

# ECCE Builder 4.5 Installation

## Overview

Before installing the ECCE Builder we highly recommend reviewing the [platform requirements](#) in order to save unnecessary aggravation should the system you wish to install on not meet these specifications for operating system version, memory, disk space, graphics hardware, etc.

The ECCE Molecule Builder runs on Linux and UNIX workstations under the X Window System and OpenGL. These machines can only be Intel Pentium and Itanium, AMD Athlon and Opteron processor Linux PCs, and SGI workstations, all constrained by the minimum platform requirements referenced above. The ECCE Builder software can be installed on each individual workstation on which it will be run, or preferably in a multi-user environment, on a shared file system such as NFS or AFS that each workstation accesses.

The installation procedures assume a basic familiarity with UNIX system administration. Commands given are for csh and should also apply to tcsh; if you are using another shell such as Bourne sh or ksh, you will need to adjust the syntax accordingly. The example installations described in this document are for a Linux workstation. If you are installing on an SGI workstation instead, you would replace the obvious Linux name references, such as “i686\_Linux\_glibc2.3”, with the appropriate IRIX names.

## Install Third-Party Software

These PREREQUISITE software packages should be installed by a system administrator on all hosts where the ECCE Builder will be run. Please make sure you have obtained and properly installed these third-party applications before installing the Builder. The required packages are:

- **Perl:** Although it is not used at runtime, the ECCE Builder cannot be installed without Perl being installed and in the path. Establish whether Perl is on your machine using the command:

```
prompt% which perl
```

- **Netscape, Mozilla, or Firefox:** Locate or install netscape, mozilla, or firefox on your machine and make sure it is in a directory in the PATH for each user. Online help and the user support request web page rely on one of these web browsers; which one is determined by installation settings.
- **OpenGL:**

Linux: The Builder works with desktops and laptops using either Mesa OpenGL software rendering or hardware OpenGL rendering using a graphics card along with the associated Linux driver software. We suggest using Linux PCs with hardware graphics cards supporting OpenGL whenever possible, with the NVIDIA and ATI cards outfitted with the most on-board memory available, being our top

recommendations when purchasing new systems for use with ECCE. If you need to use software graphics rendering, the Mesa OpenGL library will most likely be included with your version of Linux depending upon the vendor and version.

SGI: Normally all IRIX workstations have OpenGL installed along with another graphics library needed by ECCE, OpenInventor, as part of the window system software. Some IRIX compute platforms such as the Power Challenge will not have the libraries installed although they are available. On a related note, the Power Challenge platform normally does not come with the graphics hardware required so you will need to verify whether you have this hardware as well as the OpenGL and OpenInventor libraries, if you plan to run the ECCE Builder on a Power Challenge. You must obtain the OpenGL and OpenInventor libraries from SGI and install them using the SGI “inst” command. You can proceed to install the Builder and then determine whether you have the required graphics hardware based on whether chemical systems are displayed in the workspace area or not when the Builder is run. If the OpenGL and/or OpenInventor libraries have not been installed you will get missing shared library error messages when starting the Builder.

## **Register and Download the ECCE Builder Distribution**

You must provide the information asked for in the EMSL User System and then submit a software user agreement as directed in the EMSL User System before you can download the ECCE Builder distribution. See the [ECCE registration page](#) for details. One approved at EMSL, you will be provided with download instructions. Using a web browser, download the appropriate ECCE Builder distribution for your platform to a local disk directory (or download multiple distributions if you will be running the Builder from more than one platform). The download web page provides information on which distribution is appropriate for your platform. File size for downloading is displayed on the web page although having sufficient additional free disk space during installation is critical since uncompress and untar steps will multiply the size requirements temporarily.

The Builder distribution is compressed using GNU gzip. For SGI, gunzip is not included with the operating system. If you do not already have gunzip, a link on the ECCE download web page points to miscellaneous download files, including the gunzip executable in standard UNIX “.Z” compressed format. Download, uncompress, and make sure gunzip is in your path when running the Builder install script. The gunzip utility is already provided with all Linux operating systems.

