Ecce Version 3.0 Release Notes - November 13, 2002

EMSL Release - December 4, 2002

The intent of this page is to provide information specific to version 3.0 of Ecce. Except as mentioned herein release notes from previous versions of Ecce still apply so please do not consider this as a standalone reference.

Version 3.0 supports Ecce application software on the Linux operating system for many, though not all, machine configurations. A Java-based inter-process messaging server has been added to replace a technology freely available only for SGI and Sun. The Ecce distribution packaging and installation script have been redesigned combining the previous application and server software distributions into a single unified distribution. Many other enhancements and bug fixes have been made as described in these release notes.

Note: Ecce version 3.0 requires NWChem 4.0 or newer due to changes in the NWChem input and output file formats.

Release Notes for Recent Previous Versions

Version 2.1 Release Notes - February 11, 2002
Version 2.0 Release Notes - July 17, 2001
Version 1.5 Release Notes - December 1, 1999

What's New?   What's Fixed? What's Broken?

What's New?

User Notes:

1. **(v3.0 patch) Passphrase can be changed without losing configured passwords**
2. **(v3.0 patch) New runtime_setup.sh file for sh, bash, ksh users**
3. **Ecce is now available on Linux platforms**
4. **Support for Solaris 2.8 and 2.9--Solaris 2.6 and 2.7 dropped**
5. **Machines now have reference names allowing multiple registrations of the same machine**
6. **Online help updated**
7. **Basis set reference library updated**
8. **Basis set names are used in input files**
9. **Calculation Editor toggle for using basis set names or explicit exponents and coefficients**
10. **Imports recognize basis set names**
11. **Improved error messaging during calculation imports**

12. **Imported calculations can now be aborted while importing**
13. **NQE/NQS $TMPDIR supported**
14. **Spherical harmonics up to F functions supported in Calculation Viewer**
15. **Localized cleans are supported in the Builder**
16. **Fragments are centered when added to empty Builder**
17. **Gaussian Cube formatted files can be displayed**
18. **Modified PDB reader**
19. **Multiple bonded hydrogens are not allowed**
20. **Builder auto-normalize option enabled by default for new users**
21. **Remote xterm shells started with users default shell**
22. **Machine Browser and Job Launcher allow selection of either configured or all registered machines**
23. **Calculation Manager Manage Files dialog redesigned**
24. **Support for concurrent usage of Ecce v2.1 and v3.0**
25. **Lighting dialog removed from Builder and Calculation Viewer**
26. **Changes to the Gateway toolbar**
27. **Imported calculations now named based on file being imported.**

Site Administrator Notes:

1. **(v3.0 patch) Automatic creation of Ecce server accounts and synchronization of passwords**
2. **Single Ecce application and server distribution and installation script, prompting simplified, improved error checking**
3. **Single U.S. and international distribution of Ecce**
4. **New Java-based messaging service added**
5. **Ecce Apache web server enhancements**
6. **Improved documentation for updating DataServers file**
7. **Code registration enhancements**
8. **Machine Registration "Architecture" field removed**
9. **Job monitoring error detection enhancements**
10. **Remote communications debug logging**
11. **Support for LSF improved**
12. **Support for compute servers using RMS prun**
13. **OpenGL hardware limits on number of viewers specified in GLLimits.xml**
14. **Usage tracking disabled outside EMSL**

What's Fixed?

1. Calculation Editor details dialogs incompatible with Linux KDE window manager
2. Square Pyramidal geometry could not be selected
3. Builder crashes for validate structure on large systems
4. Trailing blanks in residue names confuse Builder
5. Prepending residues now works correctly
6. Invoking Basis Set Tool from Calculation Editor works on first mouse click
7. Applications now properly uniconified when question dialogs need to be displayed
8. Can no longer exit Job Launcher during launch process
9. Periodic Table electron affinity field more readable
10. Name of current application now correctly passed to the Feedback web page
11. Help buttons in Ecce dialogs no longer have the potential to crash applications
12. Crashes related to passphrase prompting fixed
13. Absolute paths to remote shell commands can now be specified in remote_shells.site
14. Improved support for calculations with large orbital data sets
15. Normal Modes panel shows more frequencies
16. MO computation error fixed (applies to generally contracted basis sets only).

What's Broken?

