

Ecce Version 3.1 Release Notes – August 15, 2003

EMSL Release - August 20, 2003

The intent of this page is to provide information specific to version 3.1 of Ecce. Version 3.1 contains a redesigned code registration user interface toolkit along with numerous other enhancements and bug fixes since the initial v3.0 release supporting the Linux operating system.

Note: Ecce version 3.1 requires NWChem 4.0 or newer (NWChem 4.5 preferred) due to changes in the NWChem input and output file formats.

Release Notes for Recent Previous Versions

[Version 3.0 Release Notes – November 13, 2002](#)

[Version 2.1 Release Notes - February 11, 2002](#)

[Version 2.0 Release Notes - July 17, 2001](#)

WHAT'S NEW

Debian Linux Support

(9/15 patch) Support has been added for the Debian Linux operating system. However, the current "stable" version of Debian that was released in December 2002 is not compatible. A kernel upgrade is required to run Ecce. The stable release kernel version that does not work with Ecce is 2.2.20. You must run at least the 2.4.20-3 kernel. We have also successfully tested 2.4.21-4. If you install and run Ecce with a kernel that is too old, you will see error messages like the following when starting the Ecce server or applications:

```
relocation error:/lib/libc.so.6:symbols __libc_stack_end, version GLIBC_PRIVATE not defined
```

This is an immediate indication that you must update your kernel if you wish to run Ecce. Once the kernel is updated, both the Ecce server and applications should run normally. The default kernel that comes with the current "test" release of Debian named "Sarge" also requires this kernel upgrade. The "apt-get" program can be used to upgrade the kernel. Ecce has also been successfully run under Knoppix, which is derived from Debian and allows Linux to be booted from a CD rather than installed on hard disk.

Data Access Control

(9/15 patch) Users can now selectively grant read or read-write access to other users for their data maintained on the Ecce data server without giving out their password. A new tab on the Calculation Manager Preferences dialog labeled "Access Control" has two type-in fields for specifying a list of "Read-Only" and "Read Write" users. By default only the owner of the data has read-write access. Granting access to other users changes the .htaccess file on the web server, which remains in effect between Ecce sessions until changed through this same dialog. At this time it is only possible to set access for the extent of a user's data rather than at a sub-project level. This feature is implemented on the

server by a cgi-bin script that must be run by an authenticated user to avoid the possibility of hijacking data.

Linux Vendor Support

Version 3.1 of Ecce has been tested on PCs running the following varieties of Linux:

- Redhat 7.3, 7.2, 7.1, 7.0 (Ecce is currently compiled under Redhat 7.3)
- Redhat 9
- Redhat 8
- Redhat 6.x
- Mandrake 8.x (Mandrake 9.x not yet tested)
- ALT Linux 2.x

You are welcome to try running Ecce under Linux from other vendors and report back the results to us. At this time, only Redhat 7.x and Redhat 9 are supported by the Ecce team.

Molecule Builder Distribution

The Ecce Molecule Builder can now be downloaded and installed as a standalone application independent of the other Ecce application and server software. All features supported in the Builder when used with the rest of Ecce are also available in the standalone version. The Structure Library files are included with the standalone Builder installation under the data/client/StructureLibrary directory rather than being located on the Ecce server. The File menu “Import...” and “Export...” options are used to open and save chemical systems. Builder installation documentation separate from the full Ecce installation documentation is available at <http://ecce.emsl.pnl.gov/docs/Builder-2864B-Install.pdf>. Installing and maintaining the standalone Builder is significantly easier than the full Ecce distribution as there is no data and messaging server. Online help for the standalone Builder uses the public web server located within EMSL at Pacific Northwest National Laboratory and thus, may be quite slow dependent upon your internet connection and distance from PNNL. Those sites seeking a three-dimensional direct manipulation molecule building capability and not interested in graphical interfaces for setting up, running, and viewing the results from electronic structure calculations are strongly encouraged to install the standalone Builder instead of the full Ecce software suite.

Online Help Updated

The web-based online help, available from all Ecce applications under the “Help” menu and with the “F1” key for context sensitive help, has been updated for v3.1. In addition to documenting new functionality for v3.1, the left-hand navigation frame has been reworked to eliminate references to functionality that was never implemented. The Ecce online help should be used as the primary means for users to learn about Ecce, being far superior to typical application help systems.

