ECCE Installation and Administration

Overview

ECCE can be installed and run on most Linux 32- and 64-bit operating systems such as Red Hat Enterprise Linux, Debian, Ubuntu, OpenSUSE, and Mint. This includes both native and virtual machine Linux installs using VirtualBox (http://www.virtualbox.org) or VMware (http://www.vmware.com). Installing Linux as virtual machine allows sites with only Windows or Macintosh OS X workstations to run ECCE. A minimum of 2 GB of memory is needed to run both your Linux operating system and ECCE although 4 GB or more is recommended. The minimum free disk space needed to install both the ECCE application and server software is 500 MB. However, the ECCE server maintains job input and output files for all calculations setup and run using ECCE. Therefore additional free disk space is recommended from several gigabytes on up the terabyte range depending upon the size of calculations run and the number of users sharing the ECCE server.

When running ECCE three distinct types of hosts are used:

- Desktop workstations running ECCE client graphical user interface applications
- Data and messaging servers
- Compute resources running chemistry codes

ECCE client application software such as the Builder, Organizer, Electronic Structure Editor, and Viewer run on Linux workstations using the wxWidgets GUI toolkit, which is built on the Gtk toolkit with the base X Window System. These workstations must run either 32-bit i686 processors or 64-bit x86_64 processors, constrained by the minimum platform requirements mentioned above. The application software can be installed on each individual workstation running ECCE, or preferably for a multi-user install, on a shared file system such as NFS or AFS that each workstation accesses.

The ECCE data and messaging server are packaged together to run on the same host. The data server is an open source Apache2 web server (http://httpd.apache.org) compiled with the optional mod_dav module to support distributed collaborative data management. The mod_dav module implements the Distributed Authoring and Versioning (DAV) protocol (http://www.webdav.org/) for maintaining files with associated metadata on a web server. The messaging server relies on an open source client/server implementation of the Java standard for inter-process communication (Java Messaging Service), named ActiveMQ (http://activemq.apache.org), to manage communications between the separate applications running in an ECCE session. ECCE has applied this technology to C++ applications by embedding a Java virtual machine inside the main Gateway toolbar application. In addition to the data and messaging server software, ECCE reference data libraries (basis set and structure libraries) and a small number of ECCE server administration scripts are provided. Typically a single data and messaging server (referred to collectively as an ECCE server) can be installed at a site serving all workstations running the ECCE application software, although multiple ECCE servers can be installed with user access to each being configured by the ECCE site administrator.

The compute resources where chemistry codes run range from single processor desktop workstations to massively parallel supercomputers and clusters running a variety of batch queue scheduling systems. They are not as tightly constrained as the Linux platforms on which the ECCE application and server software must be run, although they must run UNIX, Linux, or Macintosh OS X with C shell (csh) and the Perl scripting language available. The NWChem code is bundled with the ECCE binary distribution and may be used to run chemistry jobs on the same host as ECCE client applications. However, for shared file system installations of ECCE client application software, NWChem performance is severely degraded and may prove impractical. More than likely you will want to run NWChem and other chemistry codes on higher performance dedicated compute resources rather than where ECCE client applications are installed. This will require separate installation of the chemistry code from ECCE as well as registration of the compute resource in ECCE as described later in this document.

It is important to understand that each of these three host types is distinct within ECCE. It is possible for a single desktop workstation to function as all three of these for an ECCE installation and represent the extent of the ECCE configuration at a site. Conversely, there may be dozens of workstations running the application software, accessing several ECCE servers, and farming out chemistry jobs to compute resources both at the site and around the world.

Download ECCE Binary Distribution or Build ECCE Source Distribution

Instructions for obtaining ECCE can be found on the ECCE website at http://ecce.pnl.gov. The download website has both 32- and 64-bit binary distributions and a source code distribution. Binary distributions are provided for both the full ECCE software suite and the standalone ECCE Builder application. Although these binary distributions are built on Red Hat Enterprise Linux (the operating system supported for the EMSL where ECCE is developed), this distribution should run on a variety of Linux operating systems. This is possible by bundling all the shared libraries required for the different ECCE applications including system libraries that are normally present on most Linux systems, but may not be fully compatible with what was used to create the ECCE binary distributions on Red Hat. These binary distributions have been tested with operating systems including Debian, Ubuntu, OpenSUSE, and Mint in addition to Red Hat.

Sites having difficulty using the ECCE binary distributions, those considering modifying or adding to ECCE code, or those just wanting a better understanding of the ECCE software can download and build ECCE from the source code distribution. The results from completing an ECCE source code build as documented in the build/README file in that distribution (the build directory is not included with ECCE binary distributions) will be an ECCE binary distribution specific to the Linux operating system and hard platform on which it was built. This new ECCE binary distribution is identical in structure to those downloadable from the ECCE website and thus the install documentation herein should be followed to complete the installation.