1. Viewing molecular orbitals in the Calculation Viewer while a calculation is running results in coordinates that do not match the orbitals
2. Refresh the Molecule Builder geometry table in order to see the new coordinates that result from using the bond or atom manipulators
3. Molecule Builder sphere radius selection does not work
4. Rings are not displayed in the Molecule Builder and Calculation Viewer
5. Cannot add measures in the Calculation Viewer to a property that is animating
6. Color and Pixmap allocation can fail on SGIs leading to warnings or crashes
7. access_log file for SGI web server does not show proper IP addresses for connections
8. Vizualization fonts on Solaris are garbled
9. Panels in the Calculation Viewer can no longer be "floated" on Solaris
10. Panels in the Calculation Viewer do not automatically resize on Linux
11. Graphics support on Linux will vary depending on your graphics card and driver.

What's New?

1. (v3.0 patch) The initial Ecce passphrase dialog has been redesigned to allow passphrases to be changed without losing previously configured compute server and Ecce server passwords. A button labeled "Change" has been added, while the button formerly labeled "New", is now labeled "Clear" to better indicate its function. To change your passphrase, you first must enter your existing passphrase and then select the "Change" button. A field labeled "New passphrase" will be shown below the existing passphrase field. Enter your new passphrase (4 characters minimum) and hit return or the "OK" button. A confirmation dialog allows you to cancel the change before all configured passwords are converted to work with the new passphrase. The "Clear" button works like the old "New" button except you select the button first and then enter your passphrase in the "New passphrase" field. Any text entered in the existing passphrase field before hitting the "Clear" button will be ignored. A confirmation dialog is also shown for clearing your passphrase, indicating that all configured passwords will be lost.

2. (v3.0 patch) A Bourne shell version of the runtime_setup Ecce user setup script, named runtime_setup.sh, has been created. The original runtime_setup script is only compatible with csh and tcsh environments. Now users of Bourne shell (sh), Bourne Again shell (bash), and Korn shell (ksh), can use Ecce without changing shells. The runtime_setup.sh file is normally sourced from a user's login environment files similarly to runtime_setup.

3. Version 3.0 of Ecce supports PCs running Linux for the first time. Only Redhat 7.x (7.3 recommended) is supported although Ecce has been successfully run on at least the following Linux operating systems:
   - Redhat 7.3, 7.2, 7.1, 7.0
   - Redhat 8.0
   - Redhat 6.x
   - Mandrake 8.x (Mandrake 9.0 not yet tested)
   - ALT Linux 2.0

   Ecce runs under the KDE and GNOME window managers and most likely others. The XFree86 X Server software is required with the version included in Redhat 7.x and Mandrake 8.x (XFree86 4.x). Older versions of XFree86 may need to be upgraded although XFree86 3.x has also been shown to work at least in some configurations. A hardware graphics card supporting OpenGL is strongly recommended (NVidia GeForce2 and Quadro being our top recommendations for purcasing new hardware), although Mesa software OpenGL rendering is also acceptable. Ecce has been successfully run on Intel Pentium, Intel 64-bit Itanium, and AMD Athlon processors. For Itaniums, the same executables that are used for 32-bit platforms are run because Ecce cannot be compiled with 64-bit processors. The required graphical user interface development tools are currently not being supported under the 64-bit compiler.

   The Ecce application software includes all required shared system libraries except OpenGL. This is to support the many different operating system vendors and versions, as well as kernel and glibc configurations. Ecce also requires a newer version of the g++ compiler and glibc than is being shipped with Linux operating systems. The Ecce server software, specifically the Apache2 web

server, is built with standard versions of gcc and glibc, and thus depends on the operating system supplied versions of certain shared libraries. It is thus possible that specific configurations of Linux workstations used as Ecce servers will need libraries we do not currently distribute. Contact ecce-support@emsl.pnl.gov in this instance.

