ECCE 4.x RELEASE NOTES

Version 4.0—September 29, 2006
Version 4.0.1—November 6, 2006
Version 4.0.2—February 7, 2007
Version 4.5—November 15, 2007
Version 4.5.1—December 27, 2007

The intent of this page is to provide information specific to the 4.x versions of ECCE. Version 4.0 supports the NWChem molecular dynamics module for setting up, running, and viewing results of molecular dynamics simulations. New protein rendering styles for large bio-molecules are available and overall data management and visualization capabilities have been upgraded in ECCE 4.0 to handle 100,000+ atom chemical systems and the volume of output data typical of molecular dynamics studies in addition to existing support for electronic structure calculations. All new development starting with ECCE 4.0 is being done with a cross platform graphical user interface development toolkit in order to support platforms beyond Linux and UNIX in the future. With each successive 4.x release, additional existing "legacy" ECCE applications will also be migrated to this cross platform toolkit. Version 4.0.1 fixes several issues that existed in the initial 4.0 release including loss of property data in the Calculation Viewer while a simulation is running and improvements to the reliability of Java based inter-process messaging. Version 4.0.2 supports ECCE users outside the EMSL facility running jobs on the EMSL HP Itanium cluster, mpp2. Version 4.5 features a completely redesigned Molecule Builder user interface, cross platform toolkit ports of three more major ECCE applications, additional molecular dynamics capability, NWFS archive support for EMSL users, and a new messaging server implementation. Version 4.5.1 bundles the new NWChem 5.1 release and adds some Builder and Calculation Viewer enhancements. Version 4.5.1 notes, the latest release, have titles highlighted in **green text**.

RELEASE NOTES FOR PREVIOUS VERSIONS

Version 3.2.x Release Notes – April 5, 2006
Version 3.1 Release Notes – August 15, 2003
Version 3.0 Release Notes – November 13, 2002

WHAT'S NEW

Changing the Chemistry Code

(4.5.1) The Calculation Editor now supports changing the underlying computational code (NWChem, GAMESS UK, etc.) for existing calculations. Previously the code was

set when the calculation was first created and could not be changed after that point. Now, the code is still set when the calculation is initially created, but can be reset to use a different code from within the Calculation Editor. The top of the Calculation Editor main window has an icon button for each ECCE registered code that act like a radio button group for selecting the current code. By selecting a different code than what is currently set, all theory and runtype details parameter settings will be lost. However, the chemical system and basis set will be preserved when the code is changed. Additionally, the level of theory and the runtype will also be preserved if the newly selected code supports them. If not, the level of theory and runtype will be reset to values that are supported by the new code. This code change feature allows calculations to be easily setup for multiple codes sharing the chemical system and basis set configuration. Because changing the code is considered a fundamental change to the calculation and can result in loss of detail dialog parameter settings, a prompt is issued in the Calculation Editor to confirm the action before making the change.

NWChem 5.1 Bundled

(4.5.1) ECCE binary distributions for both Linux and SGI IRIX now include NWChem 5.1. Additionally the registration for the EMSL 12-teraflop HP Linux cluster mpp2 has been updated to run NWChem 5.1 for jobs launched from ECCE. No changes have been made to the NWChem code registration in ECCE specifically for NWChem 5.1 as input and output files are compatible with the previous NWChem 5.0 release. As with past releases of ECCE that have bundled NWChem, it is recommended that sites wishing to improve the performance of the computational code download and use a distribution of NWChem separate from the one bundled with ECCE. This allows NWChem to be tailored to the specific hardware platform where the distribution bundled with ECCE is more generic. For example, the Linux distribution of NWChem bundled with ECCE is a 32-bit executable even for 64-bit platforms and thus will perform poorly on higher performance Linux workstations. It is a straightforward matter to configure ECCE to run separately installed NWChem distributions using the Machine Registration application. ECCE bundles NWChem as a matter of convenience for those evaluating either ECCE or NWChem with the intent that users running the software for actual research will install NWChem separately. For less demanding computational applications on low-end hardware, it may be feasible though to continue using the ECCE bundled NWChem distribution.