Using a web browser, download the desired ECCE distribution for your platform to a local disk directory. File size for downloading is displayed on the web page although having sufficient additional free disk space during installation is critical since ECCE distributions are compressed and extraction will multiply

the size requirements. This document assumes that either a full ECCE binary distribution is downloaded or that a source code distribution has been downloaded, built, and a new ECCE binary distribution has been generated from that build as the starting point for the installation procedures given below. ECCE Builder binary distribution installations are documented separately. Full ECCE binary distributions include both the ECCE application software and server, although installation options allow you to selectively install only applications or the server, as well as both. This gives flexibility that allows, for example, sharing one ECCE server for separate 32-bit and 64-bit application software installations. As a benefit of the web server technology underlying ECCE data management, the ECCE server can be installed on a machine of your choosing provided it is accessible via http from the machines where ECCE application software is run (shared file systems aren't needed between server and application machines).

Install ECCE

The installation procedures assume a basic familiarity with UNIX/Linux system administration. Commands given are for sh and also apply to bash; if you are using another shell such as csh or tcsh, you may need to adjust the syntax.

In order to maintain the integrity of the installation, we recommend creating an account named ecceadm, for "ECCE Administrator", or something similar and installing as that user. There are many configuration files, along with executables and libraries distributed with ECCE that if removed or improperly modified will corrupt the installation.

The ECCE binary distribution itself is a self-extracting C shell installation script along with the application software and server bzip2 format compressed tar files. The installation script has a main menu allowing you to select the type of install to be performed. Normally a "full" installation of both the application and server software is done. This option is appropriate for either standalone or networked hosts. Further options allow the application software and server to be installed independently. These options accommodate application software being installed on all desired platforms (by downloading and running the binary distribution script on each platform), with the server installed on just a single platform, among other scenarios. The main menu allows both new installations and upgrades of older releases of ECCE to the newest version.

Depending upon the policies at your site, you may need to do the server side of the installation as another user rather than ecceadm. If you install as root the Apache httpd daemon will automatically run as the unprivileged "nobody" user, an additional security benefit when your network, firewall, and web server configuration allows external access. If you wish to do a server install as root, you may either install all of ECCE as root ("full install"), or you can install the application software first as ecceadm (or another user) selecting "Application software only" from the main menu, and then doing a second install as root selecting "Server install" from the main menu.

The following steps document sample installations of ECCE on a Linux host for two common scenarios--a full install and a full upgrade. If you are doing other than a full ECCE install or upgrade, then the prompts below will vary somewhat.

- **Full ECCE Install**

  Run the install_ecce.*.csh script in the directory where it was downloaded. You may need to add execute permission to the file first. Note that values in square brackets are defaults and you may simply hit return to use a default. For clarity, values are always explicitly entered for the prompts in these sample installs even when the default value is used. Here is the first sample invocation of install_ecce.*.csh, a full install, run as ecceadm with links to notes describing how to determine appropriate values for each of the configuration settings:

  prompt$ **cd /myfiles**
  prompt$ **chmod +x ./install_ecce.v6.4.rhel5-gcc4.1.2-m64.csh**
  prompt$ **./install_ecce.v6.4.rhel5-gcc4.1.2-m64.csh**

  Extracting ECCE distribution from ./install_ecce.v6.4.rhel5-gcc4.1.2-m64.csh...

  Main ECCE installation menu
  ==========
  1) Help on main menu options
  2) Prerequisite software check
  3) Full install
  4) Full upgrade
  5) Application software install
  6) Application software upgrade
  7) Server install
  8) Server upgrade

  IMPORTANT: If you are uncertain about any aspect of installing
  or running ECCE at your site, please refer to the detailed
  ECCE Installation and Administration Guide at
  http://ecce.emsl.pnl.gov/docs/installation/2864B-Installation.pdf

  Hit <return> at prompts to accept the default value in brackets.

  Selection: [1] **2**

  Checking prerequisites for running ECCE…

  If any of the following packages aren't found or aren't the right
  version, hit <ctrl>-c at the prompt and either find or install
  the package before installing ECCE. The whereis command is
  useful for finding commands and libraries not in your path.

  Found java in: /usr/bin/java
  ECCE requires java 1.5.x or 1.6.x

This version: java version “1.6.0_18”
Hit return if this java is OK…

Found python in: /usr/bin/python
ECCE requires python 2.4.x or newer
This version: Python 2.6.6
Hit return if this python is OK…

Found perl in: /usr/bin/perl
ECCE requires perl 5.x.x
This is perl, v5.10.1 (*) built for x86_64-linux-gnu-thread-multi
Hit return if this perl is OK…

Pkg-config check for gtk+-2.0: Found
ECCE requires gtk+-2.0 2.x.x
This version: 2.20.1
Hit retrn if this gtk+-2.0 is OK…

Found ImageMagick mogrify in: /usr/bin/mogrify
ECCE requires mogrify 6.x.x or newer
Version: ImageMagick 6.6.0-4 2012-03-05 Q16 http://www.imagemagick.org
Hit return if this mogrify is OK…

Found xterm in: /usr/bin/xterm
Hit return if xterm was found…

Found OpenGL libGL in: libGL.so.1 (libc, x86-64, OS ABI: Linux 2.4.20) => /usr/lib/libGL.so.1
Found OpenGL libGLU in: libGLU.so.1 (libc, x86-64) => /usr/lib/libGLU.so.1
Hit return if these OpenGL libraries are OK…

Main ECCE installation menu
==========
1) Help on main menu options
2) Prerequisite software check
3) Full install
4) Full upgrade
5) Application software install
6) Application software upgrade
7) Server install
8) Server upgrade

IMPORTANT: If you are uncertain about any aspect of installing
or running ECCE at your site, please refer to the detailed
ECCE Installation and Administration Guide at

http://ecce.emsl.pnl.gov/docs/installation/2864B-Installation.pdf

Hit <return> at prompts to accept the default value in brackets.

