ECCE VERSION 3.2.x RELEASE NOTES

v3.2 – May 10, 2004
v3.2.1– July 8, 2004
v3.2.2– February 9, 2005
v3.2.3– July 28, 2005
v3.2.4– October 26, 2005
v3.2.5– April 5, 2006

The intent of this page is to provide information specific to the 3.2.x versions of Ecce. Version 3.2 contains new molecular dynamics structure setup functionality in the Builder, Gaussian 03 support, and numerous other enhancements and bug fixes since the v3.1 release. Version 3.2.1 contains new Builder toolkits for specifying structural constraints and setting up QM/MM jobs. Masses can also be set per atom and several other bug fixes have been made since the v3.2 release. Version 3.2.2 supports newer Linux operating systems such as Red Hat Fedora Core 3, as well as bug fixes and minor enhancements. Version 3.2.3 adds support for NWChem 4.7 including the Property runtype with new Calculation Viewer visualizations and other features. Version 3.2.4 contains updated basis sets and a fix to calculating molecular orbitals among other minor enhancements and fixes. Version 3.2.5 supports GAMESS-UK release 7.0, with the code registration performed by the Daresbury Laboratory Quantum Chemistry group that maintains GAMESS-UK. Release notes for versions 3.2.1, 3.2.2, 3.2.3, and 3.2.4 are indicated by the version number in parentheses preceding the description. Those notes without a version number are for changes made in version 3.2. Version 3.2.5 notes, the latest release, have titles highlighted in **green text**.

RELEASE NOTES FOR PREVIOUS VERSIONS

Version 3.1 Release Notes – August 15, 2003
Version 3.0 Release Notes – November 13, 2002
Version 2.1 Release Notes – February 11, 2002

WHAT'S NEW

GAMESS-UK Registration

(3.2.5) GAMESS-UK release 7.0 is now supported in Ecce. GAMESS-UK is a general purpose molecular quantum chemistry code maintained at CCLRC Daresbury Laboratory and Utrecht University. For details, see http://www.cfs.dl.ac.uk/ . GAMESS-UK calculations can be setup, run and output properties visualized within Ecce. Input parameters can be setup for Hartree-Fock, DFT, and MP2 calculations. Energies, geometry optimizations, and vibrational modes can be calculated. Molecular orbitals,

geometry optimization pathways, partial charges, vibrational modes, infra-red, and Raman spectra can be visualized.

Builder Usage Message

(3.2.5) Due to several support queue inquiries about how to enable Builder editing functions after reading a PDB file, a usage message is now shown where the atom editing buttons normally appear at the top-left corner of the main Builder window. The message indicates that a residue must be selected from the MD Toolkit or that all residue information must be cleared for the editing functions to be enabled. The usage message is hidden when editing a structure without residues or when a residue has been selected in the MD Toolkit, with the editing functions being displayed instead.

Basis Set Library Updated

(3.2.4) The basis set library used by the Basis Set Tool has been updated with the most recent version of data maintained by Dr. David Feller for the PNNL Environmental Molecular Sciences Laboratory (EMSL). Notable changes include updated reference information for cc-pVnZ-PP basis sets and first row transition metal coverage for the cc-pVnZ-DK basis sets. See the database revision log available from the "Atomic Bases" menu in the Basis Set Tool for details about additional changes.

POV-RAY Output Enhancements

(3.2.4) The POV-Ray output format now includes support for exporting hydrogen bonds and anti-aliasing output in the image preview available from the Export dialog. Anti-aliasing is the process of blurring sharp edges to produce a more appealing image without computer artifacts; useful for publication quality graphics. The syntax for using anti-aliasing with the povray command is also given in the output ".pov" file produced by Ecce.

Molecular Orbital Colors

(3.2.4) For each molecular orbital surface pair of colors, e.g. red/green, blue/yellow, etc., the same colors in opposite order have been added, e.g., green/red, yellow/blue, etc. Thus, the lobes of the orbitals can be colored either way. This was done to allow matches to the colors used by other visualization packages.

Message Area in Calculation Manager Access Control

(3.2.4) A message area for confirming success and reporting failures with changing access permissions has been added to the Calculation Manager Access Control dialog. Previously, errors were reported to the main Calculation Manager window message area. There were no confirmation messages at all that the permissions had been successfully updated, leaving users uncertain if any action had been taken after hitting the "Change" button. The Access Control feature is accessible from the Calculation Manager "Options" menu.

NWChem Property Runtype

(3.2.3) Extensive new support for properties was added to Ecce to reflect functionality in NWChem 4.7. The property runtype now supports calculation of electric fields at nuclei,

electric field gradients at nuclei, electron density at nuclei, shielding tensors, and Fermi contact and spin-dipole expectation values. Ecce also supports indirect spin-spin coupling, but this will not work properly until a patch is released for NWChem 4.7 that corrects the output to the ecce.out file for this property. The Calculation Viewer has also been modified to support visualization of these new properties. This includes visualizations of tensors as triads of bi-directional vectors, and shaded-atom visualizations of scalar properties that are related to individual atoms.

NWChem 4.7

(3.2.3) The NWChem distribution packaged with Ecce has been upgraded from version 4.6 to 4.7. While most sites making extensive use of NWChem will likely opt to install it themselves on dedicated compute servers, the distribution of NWChem packaged with Ecce does offer a quick way for sites to run NWChem from Ecce for uses such as evaluating Ecce and/or NWChem. Unfortunately, the binary distributions of NWChem 4.7 specifically for 64-bit processors running Linux do not run on all systems. Therefore, only the 32-bit Intel Fortran Compiler (IFC) version of NWChem 4.7 built for Redhat 7.3 is bundled with all Linux distributions of Ecce v3.2.3. This version appears to run reliably on GNU C Library 2.2 and 2.3 Linux operating systems, as well as with 32- and 64-bit processors. However, it certainly is not optimized for running on 64-bit processors and we only recommend it for evaluation and other low-demand needs.

Calculation Viewer Visualization Overlay

(3.2.3) All Calculation Viewer properties that support a visualization (indicated by the small chemical system icon to the left of the property name in the property data panel) can now be combined with any number of other property visualizations. Each property panel contains a new “push-pin” icon to the right of the property name, next to the icon for floating the property panel in its own window. Selecting the push-pin icon to enable overlay (the push-pin will be solid colored when enabled and an outline when disabled) results in that property being combined with any others that are visualized. Any property where the push-pin is selected will overlay with any others that are also selected for overlay. Push-pins can be toggled off to deselect properties for overlay. Visualizations that shade atoms, such as Mulliken charges, cannot meaningfully be combined with each other as the last property of this type that is visualized will override the previous ones. However, multiple vector/tensor properties may be combined with the new color option menu being used to distinguish them. A single property that shades atoms can be combined with any number of vector properties and also properties that calculate isosurfaces (molecular orbitals). The primary use of this feature is in creating presentation or publication graphics and thus both POV-Ray and image file (GIF, JPEG, etc.) formats support property overlays.

Calculation Viewer Vector Colors

(3.2.3) An option menu has been added to all Calculation Viewer property data panels that produce vector/tensor visualizations. The menu allows the color (for single vectors) or positive/negative color pair (for bi-directional vectors) to be selected from a fixed list. This feature allows vectors from different properties to be distinguished when used in conjunction with the new visualization overlay feature.

Property Visualization POV-Ray Support

(3.2.3) The new tensor and shaded-atom visualizations are picked up when the contents of the Calculation Viewer are exported as POV-Ray formatted files. This includes tensor color(s) as selected by the user.

Shaded Atom Visualization Color Ranges

(3.2.3) The spectrum ranges for all Calculation Viewer per-atom scalar property visualizations, such as Mulliken charges, have been made editable so that users can set the minimum and maximum values of the color ranges. This allows the user to expand the atom color (value) differences in sub-ranges of particular interest. Additionally, per-atom scalar properties that previously displayed the numeric value as a label next to the atom in the visualization no longer do so. It was too easy for these values to be written over the top of each other or otherwise become more of an annoyance than a benefit. The per-atom values are always displayed in the Calculation Viewer property data panels in a tabular spreadsheet.