PyQt Details Dialogs

The Calculation Editor code registration details dialogs have been re-implemented using the PyQt toolkit. These PyQt details dialogs replace the C++ Amulet toolkit dialogs used in past releases of Ecce. PyQt (<http://www.riverbankcomputing.co.uk/pyqt>) is the Qt C++ cross-platform GUI development framework (<http://www.trolltech.com/products/qt>) wrapped with the Python scripting language (<http://www.python.org>). Python classes for different interface objects (i.e. FloatInput, IntegerInput, MenuInput, ToggleInput, etc.) were written by the Ecce team specifically for creating details dialogs.

This conversion to PyQt was undertaken for several reasons. Foremost, all aspects of code registration can now be done through script files rather than any compiled code. As the user base of Ecce increases it is expected that sites using Ecce will contribute to code registration to a greater extent than in the past. Also, future development of capabilities for users to extend Ecce will likely be based on Python scripting so the use of a GUI toolkit embedded in Python for code registration was a natural choice.

Users of Ecce should only notice subtle changes in appearance and behavior between the old Amulet and new PyQt details dialogs for the currently registered computational codes. For instance, it is no longer necessary to hit the return key for a new numeric or text input field value to be processed. Like other Ecce applications, moving the cursor out of the field is now sufficient. Also, the clumsy “+” and “-“ buttons to resize the Amica theory dialog have been eliminated as PyQt works correctly with resizing windows through the window manager controls.

Those registering codes to Ecce will find the new PyQt-based design more intuitive and faster to use than the Amulet implementation. A preliminary version of the Ecce code registration document updated for PyQt is now available at http://ecce.emsl.pnl.gov/docs/2864B-code_reg.pdf. The directory named codereg under the top-level Ecce application software installation contains the NWChem, Gaussian-98, and Amica details dialogs used by the Ecce Calculation Editor. These can be referenced as examples for creating new details dialogs. The PyQt interface object classes used for building details dialogs are in the templates.py file in the same directory. For the Ecce v3.1 release, Python version 2.3, Qt version 3.2.0, and PyQt version 3.7 are deployed with Ecce.

Alternative Setup Workflow

In addition to the standard Ecce workflow model of creating a calculation in the Calculation Manager and then using various tools to complete the setup, users can now start with the Builder and use the "Save As" menu item to create a calculation and then continue with the normal calculation setup process. We have found many users predisposed to favor interfaces where the chemical system is defined immediately due to familiarity with other packages using this workflow. This feature simply allows those users to work in this mode within Ecce.

Machines Added and Dropped

The registered machines included in the Ecce distribution now include the new EMSL HP Linux 1900 Itanium2 processor, 11+ teraflop phase 2 cluster, mpp2. The phase 1 cluster, opus, is now out of operation and has been removed from Ecce. As with opus, mpp2 uses the LSF queue management system. The Ecce mpp2 registration runs NWChem (Gaussian is not available) on the processor local “/scratch” file system yielding much better performance than with opus. The mpp2 registration is visible to external sites running Ecce as mpp2 is available to projects with approved EMSL Grand Challenge proposals.

The EMSL Pentium Xeon cluster named legion, running Sun Grid Engine, has been registered for EMSL users.

The EMSL Dell Linux cluster named colony has also been removed from Ecce as it is no longer available to EMSL users. The NERSC Cray, mcurie.nersc.gov, has been removed from Ecce as that machine is no longer in service. Finally, the EMSL compute servers mpp1 and mulliken have been removed as those resources are no longer in service.

Builder Performance

As part of initial efforts to add support for molecular dynamics calculations, a number of performance and memory management enhancements have been added to the Builder. Users can now control the limit at which undo stacks are maintained by setting the environment variable `$ECCE_BUILDER_UNDO_MAXATOMS`. If not specified, it defaults to 5000 atoms. The Builder has been successfully tested rendering 1,000,000 atoms (wireframe) on a Linux workstation with an ATI Fire GL X1 graphics card. Results will vary depending on your graphics hardware and driver.