Selection: [1] **3**

Host name: [mymachine.mysite.mydomain] **mymachine.mysite.mydomain**
Application installation directory: [/myfiles/ecce-v6.4/apps] **/sharednfs/ecce-v6.4/apps**
Server installation directory: [/myfiles/ecce-v6.4/server] **/myfiles/ecce-v6.4/server**

ECCE v6.4 will be installed using the settings:

Installation type: [full install]
Host name: [mymachine.mysite.mydomain]
Application installation directory: [/sharednfs/ecce-v6.4/apps]
Server installation directory: [/myfiles/ecce-v6.4/server]

Are these choices correct (yes/no/quit)? [yes] **yes**

Installing ECCE application software in /sharednfs/ecce-v6.4/apps...
Extracting application distribution...
Extracting NWChem distribution…
Extracting client WebHelp distribution...
Configuring application software…
Configuring NWChem…

Installing ECCE server in /myfiles/ecce-v6.4/server...
Extracting data server in /myfiles/ecce-v6.4/server/httpd...
Extracting data libraries in /myfiles/ecce-v6.4/server/data...
Extracting messaging server in /myfiles/ecce-v6.4/server/activemq...
Configuring ECCE server...

ECCE installation succeeded.

****
!! You MUST perform the following steps in order to use ECCE !!
-- Unless only the user ‘ecceadm’ will be running ECCE,
start the ECCE server as ‘ecceadm’ with:
/myfiles/ecce-v6.4/server/ecce-admin/start_ecce_server

-- To register machines to run computational codes, please see
the installation and compute resource registration manuals
at http://ecce.pnl.gov/using/installguide.shtml

-- Before running ECCE each user must source an environment
setup script. For csh/tcsh users add this to ~/.cshrc:
if (-e /sharednfs/ecce-v6.4/apps/scripts/runtime_setup) then
source /sharednfs/ecce-v6.4/apps/scripts/runtime_setup
endif
For sh/bash users, add this to ~/.profile or ~/.bashrc:
if [-e /sharednfs/ecce-v6.4/apps/scripts/runtime_setup.sh]; then
. /sharednfs/ecce-v6.4/apps/scripts/runtime_setup.sh
fi
****
prompt$

- **Full ECCE Upgrade**

Here is the second sample invocation of install_ecce.v6.4.*.csh, a full upgrade from a release of ECCE v6.0, run as ecceadm with links to notes describing how to determine appropriate values for each of the configuration settings:

prompt$ **cd /myfiles**
prompt$ **chmod +x ./install_ecce.v6.4.rhel5-gcc4.1.2-m64.csh**
prompt$ **./install_ecce.v6.4.rhel5-gcc4.1.2-m64.csh**

Extracting ECCE distribution from ./install_ecce.v6.4.rhel5-gcc4.1.2-m64.csh...

Main ECCE installation menu
==========
1) Help on main menu options
2) Prerequisite software check
3) Full install
4) Full upgrade
5) Application software install
6) Application software upgrade
7) Server install
8) Server upgrade

IMPORTANT: If you are uncertain about any aspect of installing
or running ECCE at your site, please refer to the detailed
ECCE Installation and Administration Guide at
http://ecce.emsl.pnl.gov/docs/installation/2864B-Installation.pdf

Hit <return> at prompts to accept the default value in brackets.

Selection: [0] **4**

Host name: [mymachine.mysite.mydomain] **mymachine.mysite.mydomain**
New application installation directory: [/myfiles/ecce-v6.4/apps] **/sharednfs/ecce-v6.4/apps**
Existing application directory to upgrade: **/sharednfs/ecce-v6.0/apps**
New server installation directory: [/myfiles/ecce-v6.4/server] **/myfiles/ecce-v6.4/server**
Existing server directory to upgrade: **/myfiles/ecce-v6.0/server**
Backup existing server user data (yes/no)? [yes] **yes**

ECCE v6.4 will be installed using the settings:

Installation type: [full upgrade]
Host name: [mymachine.mysite.mydomain]
Application installation directory: [/sharednfs/ecce-v6.4/apps]
Application directory to upgrade: [/sharednfs/ecce-v6.0/apps]
Server installation directory: [/myfiles/ecce-v6.4/server]
Server directory to upgrade: [/myfiles/ecce-v6.0/server]
Backup existing server user data: [yes]

Are these choices correct (yes/no/quit)? [yes] **yes**

Installing ECCE application software in /sharednfs/ecce-v6.4/apps...
Extracting application distribution...
Extracting NWChem distribution…
Extracting client WebHelp distribution...
Configuring application software...
Configuring NWChem…

Installing ECCE server in /myfiles/ecce-v6.4/server...
Extracting data server in /myfiles/ecce-v6.4/server/httpd...
Extracting data libraries in /myfiles/ecce-v6.4/server/data...
Extracting messaging server in /myfiles/ecce-v6.4/server/activemq...
Configuring ECCE server...
Copying user data from server to be upgraded...
Copying share data from server to be upgraded...