## **Install ECCE Builder**

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 the ECCE Builder that if removed or improperly modified will corrupt the installation.

The ECCE Builder distribution itself is a self-extracting C shell installation script along with compressed tar files containing the Builder application software. The installation script prompts for configuration settings and then performs the installation.

Run the `install_ecce_builder.v4.5.*.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 below are the default and you may simply hit return to use the default. For clarity, values are always explicitly entered for the prompts in this example even when the default value is used. The host this sample installation is performed on runs a version of the Linux operating system using version 2.3.x of the GNU C Library such as Red Hat Enterprise Workstation 3 or Fedora Core 3. For other platforms, remember to modify the commands accordingly. Here is the sample invocation of `install_ecce_builder.v4.5.*.csh`, 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_builder.v4.5.i686_Linux_glibc2.3.csh
prompt% ./install_ecce_builder.v4.5.i686_Linux_glibc2.3.csh
```

Extracting ECCE Builder distribution from `./install_ecce_builder.v4.5.i686_Linux_glibc2.3.csh...`

ECCE Builder installation directory: `[/myfiles/ecce-builder-v4.5] /myfiles/ecce-builder-v4.5`

ECCE Builder v4.5 installation directory: `[/myfiles/ecce-builder-v4.5]`

Is this choice correct (yes/no/quit)? `[yes] yes`

Installing ECCE Builder in `/myfiles /ecce-builder-v4.5...`

```
Extracting ECCE Builder distribution...
Extracting client WebHelp distribution...
Configuring ECCE Builder...
```

ECCE Builder installation succeeded.

\*\*\*\*\*

**!! You MUST perform the following steps in order to use ECCE !!**

```
-- To run the ECCE Builder each user must source either the
runtime_setup (csh/tcsh) or runtime_setup.sh (sh/bash/ksh)
script in the directory /sharednfs/ecce-v4.5/apps/scripts
from their shell environment setup script. For example,
with csh or tcsh, add the following to ~/.cshrc:
    if (-e /sharednfs/ecce-builder-v4.5/scripts/runtime_setup) then
        source /sharednfs/ecce-builder-v4.5/scripts/runtime_setup
    endif
```

\*\*\*\*\*