System Error Run State

A new calculation run state, “system error”, has been added. This is used to distinguish particular types of job monitoring failures from the catch-all “monitor error” state. By default the “system error” state is displayed as a black diamond. The intent is that failures related to the current state of the compute server, such as the machine going down, be reported as a “system error”. At this time only a failure to maintain a connection to a compute server, either due to the network or server itself being unavailable, will be reported as a “system error”. All other types of failures will be reported as a “monitor error”. An important benefit of this new state is that it allows the Ecce team to determine which failures should be investigated more thoroughly due to the possibility of an Ecce job monitoring implementation bug. Within EMSL all “monitor error” failures are automatically reported to the Ecce support queue.

Molecular Orbital Energy Plot

The MO visualization panel in the Calculation Viewer has been extended to include a graph option that displays an energy level diagram. Closed-shell calculations with no symmetry show a single column of energy levels, open-shell unrestricted calculations without symmetry show separate alpha and beta energy levels, and calculations with symmetry show energy levels for each irreducible representation. There is also an option to collapse energy levels back down to a single column.

POV-Ray Image Export

An option for exporting POV-Ray formatted image files was added to the Builder and Calculation Viewer. POV-Ray files can be used to generate publication quality images. The POV-Ray files include all atoms and bonds, molecular orbitals, and any vectors, such as normal modes or energy gradients. The POV-Ray files reproduce views that are close to the views seen in Ecce, but there may be some minor differences. Users interested in creating graphics based on the POV-Ray files will need to download a copy of the POV-Ray graphics processor. More on POV-Ray can be found at <http://www.povray.org>.

Chemical System Import Formats

The Builder now supports the import of the following chemical system formats: PDB, XYZ, MVM, Alchemy, Ball and Stick, Chemical Markup Language, GAMESS Output, NWChem Output, Q-Chem Output, and UniChem XYZ.

Chemical System Export Formats

The Builder and Calculation Viewer now support the export of the following chemical system formats: PDB, XYZ, MVM, Alchemy, Ball and Stick, Chemical Markup Language, Fenske-Hall Z-Matrix, GAMESS Input, Gaussian Input, NWChem Input, Q-Chem Input, SMILES, and UniChem XYZ.

NWChem ESP Runtime

An ESP runtime was added to the NWChem Calculation Editor. This runtime is designed to assign partial charges to atoms by fitting them to the electrostatic potential obtained from the ab initio electronic density obtained using an RHF theory calculation. This runtime is supported by the new Partial Charge Toolkit in the Builder. The toolkit can be used to assign atom constraints and visualize constrained atoms. The Calculation Viewer has also been extended to include a partial charge visualization tool, similar to the Mulliken population analysis panel, that allows users to visualize the results of the different electrostatic fits and to copy the partial charges back to the original structure so that they can be used in further calculations. Partial charge data is extracted by Ecce from the <Calculation>.q file generated by NWChem. More on ESP calculations can be found in the online help and the NWChem documentation.

NWChem Property Runtime

A Property runtime was added to the NWChem Calculation Editor. At the current time, this runtime only supports calculation of NMR shielding constants. Other properties will be added in future releases of NWChem and Ecce.

Calculation Viewer Vectors and Tensors

The Calculation Viewer has been extended to support visualization of several new vector and tensor quantities. In addition to the dipole moments and normal modes, energy gradients are also displayed as atom-centered vectors, when available. Tensor quantities, such as the quadrupole moment, polarizability, or NMR shielding tensors, are displayed as a triad of orthonormal bipolar vectors oriented along the principle components of the tensor and scaled by the corresponding tensor eigenvalue.

Globus Toolkit 2.4

Support for Globus, <http://www.globus.org>, has been upgraded to Globus Toolkit 2.4 (2.2 also supported). A new parameter named “globusContact” has been added to the CONFIG.<machine> files in the application software siteconfig directory. The value for the globusContact parameter is the “Globus job manager” suffix used to submit jobs to that machine. For non-queued machines this does not normally need to be specified. A typical globusContact value for a machine named mpp2.emsl.pnl.gov running LSF, for example, could be “jobmanager-lsf”, in which case the full Globus job manager specification generated by Ecce is “mpp2.emsl.pnl.gov/jobmanager-lsf”.