ECCE installation succeeded.

****
!! You MUST complete the following steps in order to use ECCE !!
-- Unless only the user ‘ecceadm’ will be running ECCE,
start the ECCE server as ‘ecceadm’ with:
/myfiles/ecce-v6.4/server/ecce-admin/start_ecce_server

-- To register machines to run computational codes, please see

```
  the installation and compute resource registration manuals
  at http://ecce.emsl.pnl.gov/using/installguide.shtml

-- Before running ECCE each user must source an environment
  setup script.  For csh/tcsh users add this to ~/.cshrc:
    if (-e /sharednfs/ecce-v6.4/apps/scripts/runtime_setup) then
      source /sharednfs/ecce-v6.4/apps/scripts/runtime_setup
    endif
  For sh/bash users, add this to ~/.profile or ~/.bashrc:
    if [ -e /sharednfs/ecce-v6.4/apps/scripts/runtime_setup.sh ]; then
      . /sharednfs/ecce-v6.4/apps/scripts/runtime_setup.sh
    fi
*****************************************************
prompt$
```

After the install_ecce.*.csh script has completed with both the application software and server being installed as desired, you may delete the distribution script although we recommend waiting until ECCE is completely tested at your site.

The next several paragraphs describe how to choose appropriate values for the ECCE installation prompts as shown above. If you have successfully run the installation script and understand the prompts, you may skip to Post-Install Configuration to continue with the installation.

Main menu selection: There are three basic types of ECCE installations: full, application, and server. Each type can either be a from-scratch install or an upgrade of an existing installation. An upgrade is done rather than a from-scratch install, referred to as simply an "install", when you have an existing version of ECCE where you wish to incorporate the machine registrations and/or calculation data for that version into the new version. An install is done rather than an upgrade when you have either not previously installed ECCE or do not wish to incorporate data from an existing version. The following describes each of the eight main menu options:

1. Help on main menu options: Abridged version of what you are reading now.

2. Prerequisite software check: Checks for packages and libraries needed to run ECCE including whether the versions found are compatible with what ECCE needs. Unless you have either previously installed ECCE on the target machine or have built it from an ECCE source code distribution this step is highly recommended to circumvent problems.

3. Full install: Install both the ECCE application software and server without incorporating data created from a previous ECCE install, if any. This is the recommended option when special needs, as described below, do not dictate separate application and server software installations. A full install can be done either for use from a single machine on or off the network, or for use from multiple machines. For use from a single machine the host name is often entered as "localhost" if defined properly in the /etc/hosts file, to allow taking machines such as laptops on

and off networks with ECCE working in both configurations. Application software is installed to local disk for use from a single machine or to a shared file system, such as NFS or AFS, for use from multiple machines. The ECCE server is always installed to local disk, but the server will be accessible externally to the extent allowed by the network and firewall configuration of the server host. Security and performance of the ECCE server would both be compromised if it was installed to a shared file system and there are no advantages in doing so. Even when installed for use from a single machine, computational jobs may still be run to other machines with a full install, assuming a network connection exists of course.

4. Full upgrade: Install a new version of the ECCE application software and server on a machine incorporating the machine registrations and calculation data from a previous install. The large number of changes between each successive version of ECCE limits how old the version to upgrade can be, but it should always work for the same major version and usually going back to the previous major version.

5. Application software install: Install only the application software and not the server. Used when ECCE will be run from multiple platforms, but the server has been already been installed on a different platform with a full install, or will be installed with a server only install.

6. Application software upgrade: Install a new version of the application software incorporating machine registrations and other application software configuration data from a previous installation. Used for installing patches to application software when there are no server enhancements, or upgrading multiple platforms for running applications. Also can be used to only incorporate machine registrations from a previous version of ECCE without incorporating user calculation data from the previous version.

7. Server install: Install only the server and not the application software. Used when the server needs to run on a different machine or platform than where the application software is installed.

8. Server upgrade: Install a new version of the server incorporating user calculation data from a previous installation. Used for installing server-side only patches or when user calculation data from a previous version needs to be upgraded without application software being upgraded.