Molecule Builder Manipulator Tools

(4.5.1) The two “manipulator” tools allowing atoms to be dragged in 3-D space and rotating atoms around bonds that were part of the Builder prior to the wxWidgets port, have been added back into the Builder for ECCE 4.5.1. The ball or sphere manipulator lets you select a group of atoms, add a spherical wireframe around the selection and then drag and rotate the sphere to move the atoms contained inside. The rotation manipulator lets you freely rotate around a bond (or any two atoms) to move all bonded atoms. With the ECCE 4.5 release, several users lamented the loss of these tools for quickly adjusting the position of atoms. In order to use these manipulator tools, you need to first place them on your Builder toolbar, accomplished by selecting “Manipulator Toolbar” from the Tools->Toolbars menu. ECCE will remember your preference for toolbars between

invocations after the first time it is initially added. Also note that the Coordinate Operations panel newly added with the Builder wxWidgets port allows more precise translations, rotations, and alignments of atoms to be performed.

Customizing Molecular Orbital Color

(4.5.1) A simple capability has been added to allow any arbitrary color pair for molecular orbitals displayed in the Calculation Viewer. This feature is useful for tailoring orbitals for publication or presentations when the existing ECCE color choices prove too limited. To use a custom color pair, one of two different environment variables must be set to specify the desired colors prior to starting the ECCE application software. Then, once in the Calculation Viewer, the "light/dark" color pair must be selected from under the Surface menu for ECCE to know to apply the custom colors. Two environment variables are provided in order to allow the colors to be specified in two different ways. Only one of the two variables needs to be set. The first variable is named $ECCE_SURFACE_COLOR1 where values for the red-green-blue components are specified between 0.0 and 1.0 as normalized floating point values. The second variable is named $ECCE_SURFACE_COLOR255 where values for red-green-blue components are given between 0 and 255 as 8-bit or 1-byte values. Each of these environment variables consists of six different numbers making up the RGB components of the positive and negative orbital lobes. Each of the six numbers is separated by any of four different tokens: a space, a comma, a colon, or a forward slash (/). For instance, if you wanted green and blue as your color pair, from the C shell prompt you could specify "setenv ECCE_SURFACE_COLOR1 0.0,1.0,0.0/0.0,0.0,1.0". Alternatively, you could specify "setenv ECCE_SURFACE_COLOR255 0,255,0/0,0,255". Make sure if you use spaces as separators between the color components that you quote the entire value of the variable. You are free to mix the space, comma, colon, and slash separators however you wish, although using the same separator token between red, green, and blue components and then a different one between the positive and negative lobes makes the value more readable. Finally, a good reference for choosing colors is the X Window System rgb.txt database of colors, found at /usr/X11R6/lib/X11/rgb.txt on most Linux systems. This file lists the 0 to 255 format RGB components for hundreds of colors along with a name for each color.

New Molecule Builder

(4.5) The ECCE team drew on user feedback over many years on what you did and didn't like about the existing version to drive the design of the new Molecule Builder. The result is a user interface that makes it easier to find functionality, is more customizable, adds new capabilities, and has a modern toolbar and "dockable panel" layout. Although the previous Builder offered a lot of flexibility in order to build almost any desired chemical system, it was often hard to know where to find and how to use the functionality required. The new Builder better adheres to conventions established by other builders and drawing packages to make it easier to find and use functionality, especially for users new to ECCE. The ECCE development team is confident that after an initial "getting acquainted" period, even long-time ECCE users will find that the new Builder improves their productivity over the previous Builder version. The new Builder was implemented with the cross platform wxWidgets GUI toolkit continuing the

migration of all ECCE applications from proprietary GUI technologies running only on the Linux/UNIX platform to an open source release on all common desktop operating systems. The new Builder includes web browser based help available by selecting the "on Builder…" menu item from the Help menu. We especially recommend this introductory level documentation to those users familiar with the previous Builder just starting to use ECCE 4.5. The new Builder is also available as a standalone distribution separate from the rest of ECCE.