Hydrogen Bonds

(3.2.3) The generation and display of hydrogen bonds has been significantly enhanced. Previously, only the Builder contained this capability as a primitive way to generate an image of a chemical system with hydrogen bonding. The algorithm for generating hydrogen bonds also proved to be overly simplistic. This could be supplemented, by using the line drawing tool in the Builder to add more hydrogen bonds, where Ecce failed to do so, in order to arrive at the proper representation. With v3.2.3, hydrogen bonds are now available in both the Calculation Viewer and the Builder as a toggle under the View menu. The bond generation algorithm has been enhanced so that additional atom types are taken into account, with the goal of eliminating the need for manual touch-ups. The display of hydrogen bonds has been changed to make the lines thinner, to better match how other chemistry visualization packages render these bonds. Hydrogen bond generation (and breaking) can further be done during a Calculation Viewer geometry optimization animation to show hydrogen bonding changing dynamically as the chemical system relaxes. Because the calculation of hydrogen bonds can be slow with larger chemical systems during an animation of an optimization, the “Recompute Bonds” toggle in the geometry optimization property panel has to be selected in order for new hydrogen bonds to be created and existing ones to break based on changes in the geometry. Hydrogen bonds are always generated for the entire chemical system rather than for selected atoms when there was a selection made. The improved algorithm for generating hydrogen bonds eliminated the need to allow this detailed level of control. Exporting images (POV-Ray, JPEG, etc.) from either the Builder or Calculation Viewer properly displays hydrogen bonds. Image capture from the Calculation Viewer also supports hydrogen bond display for making movies showing bond formation and breaking. Finally, the Builder line drawing capability was tweaked so that the lines displayed match those for the new hydrogen bonds—thinner than they were previously.

Calculation Viewer Invisible Display Style

(3.2.3) The Calculation Viewer now supports the invisible display style for selected atoms that had been previously implemented in the Builder. By selecting atoms in the visualization and selecting the radio button labeled "Invisible" under the "Style (Selected)" item of the "Display" menu; all selected atoms are hidden from view. This is useful when hiding some atoms makes areas of interest more easily seen (e.g. removing solvent) and is useful for preparing publication or presentation graphics.

NWChem ESP Runtype Parameters

(3.2.3) The Calculation Editor Theory Details dialog default values for the NWChem ESP runtype have been modified to give better results. These values have not been modified in NWChem as of yet, so Ecce always sets these values explicitly in the NWChem input deck. The ESP runtype has also been enabled for the ROHF theory.

IGLO-II and IGLO-III Basis Sets

(3.2.3) The IGLO-II and IGLO-III basis sets are now supported in the Basis Set Tool. Because these are not yet part of the NWChem library, the explicit coefficients and exponents are exported to the input deck if these basis sets are used. These basis sets may also be used for Gaussian calculations.

EMSL Machine Registration NWChem 4.7 Updates

(3.2.3) The registration for the EMSL HP Intel Itanium Linux cluster, mpp2, has been updated to run the latest version of NWChem 4.7. This includes the patch to correctly output the spin-spin indirect coupling property for visualization in Ecce. The registration for the Linux cluster, legion, also has been updated to run NWChem 4.7, although it is currently the original 4.7 release without the patch for the spin-spin indirect coupling.

Builder Selection Move

(3.2.2) Selected atoms in the Molecule Builder can be moved in space by holding down the middle mouse button and dragging in the visualization area (atoms move in the plane perpendicular to the viewing direction). Previously atoms could only be moved indirectly by adding measures (distance, angle, torsion), manipulators (move, rotate), or by editing coordinates in the geometry table. All currently selected atoms are moved together when performing a middle mouse button drag. This is a very imprecise way of creating or editing a structure, but may be appropriate in some situations before applying other more precise operations like the measures or a force field clean. This drag-move operation is reversible by the Builder undo option.

Builder Clear Residue Information

(3.2.2) PDB files can now be imported into the Builder without the associated residue information. This allows direct manipulation of the structure with the main Builder window palette of atoms, bonds, etc. instead of through the MD Toolkit by selecting a residue. A toggle on the Builder import dialog allows residue information to be cleared immediately as the structure is imported. Structures imported in this way are treated like a simple molecule without residue information. The on/off setting of this toggle is stored as a user preference. A Builder menubar item under the Options menu also allows

residue information to be cleared at any point after the initial import. When this menu option is used, a Builder undo operation can be done to restore residue information.

Feedback/Support Web Page

(3.2.2) The feedback web page has been redesigned to be easier to use and more aesthetically pleasing. The only remaining fields on the form are for the user's email address, the subject, and the problem description. We also discovered that this web page has been non-functional since the v3.2.1 release due to a missing file in the distribution. The help menu "Feedback…" menu item label in all applications has been changed to "Support…" as many users didn't understand that the "Feedback…" option was for submitting support requests.

NWChem Solvation Model

(3.2.2) Support for the COSMO solvation model built into NWChem is available in the Calculation Editor Theory Details dialog. A toggle is used to include the COSMO solvation block in the NWChem input file. Selecting the toggle also enables a choice of solvents from an option menu, each with an associated dielectric constant. If the desired solvent is not shown, the "Other" menu option can be selected, enabling a numeric input field for entering an arbitrary dielectric constant. Note that this support for solvation within Ecce is based on a model and does not actually add solvent molecules to the chemical system.

BSSE Corrections

(3.2.2) The Builder Geometry Table now has limited support for setting up BSSE calculations in NWChem, Gaussian 03, and Gaussian 98. Selected atoms can be changed to "BQX" type behavior with an option in the Geometry Table Actions menu. Conversely, atom behavior (BQX settings) can be cleared en masse with another option in the Actions menu. The NWChem or Gaussian input file will properly reflect the BQX atom specifications needed for a BSSE calculation. BQX atoms are included as sites that contribute basis functions to the calculation but do not contribute nuclear charges or electrons.

EMSL Machine Registration Updates

(3.2.2) The registration for the SGI Altix, altix1, has been changed so that NWChem is invoked with the mpirun command rather than pam as the latter was found to be unreliable. The maximum memory for altix1 jobs was bumped up from 20 to 30 gigabytes. The registration for the Linux cluster legion no longer prepends $TMPDIR to $PATH as it was causing an incorrect version of rsh to be used by MPI. The registration for the HP Linux cluster mpp2 has been updated to run the Elan4 interconnect installation of NWChem.

Constraint/Restraint Toolkit

(3.2.1) A new toolkit for adding constraints/restraints to geometry optimizations has been added to the Builder and can be accessed from the Toolkits menu. This toolkit allows users to add constraints that will freeze the value of bonds, angles, and torsions at specified values during geometry optimizations. The toolkit supports the addition of

constraints to NWChem, Gaussian 03, and Gaussian 98 optimizations and the addition of restraints to NWChem optimizations. Restraints add a classical harmonic oscillator potential between pairs of atoms and are useful for doing optimizations in the presence of fixed atoms. More information on restraints can be found in the NWChem 4.6 documentation.

Isotope Masses

(3.2.1) Support for using different isotope masses has been added to the Builder. A new column has been added to the geometry table listing the isotopic mass of each atom. The default value is taken as the mass of the most abundant isotope. The isotope masses listed in the periodic table have also been updated to include values for more elements, particularly recent additions to the periodic table. Masses can be copied from the periodic table to the geometry table using the standard X Window System copy and paste buffer. A "Change Hydrogens to Deuterium" action has also been added to the geometry table that automatically converts all hydrogens to deuterium. Another action has been added that will reset all atomic masses back to their default values. Changing atomic masses only affects NWChem frequency calculations, at present. Only if a mass is changed from the default value shown in the geometry table will any masses be included in the NWChem input file. Further, when a mass is changed, the masses for all atoms (even those not changed) will be included. Listings of nuclear spin for each isotope have been removed from the periodic table due to difficulty in finding corresponding spin values for the new isotope data.

QM/MM Toolkit

(3.2.1) A new Builder toolkit has been added to support the setup of QM/MM calculations. At present, this support is primarily for setting up electronic structure calculations in a field of fixed point charges. The toolkit allows the user to easily label selected atoms as either "Quantum" or "Point". Quantum atoms are included in the electronic structure calculation as regular atoms with basis functions, etc. while Point atoms are included in the calculation as simple fixed charges. The toolkit also provides access to the MD "Validate Structure" method that allows the user to assign partial charges to atoms in the system based on information in MD fragment and segment files. A "Break Bonds and Fill" function automatically breaks the bonds between Quantum and Point atoms, attaches a terminating hydrogen atom to the quantum atom and removes the attached Point atom. This function also removes all remaining fixed charges with zero partial charge and adds fixed atom constraints to the bond that replaces the original Quantum-Point bond. Support for Quantum and Point atoms is also provided in the geometry table, which has been extended to include a new column called "Behavior". This column lists whether an atom is Quantum, Point, or Unspecified (blank). The default behavior is Unspecified.

