ECCE 5.x RELEASE NOTES

Version 5.1—March 10, 2009
Version 5.0.1—January 19, 2009
Version 5.0—December 12, 2008

The intent of this page is to provide information specific to the 5.x versions of ECCE. Version 5.0 completes the migration of all ECCE applications to the cross platform open source user interface toolkit, wxWidgets. Specifically the user interface for the Calculation Viewer has been completely redesigned and integrated with the Builder to create a single combined visualization capability. Version 5.0.1 primarily adds a small number of new Builder/Viewer features. Version 5.1 uses virtual operating system technology to support ECCE running on Microsoft Windows based PCs along with adding a small number of other features. Version 5.1 notes, the most recent, have titles highlighted in **green text**.

RELEASE NOTES FOR PREVIOUS VERSIONS

Version 4.x Release Notes – December 27, 2007
Version 3.2.x Release Notes – April 5, 2006

WHAT'S NEW

Windows PC Support

(5.1) A special distribution of ECCE has been created for users wishing to run ECCE on a Windows based PC. The freely available VMware Player virtual operating system software is required for using this distribution to run the Linux release of ECCE on a Windows host. The distribution includes a pre-installed version of the ECCE application and server software under the CentOS 4 (http://www.centos.org/) Linux operating system. These components are bundled as a virtual machine that is directly installed within VMware Player, which must be downloaded from the VMware website (http://www.vmware.com/products/player) and installed separately. A web browser viewable movie has also been created that documents the installation of VMware Player, the ECCE CentOS virtual machine, running ECCE in this environment, and common VMware Player configuration changes.

Once the virtual machine is installed and running, three icons for accessing ECCE are shown on the desktop. One provides access to ECCE with a local ECCE data and messaging server suitable for those running off the network or when there is only a single user at a site. In this case the local ECCE server is started automatically as needed when the ECCE application software is invoked with the "ecce" command. Thus there is

normally no need to run the start_ecce_server script explicitly as there is with a regular ECCE Linux install. The remote ECCE server icon is used to run against a shared ECCE server on another (typically native Linux) workstation. By default the remote server is configured as eccetera.emsl.pnl.gov, the production ECCE server maintained for EMSL users (not accessible outside the PNNL firewall). But, a script named config_remote_server in the $ECCE_HOME/siteconfig/RemoteServer directory can be run to setup access to any desired ECCE server. The ECCE installation supports users who start the application software with a remote server in some instances and a local server in others (such as a laptop that is taken off the network for travel). The third desktop icon is used to start just the ECCE Builder/Viewer application without the rest of the ECCE application software (nor need for an ECCE server).

The Windows VMware Player version of ECCE is distributed as a compressed archive of files in "zip" format. The movie documenting the install process is also distributed as a "zip" archive file separately from the VMware Player ECCE distribution. This same movie is also available online from the ECCE public website under http://ecce.pnl.gov/support/movie_index.shtml, although performance when viewing it online can be agonizingly slow depending upon a number of factors. Thus, we recommend downloading and viewing the movie locally. These "zip" format archive files first need to be uncompressed and extracted. Windows XP and Vista allow users to double click on these files as a "compressed zip folder" to display the contents and then drag and drop them to a regular file folder to extract them. There are also a number of separately available Windows applications that can be downloaded and installed to efficiently extract these archives. The 7-zip utility (http://www.7-zip.org) is freely available and therefore recommended. WinZip (http://www.winzip.com/prod_down.htm) is also widely used, but is a licensed commercial product with a 45-day free trial period. We highly recommend users watch the movie before attempting to install the VMware Player ECCE distribution as VMware Player provides several options for installing including hardware configuration and networking. To watch the movie after extracting the files from the "zip" archive, open the file "Installing_ECCE_VM.html" in the extracted folder from a web browser such as Internet Explorer (may require the Macromedia Flash plug-in to be installed).

The VMware Player ECCE distribution can also be used on 32- and 64-bit Linux hosts, or theoretically anywhere VMware Player can be installed. Since the movie documenting the installation procedure is targeted for Windows users, a README file is included in the folder that is extracted with the VMware Player ECCE distribution describing any Linux specific steps.