Configuring New or Old Builder Version

(4.5) Because the new Builder user interface is quite a radical change from the existing Builder, plus there are two toolkit dialogs that have not yet been implemented in the new Builder, a configuration environment variable has been created to allow sites and users to select which version to run—new or old. The two dialogs that have not been implemented for the new Builder are the Topology Viewer and Force Field Editor, both used for defining structures for molecular dynamics simulations. Other than the specific functionality contained in the Topology Viewer and Force Field Editor, the remainder of the MD Builder functionality such as the MD Toolkit has been ported to the new Builder. Thus, if you use ECCE for running the NWChem MD module, you may wish to override the default setting of this environment variable that selects the new version of the Builder. Traditional ECCE electronic structure users though would not normally need to change the default setting of this variable unless they encounter difficulty in using the new Builder version. The environment variable that controls the version of the Builder is named $ECCE_WHICH_BUILDER. It is defined and documented in the application software $ECCE_HOME/siteconfig/site_runtime configuration file. Like other site_runtime file variables, the setting in the file acts as the site default and each user can override this default by defining a value for the $ECCE_WHICH_BUILDER variable in their own environment (e.g., ~/.cshrc file). There are three possible settings for this variable. A value of "new" (the default) specifies that the new version of the Builder should be used in all cases. A value of "old" specifies that the old version of the Builder should be used in all cases. A value of "new_except_md" specifies to use the new version for all cases when using the Builder for electronic structure calculations and to use the old version for molecular dynamics calculations. With the "new_except_md" setting, the old Builder will come up when invoked from the NWChem MD Prepare Editor for instance, while the new Builder will come up from the NWChem Calculation Editor.

New Calculation Editor

(4.5) The electronic structure code (NWChem, Gaussian, etc.) Calculation Editor has been ported to the wxWidgets cross platform GUI toolkit and includes a minor user interface redesign. Only the main window of the Calculation Editor was changed, as the underlying theory and runtype detail dialogs specific to each chemistry code had previously been ported to the wxPython (wxWidgets GUIs scripted in Python) toolkit. No new documentation has been created for the new Calculation Editor, but usage will be familiar to anyone who has run the old X Window System based Calculation Editor with only a few fields on the main window having been changed. The biggest difference in the Calculation Editor is the inclusion of two dialogs or toolkits for specifying

constraints/restraints and setting up partial charge calculations. These toolkits were previously part of the Builder application because they rely heavily on selection of the chemical system. But, the port to wxWidgets provided the opportunity to move these toolkits to a more intuitive spot when setting up code input rather than defining the chemical system. Access to these toolkits is based on the current run type that is selected in the Calculation Editor. For run types that find an optimized geometry, the "Constraint Toolkit…" button will be shown next to the "Final Edit…" button near the bottom of the Calculation Editor main window. The new Constraint Toolkit user interface follows the previous Builder based version. By choosing the ESP run type for NWChem, the "Partial Charge Toolkit…" button will be shown next to the "Final Edit…" button. The Partial Charge Toolkit user interface has been changed more significantly than the Constraint Toolkit from the previous version to simplify its usage. It now maintains a running list of command directives that have been created within the toolkit that will be included in the NWChem input deck.

New Basis Set Tool

(4.5) The Basis Set Tool was also ported to the wxWidgets cross platform GUI toolkit since the last production 4.0.2 ECCE release. Again, anyone familiar with the previous X Window System Basis Set Tool should be comfortable using the new wxWidgets version. The same functionality is available in the new version as the old, although there have been some minor layout changes to the main window. Access to the Basis Set Tool has been removed from the Gateway application for ECCE 4.5. This Gateway invocation was provided for using the Basis Set Tool outside the context of an ECCE calculation where the chemical system and code were specified within the Basis Set Tool and the results were exported to a file. The EMSL Basis Set Exchange web portal, available at http://bse.pnl.gov, is now the preferred means for selecting basis sets for running codes outside ECCE.