QM/MM in Calculation Viewer

(3.2.1) The Calculation Viewer has been updated to handle systems with mixed Quantum and Point charges created using the new QM/MM toolkit. This specifically required modification of the Molecular Orbital viewer and the Mulliken charge viewer.

NWChem 4.6

(3.2.1) The NWChem distribution packaged with Ecce has been upgraded from version 4.5 to 4.6. While most sites making extensive use of NWChem will likely opt to install it themselves on dedicated compute servers, the distribution of NWChem packaged with Ecce does offer a quick way for sites to access NWChem from Ecce for uses such as evaluating Ecce and/or NWChem. Version 4.6 of NWChem is significantly larger than previous releases, which accounts for the increased size of the Ecce v3.2.1 distributions.

MD Fragment and Segment File Format

(3.2.1) The "Write Fragment File" and "Write Segment File" functions in the Builder MD Toolkit have been updated to produce NWChem 4.6 format fragment and segment files. Other operations that read fragment and segment files, such as "Validate Structure", have been modified so that they support either NWChem 4.5 or 4.6 format files.

Expanded Gaussian Cube File Support

(3.2.1) Modifications were made to the Calculation Viewer to support the detection and analysis of Gaussian Cube file(s) created as part of a calculation run. When a Gaussian Cube file is created as part of a calculation run, the Calculation Viewer will display the various electron densities (or orbitals) for the molecule represented in the Gaussian Cube file format. Creation of Gaussian Cube files in NWChem, for example, can be accomplished by utilizing the Calculation Editor's "Final Edit" option and adding NWChem's DPLOT directive to the input deck. In order for these Gaussian Cube files to be detected by the Calculation viewer, the Cube files should be named with a .cub or .cube extension.

Macintosh OS X Compute Server Support

(3.2.1) It is now possible to use Apple Macintosh workstations as Ecce compute servers. Specifically, a G5 Macintosh running NWChem has been successfully registered within EMSL. Modification of the job monitoring script was required to support OS X so previous releases of Ecce will not work with Macs. Further, Ecce still does not support running the client X Windows application software on Macs. The new support for Macs only extends to running computational jobs to a Mac from other hosts already supported by the application software.

Machine Registration Startup Context

(3.2.1) The Job Launcher and Machine Browser applications now invoke the Machine Registration application in the context of the currently selected machine. Prior to v3.2.1, the Machine Registration application always came up in the context of the first listed machine, regardless of the machine selected by the user in the Job Launcher or Machine Browser.

Molecular Dynamics Toolkit Force Field Editor

A Force Field Editor dialog has been added to the Builder MD Toolkit that allows users to edit and combine force field files that use the NWChem force field format. This editor allows users to view the contents of a force field parameter file, compare parameter

values, make changes, combine parameter files, and export the results as new parameter files. The editor can be used to complete force fields for systems containing unparameterized interactions and is especially useful when used in conjunction with the Topology Viewer dialog, which is also new to this release. More information about the Force Field Editor can be found in the Ecce online help pages.

Molecular Dynamics Toolkit Topology Viewer

A Topology Viewer dialog has been added to the Builder MD Toolkit to allow users to assess whether available force fields are sufficient to cover systems that are currently being developed for MD simulations. The Topology Viewer provides a complete listing of all atom types, bonds, angles, torsions, and improper dihedrals in the system and also indicates whether or not a particular topology element is covered by the available parameter files. The Topology Viewer is coupled to the Force Field Editor, so that as elements are added to the force field, the topology is immediately updated. This provides an intuitive and interactive environment for completing force fields for new systems not currently covered by existing force fields. More information on the Topology Viewer can be found in the Ecce online help pages.

Builder DNA Toolkit

A new tool for creating strands of DNA has been added to the Builder and can be accessed under the "Toolkits" menu. The toolkit can be used to create segments of double-stranded DNA. The simple interface requires the user to enter the DNA sequence using four buttons for the A-T, T-A, C-G, and G-C base pairs and then generate the segment once the sequence has been specified. The DNA segments correspond to the B form of DNA.

Gaussian 03 Now Supported

Gaussian 03 is now a fully supported code in Ecce. Gaussian 03 calculations can be setup, run, imported, and output properties visualized within Ecce. Gaussian 98 also remains a fully supported code while Gaussian 94 calculations can only be imported and not setup and run within Ecce. Small enhancements were made to the output parse scripts due to changes between Gaussian 98 and Gaussian 03 for properties including molecular orbitals, Fermi contact values, and vibrational frequencies.

NWChem Packaged with Ecce

The NWChem executable and libraries are now distributed and installed with Ecce application software. This supports sites desiring an easy way to get up and going with running calculations under Ecce. In addition, Ecce directly uses the NWChem segment and fragment file libraries for its molecular dynamics setup capabilities and using a bundled distribution of NWChem guarantees consistency in format. When installing Ecce application software, the host machine where Ecce is installed is now automatically registered as an NWChem compute resource. Users only need to perform the Machine Configuration step before running jobs on that host. Note that running NWChem on the machine where Ecce application software was installed may be a poor choice due to lack of processing speed, memory, disk space, etc. Most sites will have dedicated compute

resources that are better suited for real-world jobs than is the machine where Ecce applications were installed.

Sharing Calculation Data

A new Calculation Manager dialog allows users to change access to their calculation data supporting collaborations with other users. This dialog is invoked with the "Change Access Control…" menu item under the "Options" menu. Other users can selectively be granted read-only or read/write access to any project or sub-project owned by a user. A user is owner of their top-level project under the "users" area and any projects or sub-projects they create whether in their own "users" area or in the "share" area. An important caveat when setting access to a sub-project is to make sure that a user granted access also has access to any parent projects on up to the top-level project. Otherwise they will not be able to navigate to the sub-project in the Calculation Manager project tree. This can be done by only allowing read access to the parent projects even if read/write access is desired for the sub-project (i.e., allowing just enough access to navigate to the sub-project without being able to add/change data in the parent projects).

Basis Set Library Revisions

Added recent updates to the EMSL Gaussian Basis Set Library maintained by Dr. David Feller. Many Correlation Consistent basis sets were added as well as a correction to the values for Iodine in the Stuttgart RLC basis.

Calculation Editor Detail Fields

Calculation Editor theory and runtype detail dialog fields are no longer automatically reset to default values with every change to the chemical system, spin multiplicity/open shells, charge, basis set, theory, or runtype. There are some instances though where it is still necessary to reset the detail fields. A change to the level or category of theory (for example SCF to DFT, RHF to ROHF is not a theory level change) will always cause both theory and runtype detail fields to be reset. A change to the runtype will always cause the runtype detail fields to be reset but not the theory detail fields. The reason in previous releases of Ecce that the detail fields were always reset is that any change to chemical system, basis set, etc. can lead to inconsistent values in specific detail fields that are dependent upon attributes like the number of electrons or basis set functions such as the number of frozen core orbitals. Now it is the responsibility of the user whenever making a change to something on the main Calculation Editor window that the detail field values are still within range. As a reminder to check the detail fields, a warning is printed to the message area at the bottom of the Calculation Editor main window. The previous warning that detail fields have been reset is now only issued for the theory level and runtype changes outlined above.

Job Launcher GUI Changes

Job Launcher fields not supported by the currently selected machine are now hidden rather than being disabled (grayed out). This saves screen space and reduces confusion in using the interface especially as the number of possible fields grows, based on the registration requirements of new machines. Likewise, to further reduce the complexity of

using the Job Launcher, the option menu for selecting the queue to use is now hidden if there is only a single queue registered for a machine.

Data Server Password Lookup and Change

The Ecce Login Password dialog now allows the current data server password to be displayed or changed. A new “Lookup” button shows the current data server password while the “Change” button now displays two secondary buttons for selecting whether to change the login password or the data server password. This allows users to change the data server password to something more meaningful than the randomly generated password (changing the data server password to be the same as the login password is prevented). A more useful message about the purpose of the Ecce login password is now given to first-time users. All references to the word “passphrase” for authenticating to Ecce prior to v3.2, have been changed to “login password”. This is simply a GUI change to make Ecce more intuitive to new users.