Host name: This is the full domain name of the machine where you are currently running the install_ecce.*.csh script. You cannot install the ECCE server on a different machine than the one you run the script on. If you do not wish to install the server on the machine you are currently on, you must copy the install_ecce.*.csh script to the desired machine and run there. The host name prompt confirms the name detected by the installation script is correct. In the majority of cases you will simply accept the default server name as shown in the square brackets, provided it is the correct full domain name. In the instance you wish to refer to the server name by an alias, use the IP address rather than the name, or use “localhost” as the name for a machine that is taken off the network, you may enter the desired name at this prompt. Note, of course, that if you set the name as “localhost”, you will only be able to run ECCE with this server from the local machine regardless of whether it is currently on or off the network.

Application installation directory: ECCE applications are designed for installation under a single shared directory at a site, with all hosts accessing the common application installation. A local file system disk is selected for the application installation directory when ECCE will only be run from a single machine. If you wish to have multiple machines running ECCE, we strongly recommend installing the application software in a shared file system if feasible as it substantially reduces parallel administration. The directory where ECCE applications are installed is independent of the directory where the distribution script is run, although the default will be a subdirectory of the run directory. For access from multiple machines the distribution is typically downloaded to local disk to speed file transfer, and then installed to a shared file system. This file system for the application installation directory should have at least 300 megabytes free for each platform that will be installed. To install multiple platforms to a shared file system, specify the same application installation directory for each platform (requires downloading and running the installation script distribution for each platform). The ECCE installation script automatically extracts platform-dependent libraries and executables into separate subdirectories. The absolute path to the directory where ECCE applications are installed is stored in the ECCE runtime_setup and runtime_setup.sh scripts as the environment variable $ECCE_HOME. The rest of this document uses the term "ECCE application installation directory" and slight variations interchangeably with the variable $ECCE_HOME, especially when referring to file paths.

You are not allowed to overwrite an existing ECCE application installation except in the case where you are installing different platforms under the same top-level application installation directory. The installation script will verify that the directory specified is not a previous installation for the same platform and prompt for a new directory if it is. This restriction prevents the inadvertent loss of a working installation should the new one have some kind of problem. If you do wish to install a new version of the ECCE applications to the same top level directory as an existing installation for the same platform, you must move the old installation to another directory prior to running the install_ecce.*.csh script. We recommend that you only remove an existing installation after you have verified the operation of the new installation.

Server installation directory: The Apache HTTP server binaries, HTTP server data directory, Apache ActiveMQ JMS server, and a directory named ecce-admin containing some scripts to facilitate ECCE server administration, will all be placed under this directory. This directory should always be on local disk. All data created within ECCE will reside under the "data" subdirectory of the server installation directory including both the original and ECCE-formatted input and output data from all jobs run with ECCE. For this reason, we highly recommend that you dedicate a large partition or an entire disk (hundreds of gigabytes if not more) for the ECCE server, depending upon anticipated usage. If you are short on disk space, it is possible to configure multiple ECCE servers and divide users between the servers, but planning ahead will make administration easier.

Are these choices correct: Pressing return or entering "yes" results in the ECCE installation completing based on the summary of settings given before this prompt. Entering "no" results in all items being prompted for again including the main menu selection.

A list of steps of additional steps is printed at the end of the installation process. If you are installing an ECCE server, the installation script will attempt to update the ECCE application software files in the $ECCE_HOME/siteconfig directory that configure access to the new ECCE server. If this fails for some reason, such as the application software not being accessible from the machine where the ECCE server is currently being installed, the instructions will be given for manually completing this step. In the event you have multiple installations of the application software at your site (not recommended due to additional burden of maintaining installations in parallel) and you wish to share the same ECCE server, the ECCE installation script will only be able to update the application software $ECCE_HOME/siteconfig files for one of these installations. In this case, you will need to copy the add_ecce_server script from the ecce-admin directory under the server installation directory to the other hosts where the application software is installed and run it manually on each host.

Existing application directory to upgrade: Each site must customize their ECCE application installation in order to recognize the compute resources and ECCE servers available to the users at the site. This information is stored in the $ECCE_HOME/siteconfig directory. Performing an upgrade allows you to automatically copy the site-specific compute resource registrations and customizations for an existing installation into the new one. Enter the application installation $ECCE_HOME directory of the existing (old) installation at this prompt. If you specify an invalid directory for the existing installation for the given platform, a warning will be issued and you will be prompted again. As well as copying the contents of an existing siteconfig directory, this upgrade feature is also used to update files that have changed format in the new version of ECCE. Therefore, it is recommended that this feature be used instead of manually upgrading an existing installation.

Existing server directory to upgrade: Enter the path for the existing ECCE server installation at this prompt. User accounts and all data created under a previous server installation will be incorporated into the new server.

Backup existing server user data: We HIGHLY recommend making a backup copy of all user data stored under the server data directory before an upgrade between server versions is done. Hitting return or entering “yes” at this prompt will copy all data stored in the “users” and “share” subdirectories of the ECCE server data directory from the existing server installation into the new server installation. This can require considerable disk space and time, which is the reason this step is optional. If you do not make the backup copy, by entering “no” at this prompt, then the “users” and “share” data directories will simply be moved from the old to the new server installation with no possibility of continuing to use the existing server. If there is not enough disk space to make the backup, or for some other reason, you do not wish the ECCE installation script to automatically make the backup, you should make a backup manually (such as a tar.bz2 file) to disk or another storage device prior to doing the upgrade.