Support for Potential of Mean Force (PMF) MD Calculations

(4.5) The ECCE development team has continued to work on extending its support for different MD calculations by including options for setting up, running, and looking at the results of Potential of Mean Force (PMF) free energy calculations. This includes an additional tabbed panel in the MD Prepare task editor that allows users to add various PMF directives to the NWChem Prepare module input deck and new tabbed panels in the MD Optimize and MD Dynamics task editors that allow users to include options that control the number of windows, etc. in each calculation. For examining output from PMF calculations, the new PMF Grapher available from the Calculation Viewer lets the user select the PMF directive of interest and a subset of the PMF frames to graph. Energy distributions, coordinate distributions, and energy vs. coordinate can be graphed within the same plot or separately.

Enhanced MD Property Graphing

(4.5) The new MD Property Grapher allows the user to plot a single property against one or more other properties in an XY scatter plot, all of which appear in the same plot. Two lists of properties are shown in the user interface for the MD Property Grapher, which is invoked from the Calculation Viewer. One property is selected for the X-axis and one or more properties for the Y-axis before hitting the "Graph" button. Both the Property Grapher and the previously mentioned PMF Grapher use the Gnuplot package (http://www.gnuplot.info) to produce output graphs, allowing additional capabilites such as interrogating plotted data points for exact values. Additionally, both the Property and PMF Graphers can be run outside of the Calculation Viewer from the command line using the commands "eprp" and "epmf", respectively. The names of the .prp and .pmf type files to graph are passed on the command line to the scripts, usually with a wildcard file specification. This allows users who prefer to run NWChem MD simulations outside ECCE to use a portion of the ECCE MD analysis capability.

NWFS Archive Support

(4.5) Users of ECCE within EMSL now have the capability to store the large files produced by molecular dynamics calculations directly to the NWFS archive. The "Configure NWFS Archive Access…" menu item in the Organizer Edit menu is first used to specify to ECCE how to connect to the archive on behalf of the user (user name, password, and top-level directory). Then the MD Optimize and MD Dynamics task editors have a new dropdown menu under the Files/Trajectory panel for selecting to store output to the NWFS archive, the ECCE data server, or not to store output other than on the compute resource where it is calculated. All trajectory, restart, and PMF files produced by the calculation will be stored to the location specified by this menu setting. The Calculation Viewer transparently accesses this data from the location specified for each calculation (archive, data server, or compute resource) without any extra steps by the user.

External Access to EMSL mpp2 Itanium Cluster

(4.0.2) For the first time since the EMSL facility was required to restrict external access to the mpp2 cluster via a one-time login protocol, ECCE users are now able to launch and monitor jobs on mpp2. ECCE external mpp2 access is available to anyone who has obtained a time allocation on mpp2 and currently reaches mpp2 using an RSA SecurID token via the mpp2e front-end machine. To run a job on mpp2, select mpp2 from the list of ECCE registered machines in the Job Launcher, ignoring the fact that the external access to mpp2 normally goes through mpp2e. When the Launch button is hit, ECCE will display a prompt dialog for the passcode required to log onto mpp2e. Correctly entering the passcode will result in ECCE logging into mpp2e and then automatically hopping to mpp2 using the password entered in the Job Launcher Password field. The remaining steps in the ECCE job launch and monitor process, including file transfer, will proceed as usual without further passcode prompts. Other remote communication in ECCE, such as starting remote shells in the run directory, terminating calculations, updating molecular dynamics trajectories in the Calculation Viewer, and Machine Browser queries, will prompt for the mpp2e passcode when accessing mpp2. As before

the 4.0.2 release, ECCE mpp2 users inside the EMSL facility firewall where SecurID tokens are not required will not be prompted for a passcode since only the regular mpp2 password is required for access.

Calculation Viewer Histogram and Autocorrelation Plots

(4.0.1) The property data plots in the Calculation Viewer that display step series data have been extended to support two additional types of plots. These plots allow users to generate a histogram of the data values or to generate the autocorrelation function of a time series or other sequence of data points. The histogram function allows users to get a quick estimate of the average value of a property and the width of the distribution of property values. The autocorrelation function can be used to estimate decay times for property values (the autocorrelation function displays the autocorrelation of the fluctuations from the mean of the property). While these new plots are available for all properties, including those evaluated from ab initio electronic structure calculations, they are most useful for the time series properties produced by molecular dynamics simulations.

