug 26 18:06:43 2012] (1485) 13 monitored jobs
[Thu Sep 17 17:32:51 2011] (21095) Received SIGTERM!
[Thu Sep 17 17:32:51 2011] (21095) Send TERM to child ssh process
[Thu Sep 17 17:32:51 2011] (21095) distributor site monitor stopped
[Thu Sep 17 17:32:51 2011] (17348) Send TERM to child site steele proc
ess
[Thu Sep 17 17:32:51 2011] (17348) **************************
[Thu Sep 17 17:32:51 2011] (17348) * distributor job monitor stopped *
[Thu Sep 17 17:32:51 2011] (17348) **************************
```

It is imperative that the job monitor be running in order for notification of job progress to occur. If users report that their job appears to hang check to make sure the job monitor is running. If necessary take corrective action and restart the daemon.

monitorTunnel.log

The monitorTunnel.log file tracks invocation and termination of each ssh tunnel connection. If users report problems with job submission to sites accessed via an ssh tunnel this log file should be checked for indication of any possible problems.

Remote Domain Configuration

For job submission to remote sites via ssh it is necessary to configure a remote job monitor and a set of scripts to perform file transfer and batch job related functions. A set of scripts can be used for each different batch submission system or in some cases they may be combined with appropriate switching based on command line arguments. A separate job monitor is need for each batch submission system. Communication between the HUB and remote resource via ssh

requires inclusion of a public key in the authorized_keys file.

Job monitor daemon

A remote job monitor runs a daemon process and reports batch job status to a central job monitor located on the HUB. The daemon process is started by the central job monitor on demand. The daemon terminates after a configurable amount of inactivity time. The daemon code needs to be installed in the location declared in the monitors.dat file. The daemon requires some initial configuration to declare where it will store log and history files. The daemon does not require any special privileges any runs as a standard user. Typical configuration for the daemon looks like this:

The directory defined by MONITORLOGLOCATION needs to be created before the daemon is started. Sample daemon scripts used for PBS, LSF, Condor, Load Leveler, and Slurm batch systems are included in directory BatchMonitors.

File transfer and batch job scripts

The simple scripts are used to manage file transfer and batch job launching and termination. The location of the scripts is entered in sites.dat.

Examples scripts suitable for use with PBS, LSF, Condor, Load Leveler, and Slurm are included in directory Scripts. After modifications are made to monitors.dat the central job monitor must be

notified. This can be accomplished by stopping and starting the submon daemon or a HUP signal can be sent to the monitorJob.py process.

File transfer - input files

Receive compressed tar file containing input files required for the job on stdin. The file transferredTimestampFile is used to determine what newly created or modified files should be returned to the HUB.

receiveinput.sh jobWorkingDirectory transferredTimestampFile

Batch job script - submission

Submit batch job using supplied description file. If arguments beyond job working directory and batch description file are supplied an entry is added to the remote site log file. The log file provides a record relating the HUB end user to the remote batch job identifier. The log file should be placed at a location agreed upon by the remote site and HUB.

submitbatchjob.sh jobWorkingDirectory jobDescriptionFile

The jobld is returned on stdout if job submission is successful. For an unsuccessful job submission the returned jobld should be -1.

File transfer - output files

Return compressed tar file containing job output files on stdout.

transmitresults.sh jobWorkingDirectory

File transfer - cleanup

Remove job specific directory and any other dangling files

cleanupjob.sh jobWorkingDirectory

Batch job script - termination

Terminate given remote batch job. Command line arguments specify job identifier and batch system type.

killbatchjob.sh jobId jobClass

Access Control Mechanisms

By default tools and sites are configured so that access is granted to all HUB members. In some cases it is desired to restrict access to either a tool or site to a subset of the HUB membership. The keywords restrictedToUsers and restrictedToGroups provide a mechanism to apply restrictions accordingly. Each keyword should be followed by a list of comma separated values of userids (logins) or groupids (as declared when creating a new HUB group). If user or group restrictions have been declared upon invocation of submit a comparison is made between the restrictions and userid and group memberships. If both user and group restrictions are declared the user restriction will be applied first, followed by the group restriction.

In addition to applying user and group restrictions another mechanism is provided by the boolean keyword arbitraryExecutableAllowed in the sites configuration file. In cases where the executable program is not pre-staged at the remote sites the executable needs to be transferred along with the user supplied inputs to the remote site. Published tools will have their executable program located in the /apps/tools/revision/bin directory. For this reason submitted programs that reside in /apps are assumed to be validated and approved for execution. The same cannot be said for programs in other directories. The common case where such a situation arises is when a tool developer is building and testing within the HUB workspace environment. To grant a tool developer the permission to submit such arbitrary applications the site configuration must allow arbitrary executables and the tool developer must belong the system group submit.