4. Ecce v3.0 supports Sun Solaris 2.8 and 2.9. Ecce is now compiled with g++ rather than the native Sun C++ compiler on Solaris 2.8 and runs these same executables on Solaris 2.9 systems. Support for Solaris 2.6 and 2.7 has been dropped as these operating system versions are no longer supported within EMSL. Starting with v3.0, the Sun distribution of Ecce is available by special request only. As Suns become less common within EMSL and new Linux machines are added, the Ecce team needs to closely track the usage of the Sun version of Ecce to justify its continued availability. There are some further limitations unique to the Sun release of Ecce with v3.0, such as statically linked executables requiring extra memory, that make us reluctant to make it as openly available. If you do wish to use the Sun release of Ecce, send email to ecce-support@emsl.pnl.gov and instructions will be provided for downloading. SGI IRIX 6.5 support and distribution is not impacted as there continues to be significant demand for this platform.

5. Machines now have an associated "reference" name selected by the site administrator or user performing the machine registration. This "reference" name is the unique key for identifying the machine and the full machine name previously used to uniquely identify the machine is now an attribute that does not need to be unique. Thus, a machine can be registered more than once by using different "reference" names for each instance. For instance, a queued machine can be registered to run both batch and interactive jobs by registering the machine separately with each configuration. This feature also allows commonly known aliases for a machine to be used when login node names are not well known. This feature has had a broad impact on all Ecce data pertaining to machine names being saved including the v3.0 changes to preference file formats. Applications like Job Launcher and Machine Browser that display lists of machines now display these reference names rather than the full machine names.

6. Ecce online help has been updated for version 3.0. This is the first update since v2.0. As with v2.1, online help is distributed with the Ecce server. New for v3.0, the web browser to be used for each platform (Linux, SGI, Sun) can be configured as either netscape or mozilla as a site or user preference. The site administrator can do this by editing the siteconfig/site_runtime file under the top-level application software directory. Each user can override the site preference by setting the variables $ECCE_LINUXBROWSER, $ECCE_SGIBROWSER, or $ECCE_SUNBROWSER depending on which platform(s) they run on. The default web browser is mozilla for Linux and netscape for SGI and Sun. Netscape and mozilla are the only supported web browsers allowing the control over changing the displayed URL needed by Ecce. KDE Konqueror, for instance, cannot be used with Ecce. The same web browser configured for online help is also used for the web-based user feedback capability. Invalid links in the online help left-hand frame have been fixed for v3.0.

7. New basis sets have been added and minor corrections made to the Ecce basis set reference library maintained by Dr. David Feller of the PNNL Environmental Molecular Sciences Laboratory. There are currently 238 basis sets in the Ecce basis set library distributed with the Ecce v3.0 server.

8. Basis set names, instead of explicit lists of coefficients and exponents, are now used whenever possible in NWChem and Gaussian 98 input decks. NWChem uses basis set names in almost all cases, Gaussian 98 will use basis set names only for systems where all atoms are using the same basis and the basis set is listed in the Gaussian 98 basis set library. Explicit exponents and coefficients rather than basis set names will generally be used if the basis set has been modified using the Basis Set Tool or the Contraction Editor. Also, for the basis sets CRENBL ECP and CRENBS ECP, explicit exponents and coefficients will always be used because of naming discrepancies between Ecce and NWChem.

9. The Calculation Editor now has a toggle labeled, "Use Exponents & Coeffs", below the "Basis Set Tool..." button. This is used primarily if a basis set does not have an entry in the internal basis set library for NWChem. Several of the most recently added basis sets for v3.0 fall into this category. The computational code itself can be used to detect the lack of a library name by starting the job and letting it generate an error if basis set names are not recognized. By default this toggle is off so that library names will be used. Clicking the toggle on indicates to the Calculation Editor that the input file should be regenerated (saving is enabled). The next time the input file is generated it will have explicit exponents and coefficients and no basis set library names. If the Calculation Editor is restarted, this toggle will still be shown as off even though the input file may actually contain exponents and coefficients. Thus, it is important to make sure this toggle is correctly set each time an input file is generated if exponents and coefficients are desired.

10. NWChem and Gaussian 98 imports will generally recognize basis set names. The name recognition capability is more robust for NWChem than Gaussian 98, but it should be possible to import substantially more input files than previously was the case. Again, for Gaussian 98 only calculations where the basis set name is specified in the route card are supported. Imports of Gaussian 98 files where a combination of basis set names and explicit coefficient lists or where the basis set names are used in basis set field will not be able to identify the basis set. For NWChem, only orbital basis sets will be imported. Fitting basis sets, such as XC and CD, and ECP functions will be ignored (ECP functions are also ignored for Gaussian imports). The orbital basis sets are sufficient to display molecular orbitals.