Calculation Viewer Batch Trajectory File Monitoring

(4.0.1) When batched trajectory file sequences are requested (from the Files panel of the MD Task Editor) when running an MD Dynamics or MD Optimize task, the Calculation Viewer Trajectory property panel better handles newly created batch files for local job launches. When animating the trajectory, the Calculation Viewer will check for any newly created batch trajectory files when it reaches the end of the trajectory animation sequence before restarting the animation from the beginning of the sequence. Any files found will be automatically added into the trajectory animation sequence. Previously the request to check for newly created trajectory files was triggered by the user hitting the refresh icon in the upper-left corner of the Trajectory property panel. This is still necessary when running the job to a remote computer since the operation of copying new batch files to the local machine for animation can be quite time consuming and thus would interrupt a running animation. It is worth noting, however, that this remote trajectory file transfer operation has been optimized to the extent that is practical so that it does not transfer over any completed trajectory files that have been previously transferred by a refresh operation. Thus, leaving the Calculation Viewer running during a long simulation and hitting the Trajectory panel refresh button from time to time will provide updates quicker than quitting and restarting the Calculation Viewer a number of times during the simulation.

NWChem 5.0 on EMSL HP Itanium Linux Cluster mpp2

(4.0.1) ECCE now runs the recent NWChem 5.0 installation by default on mpp2.emsl.pnl.gov. This is the version installed under /home/nwchem/nwchem-5.0. Users can override this default and run a different version of NWChem by setting the $ECCE_NWCHEM environment variable to a different path for the nwchem executable in their mpp2 login environment file (e.g., .cshrc).

Organizer "Force State to Failed"

(4.0.1) A new Organizer Run Management menu item allows the state of a submitted or running calculation (or MD task) to be set to the "system error" state. In certain circumstances when ECCE job monitoring fails there may be no other recourse than using this option to allow a job to be re-run or delete it. Please be careful when using this option to make sure that both the ECCE job monitoring and the computational job are no longer running. The "Terminate Calculation…", "Check Job Monitoring", and "Reconnect Job Monitoring" options should be considered first as they perform preliminary checks of the status of the job and ECCE job monitoring rather than force an immediate state change as the "Force State to Failed" option does.

New Organizer Features

(4.0.1) The Organizer has been enhanced with several new features for ECCE 4.0.1. First, the "shift-click" operation of starting a new instance of a tool (also equivalent to a right mouse button click) as in the Gateway is now supported in the Organizer context panels. Secondly, the left hand project tree view now automatically scrolls to show all children when expanding the contents of a parent project, calculation, or study. Similarly, the MD study right hand context panel now automatically scrolls to display the last task in the active branch of the workflow tree. A new "Go" menu has been added to the menu bar and includes a history list. Finally, keyboard shortcuts or accelerators for common menu operations have been added.

Residue Label Display

(4.0.1) The Builder and Calculation Viewer include preliminary support for displaying residue labels for chemical systems with this information. These residue labels display properly when using simple rendering styles like Ball and Stick and CPK, but do not work reliably for the new protein rendering styles including ribbons and cartoons.

Molecular Dynamics Support

(4.0) The ECCE 4.0 release is focused primarily on supporting the NWChem Molecular Dynamics (MD) module. ECCE can now be used to set up and execute the MD Prepare module as well as executing MD simulation tasks such as optimizing structures, single point energy calculations, and dynamics simulations. The new NWChem version 5.0 has been bundled with the ECCE 4.0 distribution capturing the latest features supporting MD as well as electronic structure computational chemistry. Free energy calculations and the functionality in the MD analysis module are not supported in this ECCE release but will be included later. Extensive documentation for this release is not available at this time. Users are encouraged to use the narrated screen-capture demonstrations available at http://ecce.pnl.gov/support/movie_index.shtml until more comprehensive documentation is available. Questions can also be addressed to ecce-support@emsl.pnl.gov.