A new hybrid Globus and ssh job launching facility was also added for Ecce v3.1. If only Globus is used for launching jobs then a patched version of ssh/sshd supporting GSI authentication (maintained by NCSA) must be installed and run to launch Globus jobs through Ecce. Since running a non-standard version of ssh was problematic on production compute resources, the Globus-ssh hybrid job launching is now supported. In this case remote communications such as file transfer and job monitoring are done with regular ssh while also using the Globus job submission command, globusrun. When registering a machine, select “Globus-ssh” as a remote shell to support this hybrid job launching. Selecting just “Globus” as a remote shell specifies that the patched GSI version of ssh is also being used. With Globus-ssh job launching two passwords are specified for machine configuration. One is the ssh authentication password and one is the Globus proxy pass phrase. Only a single password is specified for pure Globus job launches as the patched GSI ssh accepts the Globus proxy pass phrase for authentication.

Job monitoring for Ecce Globus launches has been enhanced by more closely following the intent of Globus and issuing job status commands, “globusrun –status”, from the client side rather than the compute server. Previously in keeping with the Ecce job monitoring architecture for other queue

management systems, all status commands were issued on the compute server. This change means that Ecce no longer issues any Globus commands directly on the compute server.

Support for two additional Globus RSL directives was added to Ecce: `maxMemory` and `hostCount`.

Calculation Manager Copy/Paste

The Calculation Manager now supports copy/paste or drag and drop operations across data servers or authentication realms. This is useful to move data from one server to another (for sites using multiple data servers) or to copy data to the share area for others to view.

Changing Passphrases

Originally deployed as a patch to Ecce v3.0, 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 that 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.

Bourne Shell Users

Originally deployed as a patch to Ecce v3.0, 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`.

2D Graph Manipulation

The two-dimensional XY graphs used in the Calculation Viewer support zooming, translation, and step-wise restoration of previous views. A balloon help icon in the lower left corner of each graph provides a brief description on how to use these features. To zoom in, hold down the Shift key while using mouse to draw a zoom rectangle. Pressing the 'r' key will revert to the previous view. Additionally, the left, right, up, and down arrow keys can be used to move along the x and y axis. Pressing the 'r' key will return to the default view.

Builder New Features

A number of minor features have been added to the Builder including:

- an option (in the Options menu) to turn off molecule “spinning”
- camera style (orthographic or perspective) is saved as a user preference
- x, y, z coordinates can be edited in the geometry table
- the chemical system is no longer automatically centered around the center of mass when imported from a file or structure library. Instead, users are responsible for initiating the centering operation via a menu

item under the Options menu. This was causing problems if systems were broken up into small pieces and subsequently recombined

- several different choices for atom labels are now available. Users can choose to display the old style labels, atom names, atom types, or charges. If the information has not been assigned, the label will be empty
- the geometry table now includes an option to sum the partial charges
- options for interpreting the atom coordinates as either pico or nano meters have been added to the import dialogs and the Trajectory Toolkit

Builder Trajectory Toolkit Files

The Builder trajectory toolkit now supports the use of regular expression characters '*' and '?' to view a sequence of NWChem molecular dynamics trajectory .trj files. For example, given a set of files md001.trj...md015.trj, a specification of md*.trj will sequence through the files.

Builder Trajectory Toolkit Reset

An option in the Trajectory Toolkit now allows the user to request that the scene graph be completely reset between each frame. While this can reduce performance, it is useful in cases where the number and type of atoms may change between frames. An example is a trajectory with a solute along with the waters of solvation.

Builder Trajectory Toolkit Bonds

When viewing a trajectory file(s) in the Builder, users can now request that bonds be recomputed at each step to show the formation or breaking of bonds.

Calculation Viewer Log Scales

All graphs in the Calculation Viewer now have the option to view the graph using a linear scale, a log scale if the values are positive numbers or a log scale using the absolute value if the data contains negative but non-zero numbers.

Calculation Viewer Capture Dialog

The Capture dialog in the Calculation Viewer now supports the specification of width and height of each frame (in pixels). This capability can be used to create a set of small GIF files that can then be readily converted to an animated GIF for web page content.