11. The Calculation Manager import capability now supports better error and warning messages when problems are encountered. For instance, not being able to parse a basis set specification will result in a warning message about being unable to generate molecular orbitals for the imported calculation.

12. The Calculation Manager "Terminate Calculation" item under the Run Mgmt menu now serves to abort an active calculation import as well as terminate a submitted or running job.

13. Ecce now supports the NQE/NQS $TMPDIR environment variable for automatically setting a scratch directory for a job. If a job is being run on either an NQE or NQS compute server that supports $TMPDIR itself, Ecce will use this feature if no scratch directory is explicitly set in the Job Launcher. With jobs being run to servers running different queue management system, or no queue management system at all, an empty scratch directory field is used to specify that the scratch directory should be the same directory as the calculation run directory. It is still possible to get this behavior with NQE/NQS by explicitly setting the scratch and calculation directory fields to the same value. This

feature works with Gaussian 98 and Amica. NWChem 4.x versions supporting the new $SCRATCH_DIR environment variable will also work with this feature.

14. The Calculation Viewer will now display molecular orbitals containing D and F orbitals for spherical basis sets. Previously, only the S and P contributions were included when displaying molecular orbitals for spherical basis sets.

15. The implementation of the Universal Force Field has been completely revamped to support localized cleans in the Builder. If a subset of atoms is selected when the clean button is activated, only the coordinates of the selected atoms are updated, although the remaining atoms are included when evaluating the forces on the atoms. This functionality is aimed primarily at fixing up localized regions of larges structures, such as adding missing side chains, etc. to proteins for biological simulations. The clean function can be slow for large systems, even if only a few atoms are selected. If no atoms are selected, then the clean function works as before and all atoms are optimized. Some minor bugs in the force field were also removed.

16. Fragments added from the structure library or from a paste operation are automatically centered in the Builder. Previously, fragments retained their old coordinates, which could make them hard to find if the auto-normalization option was turned off in the Builder.

17. Gaussian Cube formatted files can now be displayed using the Calculation Viewer. To view cube files, the Calculation Viewer must be brought up standalone directly from the Gateway toolbar. Cube files can be imported into the Calculation Viewer by opening the "Grids" property panel and then pressing the "Import..." button inside this panel. The Calculation Viewer can import cube files storing single or multiple grids on orthogonal lattices. Gaussian 98 will produce cube files with multiple molecular orbitals, most other files contain only single grids. Both Gaussian 98™ and NWChem can be used to create cube files displayable with Ecce.

18. The PDB reader has been modified so that it will do a better overall job on locating the ends on protein and DNA and RNA chains. The algorithm will still make errors if non-standard residues are included in the chain and it is up to the user to check the Head, Tail, and Interior assignments in the MD Toolkit and alter them, if necessary.

19. The routine for automatically generating bonds has been altered to remove multiple bonds to hydrogen. If a multiple bond to hydrogen is encountered, the shortest bond is selected and the rest are removed. This prevents spurious bonds from appearing in hydrogen bonded structures (such double stranded DNA). Those users interested in structures such as boron hydride can still store them without losing bonding information by saving them in MVM format.

20. The Builder auto-normalize option for centering and resizing the chemical system displayed in the OpenGL visualization area every time an atom is added, is now enabled for new Ecce users. Although more advanced users will often want to disable this feature, it has proven to be a good safety feature for novice users. The value of this toggle will be saved as a Builder preference as it always has been so this change only impacts new users first running the Builder.

21. Remote xterm shells started from the Calculation Manager "shell in Calculation Run Directory..." menu item, Machine Browser "Open Shell" menu item, and Machine Configuration dialog "Open Remote Shell..." button, now use the correct user login shell. Previously Ecce always started a csh instance regardless of the user's default login shell.

22. An option menu above the list of machines in Job Launcher and Machine Browser allows the user to switch back and forth between all Ecce registered machines and only those configured by the user. In v2.1, the Job Launcher had a menubar item for this feature while Machine Browser only displayed all registered machines.

23. The Calculation Manager Manage Files interface has been redesigned to make it easier to use as well as for aesthetic reasons. The functionality of this dialog has been improved through recognizing all file names copied to the data server, rather than just the fixed input and output file names as with v2.1.