Unlike electronic structure calculations, it is not possible to extensively default the calculation setup process for molecular dynamics and considerably more user expertise is required to set up calculations that will execute successfully. Potential users are encouraged to familiarize themselves with the basics of molecular dynamics simulation methodology and to understand the role of segment and/or fragment files in creating

solute models. Some familiarity with the Amber force field (Cornell et al., *J. Am. Chem. Soc*., 5197, **117**, 1995) and the evaluation of partial charges for MD models (Fox and Kollman, *J. Phys. Chem. B*, 8070, **102**, 1998) is also desirable.

The new MD functionality employs a workflow paradigm that necessitated the development of a new application to structure the creation of these workflows. This application, known as the Organizer, replaces the old ECCE Calculation Manager as the central point for users creating and accessing their calculations. Both electronic structure calculations, which can be organized within project folders, and MD calculations, which are organized within MD workflows called studies, are supported by the Organizer application. MD calculations within workflow studies are now referred to as MD tasks. These tasks are chained together with the output data of one task serving as the input for a subsequent task. Within each study exists an arbitrary number of MD tasks. Currently, the four tasks supported in ECCE are Prepare, Optimize, Energy, and Dynamics. Each task has an associated Editor that allows users to specify input parameters.
More information on the new Organizer and how to use it is available from within the online help available under the "Help" menu of the Organizer itself. For ECCE 4.0, this is the only new web-based help content that has been created. Electronic structure calculations can only be executed as standalone tasks (no chaining of data between calculations) rather than within a workflow study like MD tasks. Due to power of the workflow paradigm though and the recognition of its applicability to electronic structure calculations as well as MD, a future release of ECCE will support workflows of electronic structure calculations as is now supported for MD.

The MD Prepare Editor can be used to add counter ions and solvent to the system as well as supporting a variety of other modifications. Most of the functionality associated with the NWChem Prepare module is supported by the ECCE Prepare Editor, the only exception is functionality associated with free energy calculations. Successful completion of a Prepare task requires a complete set of fragment and/or segment files and complete coverage of all atom, bond, angle, and torsion types in the force field. The ECCE Builder Partial Charge Toolkit and Force Field Editor can be used to complete these files. More information about this functionality can be found both in the existing Builder online help (this functionality largely existed prior to the ECCE 4.0 release) and one of the narrated demonstrations previously mentioned is devoted to this topic. Successful completion of a Prepare task is also prerequisite to running any of the other MD tasks.

The remaining MD task editors are all similar and contain many of the same options. Each divides the interface for setting up the tasks into tabbed panels with a common set of panels available across all task editors. The Optimize and Dynamics Editors, however, do have unique panels containing options not available in the other tasks. These editors allow users to specify properties of the non-bonded interactions such as the cutoff distance and whether or not to use Ewald sums for the long range interactions. They also allow users to specify whether or not constraints are to be applied to atomic motion and what kinds of output should be generated. Users are encouraged to browse through all the editors to get a better sense of what functionality is supported.

In addition to supporting the setup and execution of tasks, the ECCE Calculation Viewer has been modified to support molecular dynamics simulations. At present, most of these properties are only generated during Optimize and Dynamics tasks. Standard properties, such as the total energy, temperature, and pressure are generated continuously during simulations and can be used to monitor the progress of calculations in a manner similar to that used for electronic structure simulations. The Calculation Viewer can also be used to visualize MD trajectory files. Further, the Calculation Viewer has been modified so that measures that have been attached to a trajectory visualization can be captured and exported to a file for additional analysis and display.