Calculation Name Labels

Names of calculations displayed near the bottom of applications like Builder, Calculation Editor, and Calculation Viewer, now show the name of the data server in URL format rather than just the path to the calculation. Previously the names contained no information about the data server (always starting with "/Ecce") and could have been ambiguous if multiple servers were configured.

Lab Notebook Dropped

Removed support for the former EMSL Collaboratory project Electronic Lab Notebook (ELN) from Ecce. The code for supporting ELN had long since become obsolete from changes in the ELN architecture. Due to lack of demand in using the Ecce-ELN integration, support was dropped rather than updated to the latest ELN design. Should there be significant call for this functionality in the future, it will be added back into Ecce.

Spherical Basis Set Polarization

An attribute named “noSpherical” has been added to the code registration .edml file so each runtime can be parameterized by whether spherical polarization components are supported in the input file basis set specification. By default the noSpherical attribute is false indicating that either Cartesian or Spherical polarization components can be used. Specifying noSpherical as true in the .edml file, as with the new NWChem Property and ESP runtypes, causes only Cartesian polarization to be used. If the polarization was previously set to Spherical in the Basis Set Tool and the runtime is then changed to one only supporting Cartesian, the Basis Set Tool will be properly updated with Cartesian polarization the next time it is invoked for the calculation. The Calculation Editor summary field for the basis set polarization also indicates what will be used in the input file.

Input File Storage

At the time a calculation is launched, the input file may have to be post processed to add machine specific information or directives. Previously these changes were made only on the compute server. Now they are stored back to the data server. In addition, titles are now updated during this processing to correct any inconsistencies that could occur due to copying and pasting of existing calculations.

SITE ADMINISTRATOR WHAT’S NEW

Upgrading Previous Releases

With the release of Ecce v3.1, installation upgrades from releases of Ecce prior to v3.0, i.e., v2.0 and v2.1, are no longer supported. If you do have a pre-v3.0 release where you wish to use the calculations and machine registrations created with that release, you must first install Ecce v3.0 specifying an “upgrade” from the main installation menu. The v3.0 release will be available as a special request to ecce-support@emsl.pnl.gov for the first couple months after the v3.1 release is made. Once the upgrade to v3.0 is done each user wishing to run Ecce v3.1 must start v3.0 once in order to upgrade the format of their ~/.ECCE/MyMachines file. Alternatively, the ~/.ECCE preferences directories for each user can be manually deleted and created from scratch when v3.1 is first run. Finally, Ecce v3.1 can be installed, specifying an “upgrade” from the Ecce v3.0 installation just completed. The complexity and limited demand for supporting upgrades from arbitrary past releases of Ecce has led to this policy of directly supporting upgrades only from the most recent production release.

Auto Server Account Creation

Originally deployed as a patch to v3.0, 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/siteconfig/site_runtime 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.

A feature added since the v3.0 patch is automatically sending email to the configured Ecce feedback email address whenever a new server account is created by the cgi-bin script. This allows the Ecce site administrator to monitor who is accessing Ecce at their site (the first login only) without having to disable the automatic account creation feature.

Machine Registration Examples

The application software siteconfig directory now includes a sub-directory `CONFIG-Examples` that contains files for each type of queuing system officially supported by Ecce. As a result of these new examples, Ecce installs with fewer pre-configured machines; only those machines truly available for external use are included.

Sun Grid Engine

Added support for the Sun Grid Engine, <http://gridengine.sunsource.net>, as a queue management system. The application software siteconfig/`CONFIG-Examples/CONFIG.sge` file is an example of a configuration file for a compute server running Sun Grid Engine, referred to as SGE in the file and the Machine Registration application. The example uses MPI to launch NWChem jobs although that is specific to the compute server configuration and not tied to the use of SGE.

Apache Upgrade

The Apache web server (<http://www.apache.org/httpd>) for Ecce v3.1 has been upgraded to the most recent production version, Apache 2.0.47. This fixes several critical security related vulnerabilities in Apache. For this reason and other data and messaging server enhancements, it is important that both the Ecce v3.1 application and server software be installed for those sites upgrading from a previous Ecce release.