Software Based OpenGL Support

(5.1) Because OpenGL support as needed for the ECCE Builder/Viewer is the single most common problem experienced by ECCE users, software based OpenGL libraries are now provided with the ECCE distribution as backup if hardware graphics card OpenGL support is not available or cannot be made to work. Given the differences between hardware platforms, graphics cards, and operating systems along with the limited support the ECCE team can provide for this variation, there are some circumstances where there

is no practical alternative to using the software OpenGL libraries even when a hardware graphics card supporting OpenGL along with driver software has been installed. For instance, ECCE currently runs as 32-bit applications meaning that on 64-bit systems there must be 32-bit compatibility libraries installed including for OpenGL. Additionally, if the GLIBC version supported by the local /lib/libc.so.6 system library is significantly different from that which ECCE was built with, this can also lead to incompatibility with the hardware OpenGL driver. By default ECCE will attempt to use locally installed (hardware based) OpenGL libraries. However, by setting the $ECCE_MESA_OPENGL (Mesa, http://www.mesa3d.org, is the implementation that is bundled) variable before starting ECCE, the software OpenGL libraries bundled with ECCE will be used instead. This variable can be set in a login environment setup script (.cshrc, .bashrc) for individual users or it can be set as a site-level default in the $ECCE_HOME/siteconfig/site_runtime file (not recommended if there are multiple machines that will use the ECCE installation at a site). Unfortunately, rendering performance when using software OpenGL will be significantly slower than when a hardware graphics card with OpenGL driver is used. However, for electronic structure "small molecule" chemistry ECCE is typically used for, it likely won't be objectionable. Only with molecular dynamics (such as interactively manipulating PDB file based structures) or viewing trajectory files is the amount of information being rendered large enough to make hardware OpenGL graphics much more desirable.

NWChem 5.1.1 Bundled

(5.1) Newly released NWChem version 5.1.1 has been bundled with ECCE 5.1. This is the version that will be used when calculations are run on the host where the ECCE application software is installed. No specific changes to support new NWChem 5.1.1 features have been made to ECCE. ECCE bundles NWChem as a matter of convenience for those evaluating either ECCE or NWChem with the intent that users running the software for actual research will install NWChem separately. For less demanding computational applications on low-end hardware, it may be feasible though to continue using the ECCE bundled NWChem distribution.

Gaussian Cube File Visualization

(5.0.1) Restoring a pre-ECCE 5.0 feature for visualizing Gaussian Cube format files, the 5.0.1 Viewer handles both cube files that are part of the output from a calculation run from within ECCE and standalone cube files. Any cube files produced by an ECCE run calculation can be displayed using the new "Cube File" property panel in the Viewer similar to other properties for the calculation. To display a standalone cube file that is on the local machine where the Viewer is being run, use the "Open in new context…" menu item under the File menu after opening the Viewer from either the Gateway toolbar or the command line with the "ebuilder" command. Alternatively, the name of the cube file can be passed as a command line argument to the "ebuilder" command (the "ebuilder" command is used to bring up the integrated Builder/Viewer application whether it is to be used for building molecules or viewing calculated properties). Select the surface to display from the list on the left side of the "Cube File" property panel. Note that the property panel allows linear combinations of two different surfaces to be calculated and displayed by left mouse button clicking on the name of the first surface, right mouse

button clicking on the name of the second surface, and then entering the coefficients for the linear combination into the "A" and "B" numeric entry fields on the property panel.

MO Panel Energy Graph

(5.0.1) Another pre-ECCE 5.0 feature, this time for displaying molecular orbital occupation energies graphically, has been restored. From the Viewer "MOs" property panel select "Graph" or "Graph by Symmetries" from the dropdown option menu near the right hand side of the panel title bar. The color of each orbital on the graph denotes its occupation number as indicated by the graph legend. Note that the orbital occupation energies graphed are integrated with the MO visualization by left mouse button selecting an orbital from within the graph and hitting the "Compute" button below the graph.

Builder Atom Dragging

(5.0.1) Atoms and groups of atoms selected in the Builder can be moved (translated) in space by dragging (left mouse button selection and holding down the mouse button during the operation) over any one of the selected atoms in space. This is a quick and imprecise, although often very useful, alternative to using the other Builder manipulator tools or entering atom coordinates directly in the Atom Table. Note that any atom translations made in this way can be undone with the undo (ctrl-z) capability from the Edit menu.

Exporting Tabular Data

(5.0.1) Data in the Builder and Calculation Viewer can be exported to a comma-separated values (CSV) file using the right mouse button popup "Export…" menu item. This includes tabular data such as the atom table, residue table, MOs, vibrational frequencies, moments, etc. The Organizer also supports exporting calculation summary fields displayed in the right-hand side project context panel to a CSV file.