24. If it is necessary to run both Ecce v2.1 and v3.0 back to back for the same user, Ecce offers a simple mechanism to support switching preference files between versions. When first starting v3.0, Ecce recognizes the presence of v2.1 preference files and converts them to v3.0 format. The version 2.1 files are copied to the same names with extensions of ".v2.1" and an informational message is printed on using v2.1. By copying the ".v2.1" files back over top of the v3.0 counterparts, the older version can be run again and Ecce will re-convert the files to v3.0 format when that version is run. A new script named reformat_machines is called by Ecce to do this conversion.

25. The dialog for adding lighting to a visualization scene has been removed from both the Builder and Calculation Viewer. These dialogs were experimental in nature. The decision to terminate further development was made since other packages can be used to achieve similar visual affects.

26. A few changes have been made to the Gateway including the addition of an exit button, the legend button has been removed, a Calculation Viewer icon has been added for cube file visualization, and the Calculation Manager icon has been updated to better reflect recent design changes.

27. An imported calculation will now be named based on the filename (without extension) rather than simply defaulted to "Calculation" with a unique extension as necessary. If the default NWChem log file for Ecce, ecce.out, is imported then the calculation will be named "NWChem" with a unique extension as needed. Similarly, if a default Gaussian log file for Ecce, g98.out or g94.out, is imported then the calculation will be named "Gaussian98" or "Gaussian94", respectively.

28. (v3.0 patch) Ecce server accounts for the Apache web server can automatically be created the first time a user starts Ecce. This is a feature that can be controlled by the Ecce site administrator if there are concerns about allowing any user with access to the application software to create their own server account. By default the feature is enabled, as we believe most site administrators will appreciate not having the burden of creating accounts before a prospective user can run Ecce. The environment variable $ECCE_AUTO_ACCOUNTS defined in the $ECCE_HOME/scripts/ecce_env file (which should be writable only by the site administrator) controls whether this feature is enabled. See the documentation in that file for a description of the different possible settings. In addition to

automatically creating accounts, the Apache web server passwords are now synchronized to be the same as a user's main Ecce passphrase. Every time the passphrase is changed, the web server password is updated to match. This feature is also controlled with the $ECCE_AUTO_ACCOUNTS variable to allow automatic account creation and password synchronization, only password synchronization and not automatic account creation, or neither. Automatic account creation and password synchronization is implemented with an Apache cgi-bin script. No critical data is passed unencrypted over the Internet when making these requests. For security reasons, web server passwords will need to be manually reset by the site administrator using the ecce_htpasswd script on the Ecce server for those users who forget their passphrase and must start over by clearing it in the passphrase dialog. The confirmation dialog shown to users when the passphrase is cleared tells them to contact the site administrator to have this done. The new passphrase change feature should minimize how often this is necessary, since changing a passphrase will properly synchronize the web server password with the new passphrase.

29. The Ecce distribution packaging and installation has been overhauled for v3.0. A single, unified application and server software distribution and installation script now exists rather than the previous separate distributions and install scripts. The installation is done by invoking the downloaded Ecce distribution, as it was only for the server installation with Ecce v2.1. The distribution consists of both an installation script and the binary application and server distribution which self-extracts when run. A main menu in this installation script considerably simplifies installation by streamlining the most common scenarios such as standalone machine installation (now down to two prompts) and network machine installation (now down to four prompts). Upgrading existing installations is also more straightforward and consistent between application and server components. Better error checking has been added to the installation script. Online documentation for installation, available at http://ecce.emsl.pnl.gov/docs/2864B-Installation.pdf, has also been updated to reflect the new installation and administration procedures. The size of the Ecce distribution that must be downloaded has also been significantly reduced, especially for the Linux platform (currently 58 megabytes). This was accomplished by switching to gzip/gunzip instead of the standard UNIX compress/uncompress commands for Linux (SGI and Sun distributions of Ecce still use compress/uncompress because gzip/gunzip must be downloaded separate from the operating system on those platforms). Further, a single Java Runtime Environment is included in the distribution although for a network machine installation it will be extracted separately for both the application and server components of Ecce. Finally, the binary portion of the distribution is now a raw gzipped or compressed tar file rather than being uuencoded, with more sophisticated logic being used to extract it from the full distribution.