Post-install Configuration

- **Change the Default Web Browser**

ECCE uses a web browser for online help and the user support request web page. At this time, Firefox and Mozilla are compatible with how ECCE controls the display of web pages externally (KDE Konqueror, for instance, does not allow the control needed by ECCE). By default Firefox is configured as the web browser within ECCE. This can be changed by editing the application software $ECCE_HOME/siteconfig/site_runtime file and scrolling down to the entries for web browsers. The only valid values for the browsers are "firefox" and "mozilla".

- **Change the Apache HTTP Data or ActiveMQ Messaging Server Ports**

ECCE uses a default port number of 8096 for the Apache HTTP data server. This is a "high port" and is usually a safe value that closes off the web server from outside a firewall. However, if this value is inappropriate for your site based on firewall configuration or external access to ECCE you wish to allow or deny, it can be changed manually. First, change directory to httpd/conf under the server installation directory. Next, edit httpd.conf, search for "ECCE PORT", and follow the instructions provided there to change the default. Next, update all application software installations using this server by editing the $ECCE_HOME/siteconfig/DataServers file URL for the server.

The Apache ActiveMQ messaging server uses a default port number of 8095 as configured in ECCE. To change this value, change directory to activemq/conf under the server installation directory. Edit the file activemq.xml and search for "openwire". Change the port number at the end of the value given for the "uri" keyword in the same line. Finally, update all application software installations using this server with the new ActiveMQ port in the $ECCE_HOME/siteconfig/jndi.properties file for each installation. Near the top of this file you will see the "java.naming.provider.url" keyword that needs to be updated with the new port value.

- **Access Multiple ECCE Servers**

To configure access to more than a single ECCE server for an application software installation, you must edit the DataServers file in the application software $ECCE_HOME/siteconfig directory. Follow the documentation in this file for configuring access to multiple servers.

- **Add ECCE Server Users**

The default configuration of ECCE will automatically create an ECCE server account for each user the first time they run the ECCE application software, eliminating this extra chore of creating these accounts from the ECCE administrator. The ECCE administrator can disable this feature if there are concerns about allowing any user with access to the application software to create their own area with write permission on the server. Note that users do not automatically get read or write access to other users' data. The environment variable $ECCE_AUTO_ACCOUNTS defined in the $ECCE_HOME/siteconfig/site_runtime file (which should be editable only by the ECCE administrator like all other files under $ECCE_HOME) controls whether this feature is enabled. The automatic account creation feature is implemented with an Apache HTTP cgi-bin script with no critical data being passed unencrypted over the Internet. For security reasons, server passwords will need to be manually reset by the ECCE administrator using the ecce_htpasswd script, described below, for those users who forget their

their password. If you plan to use the automatic server account creation feature, you may skip to the next section describing the ecce_htpasswd script. Goto next section

If the automatic server account creation feature is disabled accounts must be created by the ECCE administrator. The ECCE server includes a script named add_ecce_user for this purpose. This script is located in the ecce-admin directory, under the server installation directory and must be run as the same user the installation was done as (ecceadm, if you are following the recommended install procedure). It performs the steps necessary to add a single new user account to the ECCE server per invocation. The add_ecce_user script will prompt for all input needed to make a user account and home directory. An example run, done as the ecceadm user (i.e., the ECCE server owner), is shown below. The prompt for "User name" is the machine login name corresponding to the $USER environment variable for the user on the host(s) where they are running ECCE application software. Here is the add_ecce_user run:

prompt$ /myfiles/ecce-v6.4/server/ecce-admin/add_ecce_user

First name? **Joe**
Last name? **Smith**
User name? **jsmith**

Entry confirmation:

First name: Joe
Last name: Smith
User name: jsmith

Is this information correct? [yes/no] **yes**

New password: **(text not echoed)**
Re-type new password: **(text not echoed)**
Adding password for user jsmith

ECCE uses basic web server authentication, built on standard UNIX crypt functionality. ECCE server passwords entered through add_ecce_user or as described below are independent of machine login passwords for users. We recommend passwords be chosen by some random means or using public domain tools for generating "nonsensical" words for such purposes.

It is also possible to setup users completely manually, bypassing the add_ecce_user script. The script merely simplifies the most common administrative duty of adding a new user by performing a number of small steps on your behalf. If you decide to setup access differently than is supported by the script or want to understand the process behind it, the following instructions lead you through manual user account creation. If you wish to use add_ecce_user without knowing the details you may skip to the next section describing the ecce_htpasswd script, which must be used to change passwords because the add_ecce_user script only supports adding new users. Goto next section

- **Add ECCE Server Users Manually**

The recommended configuration of ECCE for access control to data stored on the web server is to create a user name and password entry in the Apache HTTP server "users" file for each user. A default "home" directory should also be created (owned by the server data directory owner--either the ECCE server owner or "nobody" if root owns the ECCE server) under the ECCE/users directory of the data directory under the server installation. The home directory is named the same as the user name and contains an .htaccess file. This file directs the web server to require the user to authenticate with their user name and password to view and create data under their home directory.