Data Server Superuser

Added a “superuser” capability for the Ecce data server so that this user can access data maintained on the server for all users as necessary. To create a “superuser” for the Ecce data server, run the `add_ecce_user` script with `ecceadm` as the “User name”. For security reasons the `ecceadm` account cannot be created automatically with the cgi-bin script by running Ecce as is possible with normal data server accounts. Further, passwords are never updated automatically even if you are running Ecce client applications as the `ecceadm` user and change the passphrase. The `ecce_htpasswd` script must be used for password changes for `ecceadm`. The “require” statement in each users’ `.htaccess` file has an entry for both their user name and `ecceadm`. This allows an authentication to the web server as `ecceadm` to be equivalent to the user authenticating. If you are upgrading from a pre-v3.1 version of Ecce and need to access web server data for existing users, `ecceadm` must be manually added to the “require” statement of each `.htaccess` file.

Multiple Data Servers

For those sites wishing to run multiple Ecce data servers there are now scripts for starting and stopping just data servers without the Ecce messaging server. The messaging server should only be run on a single machine while data servers can be run on any number of machines. On the machine that is the main Ecce server (both data and messaging server), the “start_ecce_server” and “stop_ecce_server” scripts in the ecce-utils directory are used to start and stop the server. On other machines acting as data servers only, the “start_ecce_data_server” and “stop_ecce_data_server” scripts in the same directory should be used instead. Running multiple data servers at a site is not a typical configuration although there are valid reasons for doing so, including lack of disk space on a single server to store all user data and allowing external access to one data server for collaborations while closing off another.

tcsh Support

In addition to the csh shell, Ecce now supports the tcsh command shell for remote and local communications. When Ecce uses a remote shell command like ssh or telnet, it always creates what was a csh shell within that session in order to issue commands and process output. However, it was found that specific platforms did not work reliably with csh where switching to tcsh seemingly fixed the problems. Thus, machines can now be registered to use tcsh (csh remains the default) by manually editing the CONFIG.<machine> file in the application software siteconfig directory. A new parameter named “shell” has been added where the only accepted values are csh and tcsh. For example, add the line “shell: tcsh” in the CONFIG.<machine> file to use tcsh instead of csh for a machine. It is recommended that csh be used unless problems are encountered.

Machine sourceFile Directive

Added an option to source an environmental setup file for a compute server. The “sourceFile” directive specified in the CONFIG.<machine> file in the application software siteconfig directory is used for this. The value of the “sourceFile” directive is the name of the file that is sourced whenever remote communications are established to launch a job, start a remote shell, etc. This feature is commonly used for setting paths to commands including the queue management system. It allows Ecce to be responsible for setting up the environment to run computational jobs rather than each individual user, who may know very little about the configuration of a particular compute resource. The siteconfig/CONFIG-Examples/CONFIG.lsf file contains an example of the “sourceFile” directive.

Customized Proxy Authentication

Sites can now customize proxy authentication commands required for remote shells. The remote_shells.site file in the application software siteconfig directory documents how this is done. Some remote shells, such as Kerberized rsh, require a proxy authentication command, kauth in this case, be issued before establishing a remote connection. By specifying the syntax of the proxy command in the remote_shells.site file, users are freed from issuing these commands themselves outside of Ecce.

Remote Copy Preserve Flag

Eliminated the use of the “-p” preserve flag for remote file copy operations. This was primarily to make it easier to diagnose job monitoring problems by knowing when files were copied, rather than preserving the creation date on the original source file. The side effect of this change is that file permissions are also changed to the default for the user running Ecce. It is believed that this will not result in any problems. The application software siteconfig/remote_shell.site file documentation has been updated to indicate that the “-p” flag is no longer necessary for defining new remote copy commands.

MOLECULAR DYNAMICS WHAT'S NEW

Builder Partial Charges Preserved

Modified "create residue" functionality in the Builder MD Toolkit so that it now preserves partial charge and other information.

Builder MD Toolkit Add Hydrogens

The "Add Hydrogens" button in the Builder MD Toolkit was extensively modified to improve performance. The old algorithm had an internal nested loop that was severely degrading performance for large systems.

Builder Residue Table Selection

Selections work correctly in the Builder MD Toolkit Residue table, even if it has been sorted.

Builder Environment Index

An environment index was added to the list of atom attributes and can be edited via the geometry table in the Builder. This attribute is used in molecular dynamics simulations to identify atom centers that may contain improper dihedral functions.