30. Separate U.S. and international distributions of Ecce have been eliminated. U.S. encryption export policy in the last few years has allowed software using encryption to be exported when the encryption key is fixed not to exceed a given number of bytes. By modifying Ecce never to exceed this limit, a single distribution can be used both inside and outside the United States without jeopardizing the security of data and compute server passwords stored by Ecce.

31. The Linux port of Ecce required that the inter-process messaging between Ecce applications be redesigned as the Tooltalk technology included with the Sun Solaris and SGI IRIX operating systems is not freely available under Linux. An implementation of the standard Java IPC technolgy, Java Messaging System (JMS), named JORAM (Java Open Reliable Asynchronous Messaging, see

), was selected. A Java Virtual Machine is now embedded into the Gateway application to communicate back to the JORAM server residing on the same machine as the Apache web server. The Gateway application relays messages to all other Ecce applications through traditional socket technology which decreases the complexity and memory requirement for Ecce by not embedding a JVM in every application. A Java-based technology has the advantage of allowing future Ecce tools to themselves be developed in Java running as either web browser Applets or full Java applications. Both the Ecce server and application software environment now contain a customized version of the Java Runtime Environment (JRE) needed to run the JORAM messaging server and the Gateway client application. The Ecce JRE strips out components which aren't necessary to support JORAM such as the Java AWT and Swing GUI libraries. This significantly decreases the size of the Ecce distribution as the full JRE is very large. Because the Ecce server now consists of two components--the data server (Apache) and messaging server (JORAM)--scripts were added in the server ecce-utils directory to start and stop the combined Ecce server, named start_ecce_server and stop_ecce_server, respectively. These scripts must be run as the same user who installed the Ecce server.

32. The Ecce Apache web server now uses an Apache2 server, currently version 2.0.43, with built-in support for the WebDAV data management used by Ecce, rather than the previous Apache1 server where WebDAV was a plug-in module available separately. This further standardizes WebDAV as a core Apache server component, as well as simplifying the installation procedure for those sites wishing to compile the Apache server themselves rather than use the pre-compiled server bundled with the Ecce distribution. Ecce server administration scripts have been moved to a directory named ecce-utils under the top-level server installation directory rather than under the apache directory. A new script named ecce_htpasswd has been added into the ecce-utils directory for v3.0. It simply calls the standard Apache htpasswd utility passing the correct users file and setting the $LD_LIBRARY_PATH as required for Apache2. A utility for upgrading existing Ecce v2.0 and v2.1 server user data (calculations and structure libraries) to be compatible with the v3.0 server is also included in the ecce-utils directory when applicable. The installation process notifies the installer when and how to use this utility, named fix_all_sdbm_files. A low-level incompatibility between the WebDAV database SDBM files between the Apache1 and Apache2 versions of WebDAV mandates that this script be run before existing data can be read by a new Ecce v3.0 Apache2 server.

33. The siteconfig/DataServers file now has additional explanation for adding multiple servers. The concept that the first server listed is the "default" server where Ecce gets reference information including basis sets, and that all users of Ecce at a site must have an account created on that server is also covered.

34. The application software now includes the full NWChem and Gaussian 98 code registration user interface source code, as well as the existing Amica user interface source code, under the top-level codereg directory. This provides better samples for creating interfaces to newly registered codes. In addition, the file named properties, which used to be loaded on the Ecce server, has now been packaged with the application software in the data/client/config directory. This makes it possible to do all aspects of code registration by creating and modifying application software files rather than updating data stored on the Ecce server. Ecce code registration user interfaces now require the use of g++ 3.2, the same as the rest of Ecce. This version is not distributed by Linux operating system

vendors (no version of g++ is distributed by SGI or Sun) and will have to be downloaded and possibly compiled by any site wishing to do code registration.

35. The field labeled "Architecture" in the Machine Registration application, has been removed. It was no longer being actively used. The corresponding entries in siteconfig directory CONFIG.* files have also been deleted. Sites that have registered their own compute servers can either remove the "Architecture" value manually from CONFIG.* files, or just leave them as Ecce will simply ignore unrecognized directives.