Adding Ghost Atoms

(5.0.1) The Builder allows ghost atoms (normally used in the Symmetry panel) to be added arbitrarily as atom placeholders when building a chemical system or for any other desired purpose. Under the Build panel "More…" button the ghost atom is shown with the symbol "X" in the bottom left corner of the periodic table. Selecting this "X" element allows any number of ghost atoms to be added to the workspace by clicking in free space as with the other periodic table elements. The default bonding hybridization for ghosts is a lone atom although this can be changed in the Build panel to allow bonded ghost atoms.

BqX Atom Behavior

(5.0.1) The Builder Atom Table contains two new dropdown option menu items for setting the behavior to BqX for all currently selected atoms and clearing the behavior field for all atoms, selected or not. Additionally the different types of atom behavior (Point, Quantum, Bq, BqX) can be entered directly (case insensitive) in the behavior field of the table for an atom. BqX atoms are typically used in NWChem QM/MM calculations, although ECCE does not currently offer any additional support for this type of calculation.

Authenticating as a Different Data Server User

(5.0.1) The initial ECCE login window now contains a "Data Server Login" field above the password field. This is used for remapping from a Linux login name (specified by the $USER environment variable) to a different name on the Apache2 DAV server used by ECCE to store calculation data. The first time a user starts ECCE the "Data Server Login" field will be editable with a default value of the current Linux login name. This allows the user to change the name of the initial data server account that is created on the ECCE server (assuming automatic data server account creation is enabled). Note that if a name is specified that is an existing data server account, the user will need to give the proper data server password for that account (in a different password dialog that is displayed after the ECCE login window) in order to access that data. This allows multiple users to share the same data server account and home directory either temporarily or longer term. After the initial login to ECCE the "Data Server Login" field will be disabled so a different user name cannot be specified, although the current setting will be displayed. However, it is still possible to set a different name after the initial login by starting ECCE with the command "ecce –l <DataServerLogin>" with the new login specified after the "-l" command line option (lower case letter "el", not the number "one"). Since changing the data server login name is typically seldom needed, disabling the "Data Server Login" field after the initial login was done to keep users from inadvertently changing to a different user resulting in confusion and unintentional creation of new data server accounts.

Closing Remote Shells when Exiting

(5.0.1) A Gateway Preferences dialog toggle labeled "Close Remote Shells on Exit" has been added. Toggling the preference "on" will result in all xterm shells (tail –f on output file, shell in calculation run directory) started in the current ECCE session being closed automatically when the Gateway (session) is exited. The default behavior is still to leave these remote shells up indefinitely even after the ECCE session is gone, allowing users to continue working in them. A word of caution to those who change the default behavior to close remote shells on exit: be careful that you aren't performing tasks in these remote shell windows where you haven't saved your work when exiting from ECCE, such as editing a file or running a program. ECCE immediately terminates these remote shells when exiting the Gateway and you may lose work as a result. A related bug was also found and fixed so the "ecmd" process that ECCE creates for each remote xterm shell is now properly cleaned up from the process table when the user exits the shell or the shell is closed when ECCE exits based on the preference setting. Previously these ecmd processes lived indefinitely after the shell and even the ECCE session where it had been created no longer existed.

New Calculation Viewer

(5.0) ECCE 5.0 features a redesigned user interface for the Calculation Viewer. The Viewer is now integrated into a single application with the Builder, itself redesigned for the previous ECCE 4.5 release. A single ECCE visualization application is now used for building chemical systems and viewing calculation/task output. This design ensures that all panels that are applicable to both the Builder and the Viewer, such as the selection panel, are available when needed with reduced maintenance overhead.

The dockable panel user interface paradigm first used for the ECCE 4.5 Builder is now used for the Viewer property panels in addition to the Builder tool panels. The Viewer main window is divided into property panels along the left hand side (as with the pre-5.0 Calculation Viewer), the visualization/work area in the center, and build tools along the right hand side. For build tool panels, the panel layout is completely configurable by the user dragging the panels and docking them in different places within the main window or "floating" them outside the main window as their own windows. These build tool panel locations, including docked or floated, are saved as user preferences and restored with the next invocation. Viewer property panels are an exception to saving and restoring their layout. Their location can be changed within an invocation, but will not be saved and restored between invocations.