WHAT'S FIXED

Data Server non-English Incompatibility

(9/15 patch) Fixed bug with being able to create projects and calculations on an Ecce data server for installations of Linux using a language other than English. With certain other languages, Ecce was not able to construct a valid date and time value to put on the data server. This invalid date/time specification would result in Apache server failures trying to create projects and calculations. Within Ecce the language setting, or "locale", is now set to English whenever creating date/time values fixing the problem.

Calculation Viewer Resizing

The property panels within the left pane of the Calculation Viewer are now properly sized to fit exactly in the pane eliminating nested scroll bars. Property panels in the left pane now also have height limits.

Sun Compiler Changes

With v3.1, the Solaris build of Ecce is again using the Sun CC compiler (studio 7) rather than the GNU g++ compiler. This eliminates the need to use statically compiled libraries thus reducing system memory and swap requirements. Thus, the Sun version of Ecce is no longer a special request for v3.1.

Sun Graphics Overlays

Problems have been reported with using graphics overlays on some Sun hardware graphics platforms (e.g. Elite 3D Lite). The problem is with detection of the transparent pixel color. A multi-phased approach for determining this pixel value has been put into place. If it cannot be detected, a message will print to the terminal where Ecce was started instructing the user how to disable the use of overlays. Overlays are only used to draw the lasso selection box. The lasso selection mechanism functions even if the overlay is not used--however the lasso is not drawn.

Calculation Imports Without Basis

Calculation imports no longer fail due to the basis set not being found in the output log file. Previously the import would abort immediately. Now the import is allowed to finish and properties can be seen in the Calculation Viewer. Of course, molecular orbitals cannot be parsed since they are dependent upon the basis set definition.

Socket Job Monitoring Failures

Communications problems were found at certain sites when using sockets for monitoring job output. For v3.1 all job monitoring defaults to using remote shell communication (ssh, telnet, etc.) to circumvent this type of problem. The application software siteconfig/site_runtime file ECCE_JOB_COMMS setting defines the type of job monitoring communication used for an Ecce installation.

Details Dialogs CPU Usage

Calculation Editor details dialogs under Linux were chewing up all available CPU time when they were invoked due to an incorrect implementation of a standard X Windows function that waits for and reads input from a file. The Ecce design was switched from files to UNIX pipes, which circumvents the bug.

Babel Chemical System Typing

A logic error when reading and writing chemical system files using the babel utility software would have caused failures on certain file formats prior to v3.1.

Calculation Manager Copy/Paste or Move Failure

When using deeply nested projects and/or long project and calculation names in the Calculation Manager, it was possible to overrun a memory buffer causing a paste or move operation to fail. This has been fixed.

Remote Copy Command Incorrect

The remote shell and copy command specification allowing both the shell command and the copy command to be specified separated by a “/” was incorrectly implemented. It was ignoring the remote copy command and using the default for the specified remote shell. For instance, if “ssh/ftp” was specified, scp would actually be used since it is the default for ssh when no remote copy command is specified. The correct remote copy command is now used, ftp in this case.

Builder Clean Failures

Fixed some cases of runaway Builder UFF clean operations, particularly the case of two non-bonded atoms that are initially placed close to each other.

Job Monitoring Fixes

Made several changes to improve robustness of Ecce job monitoring. Diagnosed and fixed occasional problems with opening and writing the client-side temporary file used to store raw property data sent from the compute server. Fixed a bug with the Perl “tell” function not working correctly on certain Linux platforms by manually keeping track of bytes read in the output log file.

Redhat Linux Printer List

The method for determining the list of printers available on a Linux box has changed. As of Redhat 7.3, the old mechanism could take minutes to complete. Printer management may vary for different versions of Linux. The current implementation has been tested with Redhat 7.x and 9.

Open Inventor Font Fix

The Linux and Sun fix for specifying fonts for the Open Inventor library has been redone. Previously a symbolic link was created named /tmp/ecce_openinv_fontfix. Unfortunately, the link could not be deleted by users on a system, except by the one who initially ran Ecce creating the link. Now /tmp/ecce_openinv_fontfix is a directory with the font files copied into the directory eliminating permission problems and dangling links. This eliminates warnings often seen when starting Ecce regarding not being able to remove /tmp/ecce_openinv_fontfix.