Because the large files associated with molecular dynamics trajectories create new data storage issues for ECCE, this release provides the ECCE site administrator with more latitude with regard to instituting a storage policy for these files. Via the site_runtime file in the $ECCE_HOME/siteconfig directory, the ECCE administrator can specify whether users are allowed to store trajectory files on the ECCE data server maintained at the site. The default for this option is to allow trajectories to be stored, so sites where there will be significant usage of the new ECCE molecular dynamics capability and where storage space may be taxed by storing these files may want to consider changing this default policy. If the site policy allows the storage of trajectory files on the ECCE data server, the MD task editors will enable the user to select a toggle to indicate whether to do so for each job that they run (if the site does not support saving trajectory files on the data server, this toggle will always appear disabled). By default this toggle is set to false even when the site policy allows trajectories on the data server to avoid inadvertent storage of potentially many gigabytes of data even for a single simulation. In the event that site policy dictates trajectory files can't be stored to the ECCE data server, users should make plans to store trajectory files elsewhere. Within the EMSL installation of ECCE, the site policy is to allow storage of trajectories on the data server as there is currently sufficient free disk space. Future releases of ECCE will support more options for linking to alternative data storage for these files besides the web data server. Even when trajectories are not stored on the server either by site policy or choice of the user for a simulation, visualization can still be done using the ECCE Calculation Viewer, as long as the data resides in the location where it was when the simulation was originally run. Trajectory files can also be viewed if they have been moved from their original location by bringing the Calculation Viewer up directly from the Gateway.

Requirement for .nwchemrc File

(4.0) In order to run the NWChem Prepare module, it is necessary to have an .nwchemrc file in the home directory of whatever machine is executing the Prepare module (this is usually the same machine that the user is running ECCE from). Without this file, the NWChem Prepare task will crash. Any solvent files that are to be used by NWChem must be specified in the .nwchemrc file (there is currently no way to specify the location of these files through ECCE). The .nwchemrc file can also be used to specify the directories used to find segment and fragment files and the location of force field parameter files. However, the Force Field Configuration dialog in the ECCE Builder MD Toolkit can also be used to do this and is more easily modified by the user. If force field files are specified in both the .nwchemrc file and the ECCE Force Field Configuration dialog, then all files

from both sources are used. More information on the format and contents of the .nwchemrc file can be found in the NWChem online documentation. The solvents currently supported by NWChem that need to be listed in .nwchemrc file are SPC/E water (spce), tetrahydrofuran (thfs), chloroform (clfm), and methanol (meoh). The restart files for these solvents are available in the $NWCHEM_HOME/src/data/solvents directory. Other solvents can be created by the user as described in the NWChem documentation.

Advanced Protein Rendering

(4.0) To accommodate the visualization of large bio-molecules up to 100,000 atoms and potentially beyond, the structure visualization in ECCE has been rewritten on top of a different toolkit for chemical system display. This new toolkit, OpenMOIV (see http://www.tecn.upf.es/openMOIV), is developed externally although the ECCE team has significantly contributed to the development of recent versions. This toolkit supports rendering of structures as ribbons and cartoons (alpha helices and beta sheets) among other options. A new custom display style dialog available from the Builder and Calculation Viewer allows mixing multiple display styles, setting color schemes, and selecting other advanced rendering options. An online ECCE 4.0 demonstration covers the usage of this new protein rendering capability.

Machine Configuration Redesign

(4.0) Those users of ECCE 3.x familiar with the concept of configuring machines for launch (setting the user name, password, remote shell, run directory, etc. for each machine and then saving this information for later use) from a separate dialog will find ECCE 4.0 has simplified this process. There is no longer a separate Machine Configuration dialog and making the changes directly to the Job Launcher will save those settings either when a job is launched or when another machine is selected from the option menu of registered ECCE compute resources. The save operation is done implicitly by ECCE rather than explicitly with a “Save” menu button or the customary ECCE “dirty star” icon in the feedback area. Configuring machines independently from launching jobs has always been a point of confusion with new ECCE users, which was the motivation for making this design change although there will be some initial confusion for existing 3.x users.