Although the Builder and Viewer are actually the same executable, ECCE still maintains the distinction between the two in the Gateway toolbar and Organizer—each can be invoked separately. For a calculation or task that is being setup and run within ECCE, the run state determines whether it is a "Builder" or "Viewer" type invocation. Any calculation with a run state of Created or Ready will start a "Builder" instance regardless of whether the Builder or Viewer was selected in the Organizer. Likewise, for a calculation with a run state of Submitted, Running, or one of the completion states, a "Viewer" instance will be started regardless of whether the Builder or Viewer was selected in the Organizer. The type of instance, Builder or Viewer, simply determines which panels and operations are available to the user (cannot modify a chemical system for a running calculation for example) and whether the window title indicates a Builder or Viewer.

Like the build tool panels, in order to conserve screen space within property panels, option menus are commonly used to access functionality not on the panel itself. These option menus are displayed by hitting the left mouse button over top of the blue and white window icon near the right hand side of the property panel title bar. If you can't find functionality that was in the old Calculation Viewer in a new Viewer property panel, this is the first place to check.

The dockable panel nature of the Builder/Viewer and fussiness of the wxWidgets implementation for this capability sometimes results in undesirable if not bizarre and unusable panel layouts. In this case the "Reset Defaults Tools/Toolbars" operation in the Options menu can be used to restore sanity. After answering "Yes" to the confirmation dialog, you must exit and restart the Builder/Viewer to restore the default layout.

The Builder/Viewer is the only ECCE application that supports multiple contexts (calculations, chemical system files, trajectory animations, etc.) at the same time in a single instance of the tool. This design should be transparent to traditional ECCE users who bring up the Builder/Viewer in the context of an existing calculation to build a chemical system or visualize results and then close the application when done with their immediate task. But, for those who deviate from this usage, the multiple context design can take a bit of getting used to. Contexts mimic the design of many other visualization

tools. A “Context” panel, which shows up with the other right-hand build panels, lists the current contexts and enables quick switching between them. The “File” menu contains three menu items for controlling contexts. “New context” creates an empty context whose name initially starts with “Unnamed”. This empty context can be used, for instance, to build chemical systems from scratch or using the “Import chemical system…” menu item. “Open in new context…” combines the “New context” operation with selecting a file to display in the newly created context. The selected file can be a chemical system, but this is also the way to open and animate the frames of a trajectory file or sequence of batched trajectory files (by selecting any single file in the sequence). Finally, “Close context” will close the currently displayed context, prompting to save any work if there are unsaved changes.

The “Save as…” operation in the Builder/Viewer is more powerful than in previous releases of ECCE. “Save as…” is used for saving chemical system file formats (xyz, pdb, etc.), saving image snapshots of the visualization area (jpeg, POV-Ray, etc.), and for saving out the current context as a brand new electronic structure calculation (NWChem, etc.). A drop down menu below the file name text entry field is used to specify the type of file to generate. Saving a chemical system as an electronic structure calculation allows users to start the setup process by building their structure and then defining the chemistry code and where they want to put it on the ECCE data server. Further, if a geometry trace or trajectory is being visualized, the “Save as…” operation saves the step that is currently being displayed allowing explicit control for creating structures to serve as the starting point for additional work inside or outside ECCE.

As with previous releases, the “ebuilder” script is used to invoke the standalone version of the Builder from the command line. The “ebuilder” command is also used to open trajectory files (NWChem trj, or generic xyz format) as a “Viewer” instance of the standalone builder. The chemical system or trajectory file to load can be given as a command line argument to ebuilder. Alternatively, the “Open in new context…” (chemical systems or trajectories) or “Import chemical system…” (chemical systems only) File menu operations can be used to load a file after invoking “ebuilder” without command line arguments. Invoking the Builder from the Gateway toolbar is equivalent to an “ebuilder” invocation without any arguments while invoking the Viewer from the Gateway toolbar automatically performs an “Open in new context…” operation from the newly created application—used for opening chemical systems or trajectories. An enhancement from previous ECCE releases, the “ebuilder” script is now fully functional even in a full ECCE install. Previously the “Structure Library”, “DNA Builder”, and “Peptide Builder” would not work from “ebuilder” except when a “standalone builder” distribution of ECCE was downloaded and installed.