To add a user named Joe Smith with a login name of jsmith first create a directory named jsmith in the ECCE/users directory under the server data directory. Within that directory create an .htaccess file with the following five lines:

AuthName "ECCE-Joe.Smith"
<Limit OPTIONS HEAD GET PUT DELETE PROPFIND PROPPATCH MKCOL COPY MOVE LOCK UNLOCK POST>
Allow from all
require user jsmith ecceadm
</Limit>

It is possible to be much more sophisticated with access control than is shown with this .htaccess file. You are referred to the numerous reference sources for Apache HTTP server administration to configure more complex access control. Besides creating a home directory and .htaccess file for each new user, a user name and password must be defined, as described next.

- **Run ecce_htpasswd**

The ecce_htpasswd script included in the server ecce-admin directory is used to add user name and password pairs to the server, or change the password for an existing user. This script is a simple wrapper for the standard Apache HTTP htpasswd program that sets up the proper $LD_LIBRARY_PATH and passes the correct argument for the user password file. An example invocation of ecce_htpasswd for adding the user jsmith, again run as ecceadm, follows:

prompt$ **/myfiles/ecce-v6.4/server/ecce-admin/ecce_htpasswd jsmith**
New password: **(text not echoed)**
Re-type new password: **(text not echoed)**
Adding password for user jsmith

Changing a password for an existing user is done in the same way by passing the user name on the command line. Prompts and output from ecce_htpasswd are also similar in this case. The most common way to use ecce_htpasswd is with the user name as the only command line argument. However, other arguments supported by the standard htpasswd program can also be used with ecce_htpasswd. To see the full usage of the htpasswd program via ecce_htpasswd, type "ecce_htpasswd" with no arguments in the

ecce-admin directory. Note that the "passwordfile" argument is passed by ecce_htpasswd even though the usage description (which is for the standard htpasswd script) shows it. You may also run htpasswd directly if you set the $LD_LIBRARY_PATH to include the apache/lib directory under the server installation directory. ECCE is not compatible with MD5 or SHA password encryption when automatic account creation or password synchronization is used ($ECCE_AUTO_ACCOUNTS set to something besides "false"). Finally, it is not necessary to restart the web server to recognize changes when running add_ecce_user, ecce_htpasswd, htpasswd, or manually editing .htaccess files.

- **Remove ECCE Server Users**

Due to the risk of accidentally losing valuable data, removing users from the ECCE server is done manually. Simply edit and delete the appropriate line from the Apache server "users" file (located in the "apache" directory under the server installation directory) and then remove their home directory (located in the data/ECCE/users directory under the server installation directory). Backing up this home directory before deletion is recommended if there is any chance this data will be needed in the future. As well as ECCE-specific files, all input and output log files from jobs run under ECCE are stored with user calculations, so they may later be used outside ECCE.

- **Start the ECCE Server**

At this point you should be able to start the Apache HTTP data and ActiveMQ messaging servers that make up the ECCE server. If only a single user will be running the ECCE application software, that being the same user who performed the ECCE installation and thus owns the files, there is normally no need to explicitly start the server as described below. The other requirement for automatic server startup besides being a single user installation owned by that user is for the top-level "apps" and "server" directories to be under the same parent directory, as is the default for "full install" and "full upgrade" type installations. In this case the "ecce" script used to start the application software will also start the server if it is not already running. Note that when exiting ECCE under this scenario (as with starting the server explicitly) the server will remain running as it is needed to monitor any running jobs even when ECCE user interface applications are not running. Thus, if there is a need, the server must be stopped manually as described below. Normally though the ECCE server can be left running indefinitely and imposes very little computational demand on the host machine.

For those installations where it is necessary to start the server explicitly (muti-user or when the server is not installed in a parallel directory to the application software), this operation should be done as the ECCE server installation owner (ecceadm if you are following the recommended install procedure) in order for the httpd web server daemon to have write access to files under the server data directory. Commands to start and stop the server are located in the ecce-admin directory under the ECCE server installation directory:

To start the server:

prompt$ **/myfiles/ecce-v6.4/server/ecce-admin/start_ecce_server**

After starting the server, you may verify that the Apache httpd daemon and child httpd processes are running, as well as the ActiveMQ server:

prompt$ **ls /myfiles/ecce-v6.4/server/apache/logs/httpd.pid**
prompt$ **ps -ef | grep "java" | grep "Dorg.apache"**

To stop the server:

prompt$ **/myfiles/ecce-v6.4/server/ecce-admin/stop_ecce_server**

You may wish to have the ECCE server automatically started during the machine boot sequence, assuming your installation doesn't fall under the single-user, owned-by-user variety where the server is started automatically. Contact your system administrator to configure boot sequence startup.