```
prompt%
```

After the `install_ecce_builder.v4.5.*.csh` script has completed, you may delete the distribution script although we recommend waiting until the Builder is completely tested at your site.

The next several paragraphs describe how to choose appropriate values for the ECCE Builder 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.

**ECCE Builder installation directory:** The ECCE Builder is designed for installation under a single shared directory at a site, with all Linux and SGI hosts accessing the common installation. A local file system disk is selected for the installation directory when the Builder will only be run from a single machine. If you have a shared file system and will have multiple machines and/or platforms running the Builder, we recommend installing under the shared file system as it reduces parallel administration. The shared directory where the Builder is installed is independent of the directory where the distribution is initially downloaded, although the default will be a subdirectory of the download directory. Typically the distribution is initially downloaded to local disk to speed file transfer, and then installed to a shared file system. This shared file system should have at least 100 megabytes free for each platform that will be installed. To install multiple platforms to a shared file system, specify the same Builder installation directory for each platform (requires downloading and running the installation script distribution for each platform). The installation script automatically extracts platform-dependent libraries and executables into separate subdirectories. The absolute path to the directory where the ECCE Builder is installed is stored in the ECCE user runtime setup script as the environment variable `$ECCE_HOME`. The rest of this document uses the term “ECCE Builder installation directory” and slight variations interchangeably with `$ECCE_HOME`, especially when referring to file paths.

You are not allowed to overwrite an existing ECCE Builder installation except in the case where you are installing different platforms under the same top-level 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 Builder in 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_builder.v4.5.*.csh` script. We recommend that you only remove an existing installation after you have verified the operation of the new installation. Certain releases, such as quick turnaround patches done for individual sites, have not been tested to the extent as major releases so you may find problems severe enough that you wish to revert to the previous install.

**Is this choice correct:** Pressing return or entering “yes” results in the ECCE Builder installation completing under the specified installation directory. Entering “no” results in the installation directory being prompted for again.

## Post-install Configuration

- **Change the Default Web Browser**

The ECCE Builder uses a web browser for online help and the user support request web page. At this time, Netscape, Mozilla, and Firefox are compatible with how the ECCE Builder controls the display of web pages externally (KDE Konqueror, for instance, does not allow the control needed). By default Mozilla is configured as the web browser within the ECCE Builder for both Linux and SGI platforms. This can be changed on a per-platform basis 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 “netscape”, “mozilla”, and “firefox”.

- **Change the User Support Email Address**

Email submitted via the ECCE support request web page available from the Help menu in the Builder should be sent to someone at your site if you support multiple users. However, the default configuration sends these requests back to [ecce-support@emsl.pnl.gov](mailto:ecce-support@emsl.pnl.gov), the support queue maintained by the ECCE development team in EMSL. Should the [ecce-support@emsl.pnl.gov](mailto:ecce-support@emsl.pnl.gov) queue start receiving several support requests from a site regarding issues that should be handled by the site contact you will be asked to change your support address to redirect requests. The person doing the installation of ECCE at the site is one possible choice if they are also an ECCE user so that requests pertaining to both using and the administration of the ECCE Builder can be handled. This address may be changed at any time by editing the `site_runtime` file in the `$ECCE_HOME/siteconfig` directory and changing the value for the `ECCE_SUPPORT` entry. The site point of contact for user support may pass along problems, questions, and requests that they don't know how to handle to [ecce-support@emsl.pnl.gov](mailto:ecce-support@emsl.pnl.gov), either acting as an intermediary or judiciously setting up direct communication between the ECCE team and the user.

## Setup Users' Environment

- For `csh` and `tsh` users, add the following lines to the user's `.cshrc` (or `.mycshrc` within EMSL) file, substituting the correct path under which ECCE was installed on your host:

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

There is an equivalent script named `runtime_setup.sh` in the same directory that can be sourced for `sh`, `BASH`, and `ksh` shell users.

Hint: Within EMSL, we maintain a symbolic link named `scripts` in a top-level shared ECCE Builder directory that contains multiple releases of the Builder. The `scripts` link points to the `scripts` directory for the current production version of the ECCE Builder. This way the ECCE administrator only needs to update this link to change the version all ECCE Builder users are running. Users wishing to run other than the default version the symbolic link points to can change their `.cshrc` file to reference the `runtime_setup` script for the desired version. The path to `runtime_setup` under `/sharednfs/ecce-builder/scripts` in the example above is based upon this mechanism. In the example installation, ECCE was installed under `/sharednfs/ecce-builder-v4.5`. A symbolic link in the `/sharednfs/ecce-`

builder directory named scripts pointing to /sharednfs/ecce-builder-v4.5/scripts will make it easier for the ECCE administrator to upgrade users to new versions of the ECCE Builder. The commands to do this for the example installation are:

```
prompt% mkdir /sharednfs/ecce-builder  
prompt% cd /sharednfs/ecce-builder  
prompt% ln -s ../ecce-builder-v4.5/scripts scripts
```

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

## Run ECCE Builder

- Start the ECCE Builder by typing...

```
prompt% ebuilder
```

- Where to go for help

Check out the ECCE Builder help pages on the web at <http://ecce.emsl.pnl.gov/cgi-bin/help/toolhelp?builder>, which are also accessible from within the ECCE Builder under the menubar Help menu. Also visit the user [FAQ](#) and [Release Notes](#) for version 4.5 of ECCE. The FAQ is out of date with respect to adding new items the last several releases of ECCE, but items have been removed that are no longer pertinent.