Online Help Updated

Online help has been updated to reflect new functionality and fixes in v3.2. Help has been added for the new Builder DNA Toolkit, Force Field Editor, and Topology Viewer. Updates have been made to virtually all remaining applications.

Builder Hydrogen Bonds

The Builder has a new menu option "Generate Hydrogen Bonds" that determines where Hydrogen bonds should exist and adds a distance measure between the bonds. Once generated, these can be ignored by hitting the “remove measure” icon button.

Molecular Dynamics Toolkit Assign Residue Atoms

The “Assign Residue Atoms” function of the Builder MD Toolkit has been modified so that it updates the atoms with available information from the segment or fragment files after assigning atom names.

Calculation Manager Calculation Moves

Support for moving calculations between folders in the Calculation Manager has been improved. A single calculation can be moved by selecting it in the table view and dragging it to a destination project/folder in the left-hand project tree view.

Calculation Viewer Enhancements

A number of changes were made to the Calculation Viewer to make it more consistent with the Builder. These include: an Edit menu with selection mechanisms, support for mixed display styles, incorporation of the Geometry Table, and supporting measures at all times. The Trajectory Toolkit is also now available in the Calculation Viewer.

Calculation Viewer Shielding Tensors

The Calculation Viewer Shielding Tensor visualizations have a more flexible mechanism for selecting the atoms for which vectors should be generated. Selection may be done on individual atoms in the table, selection in the visualization area, or by a new drop down menu that supports selection of all atoms of a specific element.

Calculation Viewer Mulliken Charge Visualization
Mulliken Charge distribution spectrums in the Calculation Viewer now use a positive/negative color spectrum where negative values are a shade of red, positive values a shade of blue, and zero charges are white.

NWChem Atom Name Suffixes
Ecce now supports, especially for use with NWChem, importing into and exporting out of the Builder with suffixes on atom names instead of just the atomic symbol. The suffixes must begin with an underscore followed by numbers or text. Both XYZ and MVM format files now support these suffixes in Ecce. They will also appear in an NWChem input file and can be imported from an NWChem Ecce-format output file. The Builder Geometry Table has a column for the suffix separate from the atomic symbol (select "All Fields" from the View menu). This is an editable field so suffixes can be added to a chemical system created within the Builder. It is also possible sort the Geometry Table based on the suffix and assign a suffix "en masse" with the copy and paste cells operations.

Builder Atom Name Determination
The logic for determining atom names when editing the atom names in the Builder Geometry Table has been modified to so that new atom names are checked against the atomic symbol. If the two are compatible, then the name is accepted, otherwise it is rejected. This allows the user to type in all capital names for two character element names, such as FE, without having them confused with single character elements, e.g. FE (iron) getting mistaken for F (fluorine). Ecce automatically aligns these names correctly in the four character atom name field in the PDB file.

Builder Geometry Table Environment Index
Added a column for the "environment index" to the Builder Geometry Table. This parameter is part of the NWChem MD setup and is used to help choose centers that have an improper torsion defined on them.

Builder Fragment Moves
The rules for moving fragments that are being added to a system using the "paste" operation were modified so that a displacement occurs only if the first atom in the pasted fragment overlaps something already in the Builder. This change was made so that it is easier to reorder atoms in the Builder using the cut and paste operations without changing atom locations. These operations may be desirable when used in conjunction with the MD Toolkit "Make into Residue" function.

Builder Residue Selection
Double clicking on an atom that belongs to a residue in the Builder now selects the entire residue.

Builder Geometry Table Editing

The Geometry Table in the Builder now supports "en masse" editing of x, y, or z coordinates through the copy/paste mechanism. By selecting multiple destination cells, a single paste operation will populate all cells with the value in the copy buffer.

Builder Import of Bq Atoms

The import of XYZ files in the Builder has been modified so that it will import Bq atoms. These are converted to "ghost" atoms.

Gaussian Checkpoint File

Added checkpoint file support for Gaussian 03 and Gaussian 98. A toggle at the top of the Calculation Editor Theory Details dialog controls whether the file is created. The default is to create the checkpoint file for all Gaussian calculations.

Builder and Calculation Viewer Radius Selection

A "radius selection" feature was added to the Builder and Calculation Viewer. This feature allows selection of atoms and bonds when they are within a specified radius of the current set of highlighted atoms. Complete residues will also be included in the selection, if indicated.

Calculation Viewer Surface Caching

A cache was added to Calculation Viewer for fast switching between computed MO, Density, and Spin Density displays. The default maximum cache size is 10 surface calculations. This can be customized by a site in the site_runtime file in the application software siteconfig directory or by an individual user by setting the $ECCE_MAX_CACHED_MO environment variable to a number greater than or equal to 0. Every computed MO, Density, or Spin Density is added to the cache once the computation completes. Changing the grid size will cause a recalculation.

Calculation Viewer Image Capture

POV-Ray format is now supported in the Calculation Viewer "Image Capture" tool.

POV-Ray File Generation Format

POV-Ray file generation in the Calculation Viewer and Builder has been modified so that the colors and finishes are all declared at the top of the file for most settings instead of setting them locally for each visual element. This allows users to modify the colors, etc. easily by editing the POV-Ray file by hand.

POV-Ray Output Options

Many new finishes and display options have been added to the POV-Ray export dialog in the Calculation Viewer and Builder, including a preview function. For the preview function to work, the POV-Ray processor command must be in the user's path. New finishes include "soft", "metallic", and "wood"; options for bonds include "bicolor" and a monocolor "brass" option; and new options for isosurface finishes are also provided.

Session Preferences

The Builder and Calculation Viewer camera perspective is now saved as a preference and restored in the next session. Surface colors and grid sizes in the Calculation Viewer are also now saved as preferences. All file import and export dialogs now save both the last directory used and the file filtering pattern as session preferences.

Builder and Calculation Viewer Spinning

The Builder and Calculation Viewer now have an option to disable automatic spinning in the three-dimensional visualization area. This option is saved as a preference.

Visualization Area Thumbwheel Controls

A new Z-axis rotation thumbwheel control has been added to complement the existing X- and Y-axis thumbwheels in the Builder and Calculation Viewer. The rotation thumbwheel labels have been changed to just be the axis name (X, Y, or Z) without "Rot" being pre-pended. The thumbwheel previously labeled "Dolly" has been renamed "Zoom".

Builder Command Record/Playback

A command record/playback feature was added to the Builder. This tool can be used to record and playback sequences of Builder operations for demonstrations or to automate repetitive tasks. The capability is a prototoype only at this point.

EMSL MPP2 NWChem Jobs

For running NWChem on the mpp2 HP Linux cluster in EMSL, the Ecce job submission script now copies the NWChem executable to all allocated nodes to improve performance.

PNNL SGI Altix Supported

The new SGI Altix 3700 system at PNNL, altix1, is now supported by Ecce for running NWChem jobs. This massive shared memory 64 Itanium2 processor machine runs the LSF batch queue system. Access is available on request to all PNNL staff members.

SITE ADMINISTRATOR WHAT'S NEW

New User Message and Startup Message Capability

(3.2.5) A configurable one-time message can now be displayed to new Ecce users when Ecce is started for the first time. Additionally, a "message of the day" can also be set and displayed to each user when they start Ecce. The messages are displayed in a popup information dialog from the Gateway application. The message text is contained in the $ECCE_HOME/siteconfig files named NewUserMessage and StartupMessage. Ecce site administrators have write access to this directory and thus control over the messages displayed. No messages are displayed if these files are empty (the default for new Ecce installations). Common usages for the new user message are directing users on how to access Ecce online help and where to send support requests. Common usages for the

startup message are announcing Ecce server outages and new compute resource registrations. Normally, a site will create a NewUserMessage file and leave it in place since the message is only displayed one time, while the StartupMessage file will be empty except for a few days before outages and a few days after new capabilities are added.

New Linux 64-Bit Processor and Operating System Support

(3.2.3) Ecce now supports 64-bit Intel Itanium and AMD Opteron processors running versions of Linux using GNU C Library 2.3.X (glibc 2.3) such as Redhat Enterprise Linux Workstation 3. Sites that had tried running the 32-bit GNU C Library 2.3 distribution of Ecce v3.2.2 (i686_Linux_glibc2.3) on 64-bit processors, as suggested, often found incompatibilities with the Java Runtime Environment. Further, the Opteron processor architecture detected by the uname command, x86_64, was not mapped to paths for libraries and executables by the Ecce environment setup scripts in Ecce v3.2.2, resulting in error messages. With version 3.2.3, there is a supported ia64_Linux_glibc2.3 distribution of Ecce v3.2.3 that works for the AMD Opteron processor, as well as for the Intel Itanium processor.