Ecce Startup Scripts

The ecce startup scripts have been cleaned up to ensure that minimal environment variables are put into the user's environment. The past couple releases of Ecce had added a few extra variables although Ecce has always been designed to have a negligible impact on a user's environment.

Message Dialog Closing

It was previously possible to close certain popup message dialogs using the window manager close controls rather than the buttons on the dialog itself, and send the Ecce application into an infinite hang. This was fixed by mapping the window manager close to the proper dialog button action.

Builder and Calculation Viewer Menu Accelerators

The Calculation Viewer and Builder menus now have identical keyboard accelerators.

Two-dimensional Table Appearance

All two-dimensional tables of data in Ecce have been made consistent in appearance including the usage of fonts and colors.

MOLECULAR DYNAMICS WHAT'S FIXED

SGI Bad Fragment/Segment Files

Fixed bug that was resulting in garbled atom names and atom types to being written to fragment and segment files on SGIs.

Builder Add to Residue

Fixed bug in Builder Structure Library that was causing a crash if a structure was being added to a residue while the Edit residue box was checked.

Builder Residue Nubs

Fixed Builder atom editing so that nubs are always added to the parent atom's residue.

Builder Hydrogen Randomization

Fixed bug in the Builder automatic randomization of the orientation of molecules with a single heavy atom (e.g. water) when using the MD Toolkit "Add Hydrogen" button. The bug was resulting in incorrect bond angles between hydrogen atoms after the randomization.

Builder Empty Residue Deletes

Fixed bug in Builder delete that was causing system to lose track of the residue structure if residues containing no atoms were present in the system.

WHAT'S BROKEN

XML Property Parsing

Due to an upgrade of the XML parser in Ecce, some calculations that were completed with earlier versions of Ecce may not be able to be displayed in the Calculation Viewer due to unrecoverable errors in the XML parsing. The Calculation Viewer will startup but will exit with the text message

XML Parse FATAL error - Line: x Column: y
Look for unmatched tags - matches are case sensitive

in the terminal window used to start Ecce. The values for x and y will be filled in with the appropriate line and column numbers. One straightforward solution, assuming there are only a few calculations that exhibit this behavior and the calculations still exist on the compute server, is to select "Reconnect Job Monitoring" in the Calculation Manager for any calculations having this problem and re-parsing output. A second solution is to import the calculation back into Ecce using the Calculation Manager. However, if there are several calculations that can't be displayed in the Calculation Viewer or it would be too costly to rerun the calculations then please report the problem to the Ecce team so we can work with you to resolve the parsing issues.

The Ecce production data server within EMSL, avatar, has been scanned for these problems with the offending files patched. Therefore only external sites are likely to experience this problem.

Compound Basis Set Exporting

Certain compound basis sets in the NWChem basis set library have been incorrectly merged into a single basis. This causes problems when Ecce tries to display MOs for calculations using these basis sets. To correct this, Ecce exports these basis sets as complete lists of exponents and coefficients, even if the toggle for exporting explicit basis sets has not been set in the basis set tool. Any basis sets containing "aug", "d-aug", or "-pcv" exhibit this problem.

Linux OpenGL Support

Graphics support on Linux will vary depending on your graphics card and driver. Graphics overlay, used to display the lasso during lasso selection in the builder, does not work with all graphics drivers. 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.

Intermediate Molecular Orbitals

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

Builders Geometry Table Refresh

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

Sphere Radius Selection

The sphere radius selection mechanism in the Builder, which is initiated by clicking and dragging on an atom, currently does not work. Display of aromatic rings in the Molecule Builder and Calculation Viewer is disabled. Double and triple bond displays are still supported.

Measures While Animating

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.

SGI X Window Resource Allocation

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.

SGI Apache Access Log

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.

Sun Open Inventor Fonts

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.

Sun Calculation Viewer Hangs

The Calculation Viewer on Sun can go into an infinite hang in a number of situations. Most commonly, this will happen when first opening the Calculation Viewer. To terminate the process, issue a "ps -ef | grep calcviewer" command and use the kill command with the appropriate process ids.