Unfortunately, for the initial release there exists no additional documentation on using the ECCE 5.0 Builder/Viewer beyond these release notes. We strived to make it as intuitive and stick with names and conventions established by previous releases of ECCE where feasible. You are encouraged to play with it to see how it can be applied to your work. Finally, please don’t hesitate to ask questions or give us feedback by sending email to ecce-support@emsl.pnl.gov.

Old Builder and Viewer No Longer Distributed

(5.0) The ECCE 5.0 distribution no longer contains the old X Window Motif versions of the Molecule Builder and Calculation Viewer applications. In the ECCE 4.5.x distributions the old Builder was distributed as a backup to the new wxWidgets version. This was done in case users found problems with the new Builder significant enough that they needed to revert to the old version to accomplish their work. Plus, some rarely used components of the old Builder (e.g., the MD Topology Viewer and Force Field Editor) have not been ported to the new wxWidgets version. Since the initial ECCE 4.5 release, the new Builder, now integrated with the Viewer, has become significantly more robust and reliable and the ECCE team does not anticipate sites needing to use the old versions. This decreases the size of the distribution and installation, especially with third party libraries for only a single GUI toolkit being distributed instead of two GUI toolkits. A not unintentional side effect is that if problems are found with either the new Builder or Viewer, feedback to the ECCE team will be needed, which might not be the case if the old versions were easily available. There are a small number of what the ECCE team considers to be minor features that were not implemented in the new Viewer (conversely, there are a large number of new capabilities not previously available). If you discover a missing feature from the old Builder or Viewer that you found valuable that you would like to see added back, please contact us. We are also still able to provide these old Builder and Viewer versions on request.

Normal Modes Property Renamed

(5.0) For consistency with NWChem and other chemistry codes, the Normal Modes property panel in the Viewer has been renamed to Vibrational Frequencies. Calculations that were run prior to ECCE 5.0 will automatically display what was Normal Mode data in the Vibrational Frequencies panel.

Open Source GUI Migration

(5.0) The redesign of the Viewer porting it to the wxWidgets GUI toolkit completes the migration of all ECCE applications to rely on only freely available open source products. This effort was undertaken in 2005 with one or more applications being ported to wxWidgets (see http://www.wxwidgets.org) with each release starting with 4.0, all while continuing to simultaneously add computational chemistry domain functionality. Core ECCE applications use the wxWidgets C++ toolkit, while the code registration dialogs are implemented under wxPython, the wxWidgets binding to the Python scripting language. In addition to being an open source product, wxWidgets is a cross platform toolkit that supports all major operating systems. Eliminated are two proprietary GUI development tools for the UNIX/Linux only X Window System Motif toolkit, which date back to the first production release of ECCE: Aonix TeleUSE and Quest XRT PDS widgets. This milestone opens up several new possibilities for the future of ECCE such as collaborative and contributed code developed outside the ECCE project team (only electronic structure code registration was previously possible) and ports to different operating systems including Microsoft Windows and Macintosh OS X. While the ECCE project team is not currently scoped for completing the ports to operating systems beyond Linux, please contact us if you are interested in doing ECCE development, including porting to another operating system or adding chemistry domain functionality. At this

time there is no task to make ECCE source code available for download in a useful form; i.e., able to compile in an autoconf type environment (there are numerous third party packages ECCE relies on that make it more complex to build than lower-level software like NWChem). However, it is feasible that the identification and commitment of an outside group to extend ECCE in a way that benefits a broad base of users could justify this task of creating and documenting a build environment. Finally, of note to those who would like to run ECCE on Microsoft Windows based systems is a task planned for 2009 to make a distribution of ECCE available that runs under virtualization software such as VMware (see http://www.vmware.com) and/or VirtualBox (see http://www.virtualbox.org). While not a native operating system port, this will make running ECCE feasible at sites where Linux is not available. For sites with limited access to Linux systems, the use of X Window Server software that supports OpenGL such as Hummingbird Exceed 3D (see http://connectivity.hummingbird.com/products/nc/exceed) or Cygwin/X (see http://x.cygwin.com) already allow users to run ECCE from a backend Linux workstation displaying on Windows based desktops.