Apache Upgrade

(3.2.3) The Apache web server (**http://www.apache.org/httpd**) has been upgraded to Apache 2.0.54 for all platforms. This release of Apache is primarily a bug fix release. The httpd.conf configuration file has been modified to eliminate a minor security weakness where it would send extra information about the server in response headers and server-generated pages.

Data Server File Compression

(3.2.3) An Apache filter module, Server Side Compression (SS_COMPRESSION), has been added to the Apache web server used by the Ecce data server. This new module utilizes the zlib data-compression library (**http://www.zlib.net**) to compress calculation output files as they are being stored on the data server (i.e. Input filter) and decompress files as they are retrieved from the data server (i.e. Output filter). Enabling the SS_COMPRESSION module will result in a reduction of the amount of storage space used by the data server for all calculations created once compression is enabled (no conversion is done for existing calculations). Initial testing has shown file size reduction as high as 75% for some calculation output files. However, this percentage will vary depending on the type and size of file being stored. By default, the SS_COMPRESSION module is not enabled. SS_COMPRESSION can be enabled by modifying Apache's httpd.conf configuration file. Edit the httpd.conf file located in the apache/conf directory under the top-level server installation directory and search for "Ecce COMPRESS". Uncommenting both the "SetOutputFilter SS_COMPRESSION" and "SetInputFilter SS_COMPRESSION" directives will enable the SS_COMPRESSION module.

Java Runtime Environment 1.5

(3.2.3) The Linux distributions of Ecce v3.2.3 have all been updated to use version 1.5 of the Java Runtime Environment, JRE. This latest JRE provides better compatibility between processors (32- and 64-bit) and operating systems (GNU C Library 2.2 and 2.3).

In fact, all Linux distributions now use a single distribution of the JRE rather than needing special ones based on the processor, such as 64-bit AMD Opteron. The Java Runtime Environment is used by the Java Messaging Service JORAM implementation included with the Ecce server. This component provides inter-process communication and synchronization between the various Ecce client applications that a user runs in a session.

New Linux Operating System Support

(3.2.2) Added support for new Linux operating systems, including Red Hat Fedora Core 3, Red Hat Enterprise Linux 3, Mandrake 10.1, SUSE 9.X, and Debian 3.1. There are now two different Linux distributions for 32-bit Intel/AMD processors. The distribution of Ecce that is appropriate for a Linux operating system is determined by the version of the GNU C Library on a machine. This can be found in the first line of output when the command "/lib/libc.so.6" is issued. New Linux operating systems that are supported in Ecce v3.2.2, but were not supported in v3.2.1 (Fedora Core 3, etc.), use version 2.3.X of the GNU C Library. Older versions of the Linux operating system that were supported in Ecce v3.2.1 (Red Hat 7.X, etc.), use version 2.2.X of the GNU C Library. The two different Ecce Linux distributions available on the Ecce download web page are distinguished by the version of the GNU C Library appended to the platform portion of the distribution name, glibc2.3 and glibc2.2. As a final check, the Ecce installation script tests that the version of the GNU C Library on the installation machine matches the version of the Ecce distribution and issues a warning if it does not.

Sun Solaris and 64-bit Itanium/Opteron Support

(3.2.2) The Ecce distributions for Sun Solaris workstations and 64-bit Intel Itanium/AMD Opteron processors have both been made special requests for Ecce v3.2.2. Unless there is unanticipated demand, the next major release of Ecce, v4.0, will no longer support Sun Solaris workstations. Support for 64-bit Intel and AMD processors will be limited to those running older GNU C Library 2.2.X operating systems such as Red Hat Advanced Workstation 2.1. Those sites running a GNU C Library 2.3.X Linux operating system version on a 64-bit processor are encouraged to try the regular 32-bit processor Linux distribution for GNU C Library 2.3.X with the caveat that the Ecce team cannot fully support this if problems are found. Running Ecce application software on 64-bit processors is completely distinct from running computational jobs on these machines. Ecce will continue to fully support 64-bit Intel Itanium and AMD Opteron processor workstations and clusters as compute resources for chemistry jobs. Requests from sites using the 64-bit processor Linux distribution of Ecce will determine whether there will continue to be a separate 64-bit processor Linux distribution of Ecce v4.0 for running Ecce applications on this platform.

Ecce Download Web Page

(3.2.2) The Ecce download web page has been redesigned to simplify choosing the correct distribution for a platform. Operating systems supported by Ecce are displayed in a table with links to the corresponding Ecce distribution. The split of Linux distributions in Ecce v3.2.2 based on the GNU C Library version dictated the need to list specific operating system vendors and versions. Those sites that are running Linux operating

systems not listed in the table or that are not certain of the operating system version are provided a link to determine the appropriate distribution to download.

Xterm Window Font

(3.2.2) Some sites do not get a reasonable default font when creating xterm windows such as shells in remote calculation directories or performing a final edit. A new $ECCE_HOME/siteconfig/site_runtime variable named ECCE_XTERM_FONT passes a specific X Window System font name whenever an xterm is created within Ecce. The default is not to pass a font, so the site administrator must edit the site_runtime file to use this feature. The site_runtime file contains further documentation on how this feature works and how to select an appropriate font.

Compute Server Default Parameters

(3.2.2) Compute servers running batch queue systems can now be registered with default values to display in the Job Launcher for the number of processors, memory, time limit, and scratch space. Previously the defaults were always calculated by Ecce, sometimes leading to inappropriate values. Setting default values allows the site administrator to register what are considered to be typical values, thus reducing the burden for users who may not be as familiar with running jobs on these machines. The *.Q file key names for these new default parameters are defProcessors, defMemory, defRun (time limit), and defScratch. The Machine Registration application does not support these new parameters so they must be set by manually editing the $ECCE_HOME/siteconfig/*.Q registration file for each desired batch queue machine. If no defaults are set, then Ecce calculates the default value to display in the Job Launcher as it has in the past.

Installation Prompt Removed

(3.2.2) The Ecce installation procedure has been simplified by eliminating the prompt for the support email address. The default support email address is now initially set to ecce-support@emsl.pnl.gov for all sites. However, Ecce still allows each site to customize their support email address in the $ECCE_HOME/siteconfig/site_runtime file as described in the Ecce Installation and Administration Guide and we encourage doing so when there are multiple users at a site.

Apache Upgrade

(3.2.1) The Apache web server (http://www.apache.org/httpd) has been upgraded to Apache 2.0.49. This release of Apache is primarily a bug fix release. As well as upgrading Apache, the httpd.conf configuration file has been modified to address a possible security vulnerability unrelated to Ecce.

Improved Platform Support Detection

(3.2.1) The ecce and ebuilder scripts for invoking Ecce have been enhanced to better recognize platforms not supported by Ecce. Linux platforms running Power PC, Alpha, MIPS, M68K, and Sparc processors are now recognized and Ecce exits immediately when invoked on these architectures. This does not represent any actual change in platform support by Ecce, just better automatic detection of when it is being run on a platform where it definitely will not work.

Code Registration GUI Test Script

(3.2.1) A new script named pydi for invoking the Python code registration detail dialogs outside the rest of Ecce, has been created. The pydi script is in the $ECCE_HOME/codereg directory and the only required command line argument is the name of the Python detail dialog script. Optional arguments specify the theory, runtype, etc. See the documentation at the top of the pydi script itself for more information on command line arguments. This script allows a person doing code registration to check the appearance of the Python details dialog incrementally while it is being built.

Default Remote Shell Path

(3.2.1) The $PATH set by Ecce for all remote logins has been augmented to always include /usr/bin/X11 and /usr/X11R6/bin. These are the two most common paths to X Window System applications such as xset and xterm needed by Ecce to start remote shell windows. Compute servers registration no longer requires the path to these applications be specified manually in the CONFIG.<machine> file with the xappsPath directive, provided these commands are in one of the two directories above. There are no adverse effects if these are not valid directories on a compute server.