Register Compute Resources to Run Codes

The ECCE administrator must register each queued machine that serves as an ECCE compute resource where NWChem, GAMESS-UK, Gaussian 03, Gaussian 98, and Amica jobs will be run. Non-queued shared access machines are also typically registered by the ECCE administrator. Users may register their own personal workstations provided they don't use a queue management system. Also, compute resources shared by small groups that don't use queue managers can be registered by each user desiring access as an alternative to making them globally visible within ECCE user interfaces as is the case when the ECCE administrator performs the registration. Compute resource registration is done with a graphical interface application provided in the ECCE distribution. To use this application, you must first set up your environment to run as an ECCE user. For sh/bash users, this is done by changing either ~/.profile or ~/.bashrc for the ecceadm account (or whatever account owns the ECCE installation) as described in Setup Users' Environment and sourcing the modified file. For csh/tcsh users the ~/.cshrc file should be modified and sourced. You will also need to give yourself an ECCE server user account as described above. For security reasons, there is no automatic server account creation for ecceadm. You will need to run the add_ecce_user script to create an account if you are running as ecceadm. Finally, enter the following command to start the machine registration graphical interface:

prompt$ **ecce -admin**

Write permissions for the ECCE application software installation is required to save the compute resource registration information. We do not recommend setting global write permissions on the "siteconfig" directory where the registration information is stored, as improper changes can effectively disable ECCE for all users at the site.

Use the "Help" button to get information on using the interface, what all the input fields mean, and how to manually customize some queue management options that are not yet supported via the interface. Machines within EMSL accessible externally by EMSL collaborators are initially registered in the siteconfig directory as part of the ECCE distribution. There are examples for registering machines for each queue management system that ECCE currently supports in the CONFIG-Examples subdirectory of

siteconfig. The configuration and site usage policies of most queued machines are too complex for them to be completely registered with the "ecce –admin" application. For these machines the "ecce -admin" application can be used to create template files based on the queue management system. These must be hand edited to account for the configuration of the individual machine. A PDF document describing compute resource registration is maintained on the ECCE web site and should be consulted whenever queued machines need to be registered.

Setup Users' Environment

- For sh and bash users, add the following lines to their ~/.profile or ~/.bashrc file, substituting the correct path under which ECCE was installed on your host:

  ```
  # setup to run ECCE
  if [ -e /sharednfs/ecce/scripts/runtime_setup.sh ]; then
    . /sharednfs/ecce/scripts/runtime_setup.sh
  fi
  ```

- There is an equivalent script named runtime_setup in the same directory that can be sourced for csh and tcsh users in their ~/.cshrc (~/.mycshrc within EMSL) file, substituting the correct path under which ECCE was installed on your host:

  ```
  # setup to run ECCE
  if ( -e /sharednfs/ecce/scripts/runtime_setup) then
    source /sharednfs/ecce/scripts/runtime_setup
  endif
  ```

  Hint: Within EMSL we maintain a symbolic link named scripts in a top-level shared ECCE directory that contains multiple releases of ECCE. The scripts link points to the scripts directory for the current production version of ECCE. This way the ECCE administrator only needs to update this link to change the version all ECCE users run by default. Users wishing to run other than the default version the symbolic link points to can change their environment setup file to reference the runtime_setup.sh or runtime_setup script for the desired version. The path to runtime_setup.sh and runtime_setup under /sharednfs/ecce/scripts in the examples above is based upon this mechanism. In the example installation, ECCE was installed under /sharednfs/ecce-v6.4/apps. A symbolic link in the /sharednfs/ecce directory named scripts pointing to /sharednfs/ecce-v6.4/apps/scripts will make it easier for the ECCE administrator to upgrade users to new versions of ECCE. The commands to do this for the example installation are:

  prompt$ **mkdir /sharednfs/ecce**
  prompt$ **cd /sharednfs/ecce**
  prompt$ **ln -s ../ecce-v6.4/apps/scripts scripts**

- Logout then log back in again to make sure the environment is properly setup. Enter the command "which ecce" to make sure paths are correct.

Run ECCE

- Start ECCE by typing...

  prompt$ **ecce**

  Users will first be prompted for their data server password in a window containing the ECCE "wave" logo centered on their screen. When automatic server account creation is enabled (the default), the password prompt for the initial login will be for setting a new data server password. On subsequent invocations this data server password must be entered to gain access. If automatic server account creation has been disabled then the ECCE site administrator must create an ECCE server account for the user and give them the password prior to running ECCE. Users can also change their data server password by hitting the "Change" button on the data server password window provided they know the current password.

  ECCE caches all passwords entered during an ECCE session. The data server password entered when starting ECCE is passed via this cache between all ECCE applications that access the data server saving the user from re-entering the password each time an application is started. Similarly, compute resource (machine login) passwords are cached between applications so only a single prompt for the password is made for an ECCE session. This feature is used even within a single job launch as multiple connections are established to transfer files, start the job, and then monitor the running job in a non-GUI ECCE application (eccejobstore).

- Where to go for help

  Check out the help pages on the web at http://ecce.emsl.pnl.gov/help, which are also accessible from within ECCE applications under the menubar Help menu. Also visit the user FAQ and Release Notes for the current and previous releases of ECCE. The release notes serve as the most up-to-date and complete documentation of ECCE features.