Color Themes

(5.0) ECCE now allows colors for application windows and GUI controls to be changed at the site level and by each user. Colors can either be changed individually by type of control or one of a small number of themes can be selected. The default ECCE colors have been changed in the 5.0 release to conform to the new Pacific Northwest National Laboratory branding although the "Classic" theme can be selected to restore the familiar pre-5.0 look. Colors are specified in a configuration file in the $ECCE_HOME/siteconfig directory name AppColors. This file also documents what control type colors can be changed, what the theme names are, how to specify a color value, and how users can create their own MyAppColors file to override the site level colors. Alternatively, the Gateway toolbar Preferences dialog contains a "Color Theme" choice box that updates the user MyAppColors file, but does not allow control of the individual control colors. The ECCE login window has also been changed to match the new branding with PNNL and EMSL logos added. The color of the ECCE wave logo in the background of the login window has also been changed (now PNNL-branded copper) and will not update with changes to the AppColors or MyAppColors files (same for the animated wave logo in the ECCE Gateway toolbar).

Renamed Applications

(5.0) Several ECCE application names have been shortened or changed for consistency. The Calculation Viewer is now simply Viewer. The Job Launcher is now Launcher. The Calculation Editor is now Electronic Structure Editor in a generic sense or NWChem Editor, etc. when in the context of a chemistry code. This is more consistent with the variety of new ECCE editor applications for different fields of chemistry—molecular dynamics and upcoming support for thermodynamics. Finally, the Molecule Builder is simply Builder as most users refer to it already.

SITE ADMINISTRATOR WHAT'S NEW

Upgrades of ECCE Data and Messaging Servers

(5.0) The Apache2 HTTP server (see http://httpd.apache.org) used for the ECCE data server along with the bundled mod_dav module has been upgraded from release 2.0.59 to the latest 2.2.10. The ActiveMQ Java Messaging Server (see http://activemq.apache.org) used for the ECCE JMS messaging server has also been upgraded from release 4.1.1 to 5.1.0. When installing, we highly recommend upgrading the ECCE server to 5.0 rather than solely the application software. In fact, we have experienced messaging session disconnects with accompanying java stack trace output in the window where the ECCE application session was started when running ECCE 5.0 application software against an ECCE 4.5.x server. These problems can be attributed to incompatibilities between the ActiveMQ 5.1.0 client side java messaging libraries used by ECCE 5.0 and the ActiveMQ 4.1.1 server distributed with ECCE 4.5.x.

Upgrade of wxWidgets GUI Toolkit

(5.0) The wxWidgets C++ GUI toolkit (see http://www.wxwidgets.org) used by ECCE core applications has been upgraded to the latest stable release, 2.8.9. Likewise, the wxPython toolkit (see http://wxpython.org) used for code registration theory and runtype details dialogs has also been upgraded to use the same distribution of wxWidgets. For ECCE this wxWidgets release primarily improves on the behavior of the dockable panel capability that is integral to the Builder/Viewer application.

WHAT'S FIXED

SITE ADMINISTRATOR WHAT'S FIXED

Crashes Saving Thumbnails and Image Files from the Builder and Viewer

(5.0.1) Certain operating systems and OpenGL hardware graphics drivers do not support the OpenGL off-screen rendering feature required by ECCE to save image files (JPEG, GIF, TIFF) and the thumbnail visualizations of chemical systems that are shown for the icon to access the Builder for a calculation. Typically the X Window session will completely crash trying to use these ECCE features when off-screen rendering is not supported; returning the user to the Linux login screen. Thumbnail visualizations are created by default when saving a chemical system in the Builder so it will appear as if a "save" operation is causing the crash. The $ECCE_NO_VIZIMAGES environment variable has been created to keep ECCE from creating any image files including thumbnail visualizations. Search for "ECCE_NO_VIZIMAGES" in the $ECCE_HOME/siteconfig/site_runtime file to override the default setting where off-screen rendering is used. Without off-screen rendering the POV-Ray format for capturing images of visualizations can still be used. Since POV-Ray produces publication/presentation high quality graphics and there are utilities to translate POV-Ray

files to image formats like JPEG, the lack of off-screen rendering is an inconvenience rather than a loss of functionality.

Machine Registration Queued Machine Support

(5.0.1) Several bugs were fixed with the Machine Registration application's support for registering batch queued machines. Because of the severity of these bugs, it was not previously possible to use the GUI application to register anything other than workstation class machines. Now the Machine Registration application (accessible via "ecce –admin" for users with write permission to the $ECCE_HOME/siteconfig directory) can be used for registering both workstations and batch queued compute resources to ECCE.

WHAT'S BROKEN