Ecce Installation Simplified

The distinction between network and standalone installs of Ecce has been eliminated for v3.2. Both types of installs are now performed by selecting a "full" install or upgrade from the main installation menu. A true standalone installation, so that the host may be taken off and on the network and Ecce run either way while not allowing outside machines to connect to the server when on the network, is done by specifying the host name as "localhost". Of course the name localhost must be properly configured in the /etc/hosts file with the loopback address for a standalone installation to work. File permissions, except for the application software siteconfig directory, have been buckled down to prevent inadvertent changes even by the Ecce site administrator. If necessary, write permission can be added manually to change these files, which are not normally intended for modification by sites running Ecce. The Ecce Installation and Administration PDF document available on the Ecce website has been updated with these changes to the installation procedure.

Data Sever Passwords

Data server passwords can no longer be set to be the same as Ecce login passwords and the feature to automatically synchronize them to be the same has been removed. Security vulnerabilities with HTTP password transmission possibly leading to Ecce login passwords being compromised have necessitated this change. Data server passwords are now random pseudo-words, containing both a number and a capital letter for added security, generated the first time a user runs Ecce (assuming the $ECCE_AUTO_ACCOUNTS feature is enabled). All data server passwords that are identical to login passwords (from running Ecce v3.1) will be automatically changed by Ecce to random passwords the first time a user starts Ecce v3.2. The meaning of the $ECCE_AUTO_ACCOUNTS variable has now changed to support only automatic

server account creation (a true/false value) and not password synchronization. The application software site_runtime file in the siteconfig directory documents this change.

Ecce Server Ports Check

The script for starting the Ecce server, start_ecce_server, now checks whether the ports that would be used by the Apache data and JMS messaging servers are currently in use. If so, a warning is issued about which of the ports are busy and the startup is aborted. This feature was added to make it easier for sites to diagnose problems starting the Ecce server.

Ecce Messaging Server Scripts

Two new scripts for starting and stopping just the JMS messaging server, start_ecce_message_server and stop_ecce_message_server, have been added. These compliment the existing start_ecce_data_server/stop_ecce_data_server scripts that start and stop only the Apache data server, and the start_ecce_server/stop_ecce_server scripts that start/stop both the data and messaging servers together. Normally only the start_ecce_server/stop_ecce_server scripts should be necessary. However, should there be a problem with only the messaging server, such as it going down during use, it is now possible to address the issue without impacting the data server as well.

Java Runtime Environment Updates

The Java Runtime Environment for all platforms for both the client and server sides of Ecce has been updated to version 1.4.2. This was done primarily to address reliability problems found especially on the SGI platform with being able to start the JMS messaging server. New versions of the Redhat operating system such as Advanced Workstation 3.0 and other Linux variants also require the latest JRE.

Ecce Data Server for Itanium

The Apache data server distribution bundled with the 64-bit Intel Itanium version of Ecce is now compiled on an Itanium workstation rather than being the same Apache server distribution as the 32-bit Pentium compile. Some Linux operating systems on Itanium processors were found not to run the 32-bit Pentium Apache server.

Ecce Data Server MIME Type Support

MIME types for Ecce resources are now being defined and resolved by the Ecce data server. Previously, the Ecce client application created and maintained an application specific WebDAV property to manage MIME types for Ecce resources. MIME types are now derived by the data server and reported to the client application via the standard WebDav property - getcontenttype. Calculation input/output files were renamed to conform to the new MIME type definitions. Also, some MIME type values were modified to better conform to formats used in the chemistry community. These changes are backwards compatible with Ecce resources created under the previous MIME type definitions.

Machine Registration Enhancements

Added a couple minor features to the machine registration capability. Files can now be deleted in the job submit script prior to the computational code being invoked. This is done with a block named "PrelimFilesToRemove" that can be customized by sites in the submit.site file in the siteconfig directory. At this point, this block is used to remove the *.q partial charge file for NWChem jobs to insure that calculation restarts and reruns don't pick up the old partial charges. The new "PrelimFilesToRemove" block compliments the existing "FilesToRemove" block used to delete files after the computational code has run. Secondly, the units for the maximum memory for a job on a queued machine can now be registered rather than only supporting the default of megawords. This feature is not supported in the Machine Registration application and must be specified manually <Machine>.Q file with the memUnits keyword where any arbitrary value is supported including "MB", "KB", etc.

Job Launcher Scratch Space

The Job Launcher now supports a field for the minimum scratch disk space needed in megabytes in order to start a job on a queued machine. The LSF batch queue system and possibly others supports this attribute. The Machine Registration application allows new machines to be added with this minimum scratch space attribute.

WHAT'S FIXED

Font Display in Builder and Calculation Viewer Workspace

(3.2.5) Fonts used for atom labels, bond distances, angles, torsions, and per-atom properties were garbled on Linux platforms running GNU C Library 2.3. This has been fixed by the inclusion of a font path specification in an Ecce environment setup file.

Running jobs on EMSL Linux cluster "legion"

(3.2.5) The "-nolocal" flag has been added to the mpirun command for the "legion" Linux cluster job submission script, fixing a launch problem.

Calculation Viewer Molecular Orbital Display

(3.2.4) Errors in normalizing the basis functions in the display of molecular orbitals in the Calculation Viewer were corrected. These led to distortions in displaying orbitals containing significant contributions from higher angular momentum basis functions, sometimes making the orbitals appear asymmetric. A fix was also made to ensure the correct ordering of angular momentum functions. This normalization error applies to both NWChem and Gaussian, but was not detectable in the great majority of orbitals calculated with Ecce. Additionally, the default value for considering orbital coefficient contributions has been changed from 0.01 to 0.001 so that fewer coefficients are discarded by default.

Basis Set Optimization

(3.2.4) For some newer basis sets, in particular the correlation sets that have been recontracted by Ken Dyall for use with the spin-free modified Dirac equation (e.g. cc-

pVDZ(pt/sf/fw)), the “Optimize General Contractions” option in previous releases of the Basis Set Tool did not correctly complete the optimization reformatting.

Correlation Consistent Basis Sets Corrected

(3.2.4) Meta-data attributes associated with the aug-cc-pVnZ-PP correlation consistent basis sets have been corrected making these basis sets usable. Other basis set fixes have been made as described in the database revision log available from the “Atomic Bases” menu in the Basis Set Tool.

Calculation Manager Copy Between Users

(3.2.4) Calculations and Projects can now be copied between users in the Calculation Manager when there is only read permission. Previously read-write permissions had to be granted for one user to copy data from another’s area. A scenario illustrating this is when user “B” wants to copy a calculation or project that is owned by user “A”. That is, the object to be copied is under user “A’s” home project at some level. User “A” must first grant read permission to user “B” using the Calculation Manager Access Control dialog available from the “Options” menu. Then, user “B” can navigate to the desired calculation or project in user “A’s” area, and use the “Copy” and “Paste” functions in the “Edit” menu to create a copy under a project in their own area.

Calculation Editor “Use Exponents & Coeffs” Toggle

(3.2.4) The Calculation Editor “Use Exponents & Coeffs” toggle now saves and restores its state between sessions. Previously it would always reset to being off between Calculation Editor invocations, a nuisance to remember to override when using this feature. This toggle controls whether basis set library names or explicit exponents and coefficients should be used in the input file. Another bug fixed related to this toggle now prevents the user from modifying a read-only calculation (such as one in the running or completed state) by selecting this toggle. It is now frozen to input for read-only calculations like all other fields in the Calculation Editor.

Gateway Password Lookup

(3.2.4) When requesting the Ecce data server password from the Gateway Login Password dialog using the “Lookup” button, a dialog is always displayed now. Previously, if no data server password could be found, there was no confirmation at all that the “Lookup” button was hit. Now it will indicate in the popup dialog that a data server password could not be found.

Builder Force Field Editor Element Validation

(3.2.4) For updating parameters in the Builder Force Field Editor, those fields that required an atomic symbol to be entered now use atomic numbers. This fixes a bug when the code using the value entered needed an atomic number and it was being passed an atomic symbol.

Molecular Dynamics Toolkit Topology Viewer Hang

(3.2.3) A bug was causing the Builder Molecular Dynamics Toolkit Topology Viewer to hang when there was more than a single unassigned torsion. This has been fixed.

Molecular Dynamics Toolkit Force Field Editor Export

(3.2.3) The Builder Molecular Dynamics Toolkit Force Field Editor was not exporting force field files correctly, primarily because it was not picking up any changes made to the force field. This has been fixed so that the export function now correctly exports modifications to the force field as well as combining existing force fields with their modifications.