36. In an ongoing effort to improve job monitoring reliability and robustness, the job exit status is now more accurately determined by eccejobmaster from the eccejobstore return value rather than indirectly from the .eccejobstore.status file, which is no longer created. The number of automatic job monitoring restarts is also conditionalized based on the time between restarts. Five monitoring restarts in less than 60 seconds is now recognized as a fatal condition where monitoring aborts, instead of just the previous 25 restarts over the duration of a job. Rapid successive restarts indicate that the job is hitting the same problem each time, and that continued restart attempts will likely fail as well.

37. The underlying remote shell communication done by Ecce can be logged to the shell window where Ecce has been started for diagnosing problems. Issue the command "setenv ECCE_RCOM_LOGMODE" before starting Ecce to enable this logging. An "unsetenv ECCE_RCOM_LOGMODE" will turn off remote communication logging. Any time problems are encountered related to remote operations done by Ecce, the first step to track down the problem should be to enable this logging. If problems need to be reported to ecce-support@emsl.pnl.gov, this remote communications debug output will often need to be supplied to the Ecce team. Version 3.0 takes further steps to guarantee the output will be complete and any passwords issued in remote operations will not be logged to the shell window.

38. With the addition of a new high performance Linux cluster within EMSL running LSF, the Ecce LSF integration has been enhanced since the initial release of v2.1. The new EMSL HP Linux cluster is named opus and is available for use within EMSL for users with accounts and to those external users who have completed the approval process and been granted machine time. The LSF job submission script template for this machine, which can be used as a template for registering other LSF compute servers, is in the siteconfig/CONFIG.opus file. Several older IBM SP compute servers within EMSL, including jupiter, ecs1, and nwtest, have been removed from the list of Ecce registered machines.

39. Simple support for multi-processor machines running Resource Management System, RMS, rather than a queue management system, has been added. Jobs are submitted with the prun command which is specified in the machine CONFIG.* file. These machines are registered as regular "shell" workstations where Ecce recognizes when the job actually starts by the existence of job output log files. Thus a job blocked from execution due to the required processors being allocated, will be displayed in the submitted state within Ecce.

40. The siteconfig/GLLimits.xml file is now used to configure limits on the number of simultaneous OpenGL viewers to display within the Builder Structure Library. This file allows more control in

specifying differences between versions of software such as Hummingbird Exceed/3D. The GLLimits.xml file contains more information about using this capability. The previous mechanism for setting these limits, variables in the siteconfig/site_runtime file, is no longer used.

41. Tracking feature usage of Ecce via email has been disabled for all external sites, alleviating any privacy concerns and simplifying the installation process.

What's Fixed?

1. A bug in the public domain Amulet GUI toolkit has been fixed allowing Ecce code registration theory and runtype details dialogs to be displayed from the Linux KDE window manager. This bug impacted running Ecce either directly on a Linux host or remotely logged in to an SGI or Sun and displaying back to KDE.

2. The square pyramidal geometry could not actually be selected and applied to an atom due to an internal name mismatch. This has been corrected.

3. A memory leak was causing the Builder to crash if the "Validate Structure" command was run on a very large system. The leak has been eliminated.

4. Trailing blanks in residue names, such as when a left justified atomic symbol is used for the residue name, were confusing the MD toolkit when searching for the corresponding segment or fragment file. The Builder now removes blanks from both sides of the residue name before looking for the segment/fragment files.

5. The function for prepending residues was not working correctly and was mixing up internal pointers. This resulted in garbled structures when using the structure library to build protein and/or DNA or RNA chains.

6. A long-standing bug with invoking the Basis Set Tool requiring two button pushes in the Calculation Editor under certain circumstances, has been fixed. The Basis Set Tool now comes up with the first button click in all instances.

7. All Ecce applications will uniconify when popup message dialogs need to be displayed. There are several conditions when these popups are displayed including exitting Ecce when there are unsaved changes and changing calculation context.

8. The Job Launcher no longer exits when requested by the user or when Ecce is quit from the Gateway while a job is currently being launched. It will immediately exit when it is safe to do so when the job launch is done and monitoring has been started.

9. Values displayed for electron affinities in the Periodic Table atomic data are no longer clipped such that they are difficult or impossible to see. Any clipped values can now be scrolled by selecting and dragging with the left mouse button, although this should not normally be necessary.

10. The name of the current application is now correctly passed to the web browser Feedback page when invoked from the Help menu of that application. This value is then used to set the default value for the application where the problem is being reported.

11. Hitting the Help button for dialog windows no longer causes application crashes for those windows where only the default online help page should be displayed. A bug related to invoking the "fallback" web page resulted in crashes when no specific help web page has been created for the window. These Help buttons now properly map to the fallback main Ecce online help page.

12. Memory management problems related to the initial Gateway passphrase prompt dialog have been fixed. These would cause Ecce to exit either during or after entering a passphrase.

13. Absolute paths to remote shells can be specified in the siteconfig directory remote_shells.site file. Previously the slash, "/", delimiter between directory names was recognized as the separator between a remote shell and remote copy command when not using the default remote copy command corresponding to each remote shell command (e.g., ssh/ftp). The new separator between remote shell and copy commands is now a backslash, "\" (e.g., ssh\ftp). Absolute paths in remote_shells.site file commands can be used, for instance, to override the version of a command that would normally be found with a user's $PATH variable.

14. Improvements and bug fixes were made to the parsing and storing of calculations with large orbital data sets. This is especially recognizable when importing calculations. For example, calculations with 1000+ basis functions can now be imported in a minute or two depending on system and network configurations.

15. The Calculation Viewer normal mode panel has been increased in size to show up to seven frequencies at a time. Previously, only three were visible.

16. The Calculation Viewer now computes molecular orbitals correctly for systems with generally contracted basis sets. Previously, the MO computation was incorrectly optimizing their contractions (in some cases, certain 0.0 coefficients were being omitted). Other basis sets were not affected by this error.

What's Broken?

1. If you are viewing molecular orbitals as a calculation is currently running, the coordinates might not match the orbitals.

2. You must manually refresh the geometry table after using the bond rotator or the atom manipulator to update the coordinates.

3. The sphere radius selection mechanism in the Molecule Builder, which is initiated by clicking and dragging on an atom, currently does not work.

4. Display of aromatic rings in the Molecule Builder and Calculation Viewer is disabled. Double and triple bond displays are still supported.

5. Do not try to select atoms to use with measures while a calculation property is animating. Press stop, select the atoms you are interested in, and then start the animation again.

6. There has been an ongoing X Windows Server resource problem on SGIs where allocating colors and/or pixmaps can fail. This is dependent upon the X server resource requirements for all applications currently being run, Ecce applications and others, and the hardware (model, memory, graphics card) configuration of the workstation. Usually, a series of X Windows allocation failure warnings will be printed to the window where Ecce was started and you may notice certain colors/pixmaps are missing from applications. However, it is also possible for applications to crash from the failure to allocate colors or pixmaps. The workaround to this is to close any unneeded applications, both Ecce applications and others--especially those which allocate many colors such as Netscape. Logging out from the workstation (thus shutting down the window manager session), and then back in again, is another means to free up resources.

7. There is a known bug where the access_log file for an Apache web server running on an SGI will not show correct IP addresses for clients connecting but show 255.255.255.255 instead. This is not something the Ecce team can fix. According to reports, it is a deficiency in the IRIX libraries/compiler so SGI will need to resolve this. If you are concerned, please consider using a data server running on Linux or a Sun.

8. Ecce now uses the open source version of Open Inventor for all platforms. The fonts for atom and bond labels in the Builder and Calculation Viewer appear garbled in the Solaris distribution.

9. The "Float" and "Unfloat" menus associated with each property panel in the left pane of the Calculation Viewer are currently disabled in the Solaris distribution.

10. The property panels in the left pane of the Calculation Viewer do not automatically resize to fit the width of the pane on Linux. The scroll bars can be used or resize the Calculation Viewer and use the pane resize sash (small green box on the vertical line) to adjust the relative sizes of the left and right panes.

11. Graphics support on Linux will vary depending on your graphics card and driver. Graphics overlays, used to display the lasso during lasso selection in the builder, currently do not work. The lasso selection mechanism works but the lasso will not be visible. Other potential problems include non-functional dialogs for setting foreground and background colors and possible crashes when trying to use the Structure Library. In the latter case, see the release note on OpenGL hardware limits here. If you experience these or similar problems, check the availability of a more recent graphics driver for your hardware.