Spreadsheet Tabular Data Font

(3.2.3) Data displayed in Ecce client applications in spreadsheet style tables, such as the Builder Geometry Table and many of the Calculation Viewer property data panels, is now shown with a different fixed width font. The Courier font family replaces Lucida that was previously used and found to be missing on some platforms. The Courier font appears to be standard with all X Window System installations. When Lucida was used and the font was not available, data was rendered as unintelligible "hieroglyphics".

Calculation Editor Theory Change

(3.2.3) Previously only a change to the level of theory (e.g. SCF to DFT) would reset the values of detail dialog fields back to defaults, not a change to the theory name within a level (e.g. RHF to UHF). This resulted in problems when logic in the details dialog Python scripts needed to distinguish between theory names, potentially resulting in improper code input files. Any change to a theory name now results in all detail dialog fields being reset.

Ecce Startup Failure

(3.2.2) In certain circumstances related to the network configuration outside Ecce, the name of the local host on which Ecce is being invoked cannot be determined. In this case, Ecce was adding an invalid entry to the user's ~/.ECCE/MyMachines preference file in an attempt to register the local machine for running and importing calculations. This invalid entry effectively disabled Ecce from starting for that user since reading the MyMachines file is part of the Ecce Gateway initialization. This situation is now recognized, so invalid entries are not added to the MyMachines file and users will not be shut out of Ecce.

Gaussian Calculation Imports

(3.2.2) The output file parse scripts have been corrected to properly skip over the header section containing the Gaussian code version information. This section in the Gaussian output file is separated by a series of asterisks and the number of asterisks being matched was too few in some instances before this fix, causing failures to import some calculations. This fix has been made to all supported versions of Gaussian for importing calculations: 03, 98, and 94.

Window Location Creep

(3.2.2) The code to save and restore the previous window location between invocations of Ecce applications sometimes resulted in incorrect placement of windows by a few pixels and sometimes more. The number of pixels varied based on the window manager

being used. Over many invocations, this would slowly cause the window to start creeping down and to the right on the screen. More problematic, certain secondary windows that aren't displayed except as requested, such as the Builder Partial Charge Toolkit, would be offset by the entire width and height of their window frame with each invocation (even when not displayed) instead of just a few pixels and could migrate entirely off the screen.

Calculation Directory Path Validation

(3.2.1) The calculation and scratch directory paths specified in the Job Launcher and now checked to make sure they are absolute rather than relative paths. Prior to v3.2.1, a user could specify a relative path (not beginning with "/" or "~") and the job would submit successfully. However, when the job started running, sometimes days later on queued machines, it would fail when the submit script tried to reference the relative path. Relative paths are now flagged as errors immediately when launching a job.

Job Rerun, Restart and Reconnect

(3.2.1) In version 3.2, jobs that were rerun, restarted, or where job monitoring was reconnected would often come back with Job Launcher errors due to file transfer failures. Specific files that were being copied on a job rerun, etc., including the eccejobmonitor script and the code parse descriptor file, had read-only file permissions on the compute server preventing them from being overwritten. File permissions are now set to read-write for the calculation owner so operations requiring these files to be overwritten will succeed.

Remote Login Failures

(3.2.1) For a very select number of machines, attempts to remotely login such as for a job launch would fail sporadically. The protocol that Ecce uses to recognize a valid remote login, specifically recognizing the C shell command prompt, has been slightly changed in order to work more reliably for all compute servers.

Calculation Editor Toggle

(3.2.1) The "Use Exponents and Coeffs" toggle for controlling basis set format when the Calculation Editor generates an input file has been fixed so that it does not arbitrarily reset. Minor changes such as to the chemical system were resetting the user selection for this toggle when it was not necessary. Further, quitting the Calculation Editor and restarting it with the same calculation would also reset the toggle.

Job Monitoring Failures

A bug in versions 3.0 and 3.1 of Ecce since switching to the Java Messaging System for inter-process communication, would sometimes result in a job monitoring failure (calculations in the "monitor error" state in the Calculation Manager). This would occur when Ecce was exited and then restarted while the job was in the submitted or running states. The logic to reconnect messaging in the job monitoring process on the client, eccejobstore, would fail, subsequent output would not be parsed, and the calculation would be reported as a "monitor error". Exiting and restarting Ecce client applications any number of times while a job or jobs are being monitored is now handled correctly.

Calculation Viewer Gaussian Inconsistencies

For Gaussian calculations, some properties are computed with respect to the initial coordinates and others are computed with respect to standard coordinates. Ecce does not parse initial coordinates so properties that must be visualized with respect to the initial coordinates are no longer supported in the Calculation Viewer. This list includes polarizabilities and the energy gradient vector for optimizations. For single point calculations, the properties can be supported since the single initial coordinates are known.

Gaussian ECP Basis Set Calculations

The input files for Gaussian 98 and Gaussian 03 calculations that used ECP basis sets were incorrectly formatted prior to v3.2. An extra blank line in the basis set specification was causing Gaussian to skip part of the basis set specification. The basis set input is now properly formatted for Gaussian to use ECP basis sets.

Gaussian MP Theory Energy Values

For Gaussian 98 and Gaussian 03 calculations run in Ecce, several scalar value types of energies such as CCSD were not being parsed from the output file for MP calculations. New Gaussian calculations run with Ecce v3.2 will parse and display these energies in the Calculation Viewer.

NWChem MP2 Dipole Moments

MP2 dipole moments computed by NWChem were incorrectly parsed from output files and displayed by the Calculation Viewer as identical to the SCF dipole moments. This has been fixed.

Gaussian Imported Calculations

Parsing of auxiliary output files when importing calculations, notably the fort.7 molecular orbital file generated by Gaussian was broken in Ecce v3.1. Version 3.2 correctly imports these calculations with auxiliary output files.

Calculation Editor Semi-Empirical Calculations

A logic inconsistency in the Calculation Editor allowed a basis set to be specified under certain conditions for semi-empirical Gaussian calculations. An explicit basis set should never be used with a semi-empirical calculation of course and this has been fixed for v3.2.

Calculation Manager Importing Spherical Basis Sets

When importing calculations through the Calculation Manager, if spherical basis sets were used, the spherical flag was not detected in some cases causing MO visualizations to fail. This has been fixed.

Basis Set Tool Optimize General Contractions

The input file for NWChem and Gaussian jobs has been fixed to properly reflect the user's choice for optimizing general contractions in the Basis Set Tool. Unfortunately,

there is no way to use the built-in basis set library names for either NWChem or Gaussian unless contractions are optimized so the only solution is to force explicit exponents and coefficients in the input file when not optimizing contractions.

Calculation Manager Simultaneous Imports

It is now possible to import several calculations simultaneously in the Calculation Manager. Conflicts in file paths being shared between imports caused this to fail often in previous releases.

Calculation Manager Duplicate

When using "Duplicate Setup with Last Geometry" on a calculation in the "created" state, the state of the new duplicated calculation was incorrectly set to "ready". This has been corrected so that the state of the duplicated calculation is set to "created". Similarly, using “Duplicate” on a calculation in the "completed" state was, in some cases, not correctly resetting the state back to "ready". This has also been fixed.

Calculation Manager Session Restore

When starting the Calculation Manager, the last project that a user worked in is restored as the displayed project. However, the left-hand project tree view did not scroll to this location. The tree now automatically scrolls this project into view.

Calculation Viewer Gaussian Cube File Import

The comparison of geometries in Gaussian cube files in the Grid import module of the Calculation Viewer has been modified so that files containing different geometries are imported as completely different systems. Previously, systems containing geometries with the same chemical formula and the same grid dimensions where treated as being different grid data for the same geometry.

Calculation Editor Final Edit

Calculation Editor Final Edit changes are now captured immediately when the file is written instead of only when the edit window is dismissed. This eliminates past confusion when a user writes out a modified input file opened with Final Edit, leaves the edit window up, launches the job and then finds that their Final Edit changes were not included in the input file of the submitted job.

Input File Formatting

The Calculation Editor now removes multiple blank lines whenever generating input files for any code. This is a special post-processing step applied after the input file is first generated. The input file templates, especially for NWChem, would often produce several meaningless blank lines between blocks of actual input directives making the files hard to read and often confusing when valid input was below view when using Final Edit. This post-processing step can easily be extended in the future as necessary to support other code-independent input file modifications.

Data Server Authentication Dialog Crash
Fixed crash in the Data Server Authentication Dialog when hitting the OK button with an empty password field.

Builder PDB Export
The Builder export of PDB files has been modified so that residues are not permanently added to the system if no residues were present before the export was done. Previously, exporting a PDB file resulted in the creation of residues (if none were present beforehand) and disabled all editing functions in the Builder.

Builder PDB File HOH Residues
The name of O atoms in HOH residues in PDB files imported into the Builder is automatically changed to OW.

Partial Charge Toolkit Input File Generation
The Builder Partial Charge Toolkit was not creating charge groups using the correct format in NWChem input files. Both the Partial Charge Toolkit and the input file generation have been modified so that the correct format is used.

Trajectory Toolkit Bond Display
A bond is not displayed with the Calculation Viewer and Builder Trajectory Toolkit if neither atom at the end of the bond is displayed.

Periodic Table Atomic Energies Removed
The atomic energies table previously under the Periodic Table "Atomic Data…" menu item has been eliminated for v3.2. It was found that the underlying data was not being parsed correctly in all cases for different theory levels resulting in incorrect energy values. The effort required to remedy the problem would have exceeded the perceived value of this data to users so it was decided to drop the feature.

Job Launcher and Machine Browser Machine List
Removed duplicate entries of registered machine names in the Job Launcher and Machine Browser. This occurred when both the site and the user had registered the same machine. Now, the user's registration will override the site registration for that machine and only a single entry will be shown in the list of machines.

Job Launcher Automatic Display of Registered Machines
Whenever there are no currently configured machines for the code being used, the Job Launcher now automatically switches to displaying all registered machines rather than displaying an empty configured machines list. This eliminates some confusion for novice users with how to proceed when no machines are displayed.

Calculation Viewer Clipboard
In the Calculation Viewer, scenes copied into the Clipboard now correctly copy the camera settings for both perspective and orthographic style cameras. Previously, all Clipboard scenes used the perspective camera.

Calculation Viewer Table Export Crash
Fixed crash in the Calculation Viewer for exporting tabular properties to a file. The option menu for selecting the file format (ASCII or SYLK) was not being properly initialized resulting in crashes.

Calculation Viewer Property Options Menu
To save space, the drop down menu in the top-right corner of Calculation Viewer property panels no longer has the “Options” label, but just the arrow icon pointing downward indicating a menu.

Calculation Viewer Property Pane
When opening a property panel in the left pane of the Calculation Viewer, the left pane now automatically scrolls such that the entire panel is visible.

Builder Structure Library
User-created Structure Library entries have been fixed to support names with space characters. This is done by performing URL encoding/decoding of all request/response URL's send to and received by the Ecce data server. Previously, these new Structure Library entries would look to be added correctly, but would disappear the next time the Builder was invoked.

Builder Atom/Bond Display Style
The Builder display style of atoms and bonds is remembered after making them invisible and then visible again. Previously, styles reverted to a system default when visibility was restored.

Date and Number Format Incompatibilities
Dates and floating point numeric values (different radix) now always conform to the portable "C" or "POSIX" locale throughout Ecce. This corrected problems at sites, normally outside the U.S., configured for other locales.

Dialog Windows Hidden
Import and Export dialog windows such as in the Builder, Calculation Viewer, and Calculation Manager are placed such that they cannot be hidden or lost below other windows on the desktop. They are now always on top.

Visualization Background and Foreground Colors
Problems saving certain preferences such as visualization background and foreground colors in the Builder and Calculation Viewer have been fixed.

EMSL Remote Shell ssh2_emsl Removed
The remote shell named “ssh2_emsl” is no longer available within the EMSL deployed version of Ecce. The EMSL UNIX CaNS group now runs secure shell version 2 protocol compliant ssh and scp client programs in the user default path obviating the need for the

ssh2_emsl remote shell, which specified a hardwired path to ssh/scp instead of running the standard versions.

SITE ADMINSTRATOR WHAT'S FIXED

Code Registration Basis Set Library Name Usage
(3.2.4) A new EDML file element named "LibraryNames" controls whether to allow the use of basis set library names or explicit exponents and coefficients in the code input file. This element is part of the "GaussianBasisSetRules" block of the code registration .edml file. The default value is to allow library names, so this element only needs to be included when library names should never be used. Setting the value of the element to "False", i.e. "<LibraryNames>False</LibraryNames>", means exponents and coefficients will always be used. Further, the Calculation Editor "Use Exponents & Coeffs" toggle will be disabled when library names can't be used based on the .edml file registration, indicating that the user cannot override this setting.

Code Registration File Name Hardwired
(3.2.4) The name of the code registration parse descriptor ".desc" file was found to be hardwired based on the name of the code, rather than being derived from the name specified in the ".edml" registration file.

New System Library Bundled for "Rocks Cluster" Linux
(3.2.4) The Linux system library libgcc_s.so.1 is now bundled with the Ecce glibc 2.3 distribution. The version of this library already included with the "Rocks Cluster" operating system was found to be incompatible with other system libraries bundled with Ecce. Including the library allows Ecce to run on this operating system.

XMODIFIERS Environment Variable on SUSE Linux
(3.2.4) Under the SUSE operating system it was found that setting the $XMODIFIERS environment variable would prevent Ecce from running. This variable is now unset in the setup script when starting Ecce on all Linux operating systems in case it happens to conflict with any other Linux versions.

Netscape Startup for Online Help on SGI and Sun
(3.2.4) On some SGI systems, and potentially Sun as well, the Netscape web browser failed to start when requesting Ecce online help or the support web form. This was the result of a conflict between Netscape and the $LANG "localization" environment variable. Unsetting this variable within Ecce just prior to starting Netscape resolves the issue and invoking Netscape for Ecce online help on SGI should no longer be an issue.

Automatic Server Account Creation
(3.2.2) The site configuration variable that determines whether to automatically create an Ecce server account the first time a user runs Ecce originally allowed individual users to override the setting for themselves. This defeated the purpose if a knowledgeable user

could always create an account simply by setting an environment variable to circumvent the site administrator's policy. To fix this, the variable ECCE_AUTO_ACCOUNTS can no longer be overridden by users and the value specified in the $ECCE_HOME/siteconfig/site_runtime file is always used. The default for new Ecce installations remains the same to automatically create new Ecce server accounts.

Invalid Job Submit Scripts

(3.2.1) A potential error in generating job submit scripts has been fixed by including additional blank lines in the submit script. Depending on whether certain submit script "blocks" such as "FilesToRemove" were omitted by a site registering a compute server, it was possible for lines in the generated submit script to be inappropriately joined together without needed carriage returns. In the particular case where this problem was found, jobs would still run but the completion state would always be set to "Killed".

Gaussian Job Submit Scripts

(3.2.1) The Ecce generated Gaussian 03 job submit script has been updated to be identical in format to the Gaussian 98 script. In the Ecce v3.2 release, Gaussian 03 job submit scripts inadvertently omitted the "FilesToRemove" block. Further, both the Gaussian 98 and Gaussian 03 job submit scripts no longer set $LD_LIBRARY_PATH as this was an EMSL-specific requirement.

Job Launcher Post-Processing Fixes

Job Launcher post-processing scripts (*.launchpp files in the scripts/parsers directory) now take parameters from a file instead of the command line. This eliminates failures in job launches due to the command length exceeding the fixed 256 character C shell buffer. This would happen often when either or both the installed path to the Ecce application software or the calculation path in the data server project tree for the job being launched was particularly long.

Data Server File Transfer

All file operations to and from the Ecce data server now use temporary files instead of in-memory buffers to avoid memory limitation problems.

WHAT'S BROKEN

NWChem Spin-Spin Indirect Coupling

(3.2.3) The NWChem spin-spin indirect coupling is not currently parsed correctly if this property is calculated. This is due to a bug in the output to the ecce.out file that should be fixed when either a patch to NWChem 4.7 or subsequent version after 4.7 is released. This bug also results in other valid properties occurring after the spin-spin coupling in the ecce.out file not being parsed. The workaround is to deselect the Spin-Spin Indirect Coupling toggle in the Calculation Editor Runtype Details dialog that is enabled by default for unrestricted Hartree-Fock and Density Functional Theory calculations when running NWChem 4.7 without the proper patch.

Basis Set Tool Import Fragment Disabled

The Import Fragment feature available when invoking the Basis Set Tool from the Gateway outside the context of a calculation has been disabled. Multiple problems were found with this capability and the usage level of this feature did not justify the effort to fix them.