Cross Platform Migration

(4.0) In addition to comprehensive support for NWChem molecular dynamics, ECCE 4.0 also introduces the first major steps towards migrating the application software from the Linux/UNIX environment to support multiple platforms including Microsoft Windows and Macintosh OS X, as well as continued support for Linux and UNIX. As the largest component of this migration, user interfaces are being developed using the cross-platform open source wxWidgets toolkit instead of the X Window System Motif toolkit that has previously served as the basis for all ECCE application user interfaces. Due to the volume of ECCE software, this migration must be done in a staged effort. For ECCE 4.0, all new development for supporting molecular dynamics has been done using wxWidgets. Additionally, the Organizer has been developed with wxWidgets, replacing the X/Motif based Calculation Manager. Finally, several “legacy” ECCE applications have already

been ported to wxWidgets including the Gateway, Job Launcher, Machine Browser, Machine Registration, and Periodic Table. Electronic structure code registration theory and runtype details dialogs have been migrated from the PyQt toolkit to the wxWidgets based integration with Python, wxPython. The user interfaces to most of these legacy applications ported to wxWidgets will look very familiar. Besides the changes already described for the Job Launcher, only the Machine Browser is significantly different. The new Machine Browser provides more at-a-glance information to the user about registered ECCE machines as well as being significantly more intuitive to use. The next major release after ECCE 4.0 will contain wxWidgets based versions of more legacy applications such as Basis Set Tool and Calculation Editor.

SITE ADMINISTRATOR WHAT'S NEW

Elimination of 64-bit Itanium Distribution

(4.5.1) A single distribution of ECCE is now used for all Linux platforms. Previously 64-bit Itanium processor (ia64) based Linux platforms used a special distribution of ECCE separate from all other 32- and 64-bit platforms. With the ECCE 4.5.1 release, the Itanium processor ia64 release has been eliminated. Only the distribution of NWChem bundled with ECCE was different between the two Linux distributions available for ECCE 4.5. The ECCE Linux distribution consists of 32-bit applications that run on 32- and 64-bit platforms. This requires the installation and use of 32-bit compatibility libraries on some 64-bit systems that otherwise cannot run 32-bit applications. Because of the system log warning messages that are issued from running a 32-bit version of NWChem on an ia64 workstation (see below release note on the Itanium distribution), it is recommended that users download and install a distribution of NWChem specifically built for that platform.

New Java Messaging Server Implementation

(4.5) The previous JORAM server implementing the Java Messaging Service has been changed out in favor of the Apache supported ActiveMQ server in ECCE 4.5. The most important reason for making this change was eliminating a pervasive problem experienced by many sites where the client side messaging session disconnected from the messaging server. Often that would happen when leaving an ECCE session running idle such as overnight and then returning to use it the next day. At that point any running ECCE applications would no longer function properly and it was not possible to start new applications. A slew of Java "out of bounds" error messages to the console where the session was started also accompanied this problem. The only workaround was to quit out of each ECCE application separately and restart the session. The new ActiveMQ server (http://activemq.apache.org) has become a more widely used JMS implementation than JORAM over the many years since ECCE adopted JMS for inter-process communication (ActiveMQ did not exist when ECCE first selected a JMS implementation). Configuring ActiveMQ is also a bit simpler than JORAM with only a single client side configuration file (jndi.properties) and a single server side configuration file (activemq.xml). The ECCE distribution installation script makes the necessary updates for these two files and site administrators normally do not need to be aware of these details. You will notice that

the console output from starting the ActiveMQ server is different than from JORAM, but it is really only necessary to scan this output for errors, usually in the form of Java tracebacks. Another advantage with ActiveMQ is that only one socket port is used for messaging rather than the three ports needed for JORAM. By default ECCE uses the port 8088 for ActiveMQ, which was also one of the three used for JORAM. The installation and administration manual describes how to change this port if needed. Finally, the server "upgrade" option available from the installation script main menu does support upgrading what was previously a JORAM messaging server to become an ActiveMQ server so the changeover to the new JMS implementation should be transparent to both the ECCE site administrator and users.

One-time Login Compute Resource Support

(4.0.2) In order to support external access to the EMSL mpp2 cluster, extensive changes were made to the ECCE remote communications subsystem. Changes include support for interactive prompting while remote communication shells are being created, high-speed and reliable file transfer over a remote shell connection (e.g. ssh) instead of a remote copy command (e.g. scp), and sharing remote shell connections between ECCE applications that were previously distinct processes. These changes were dictated by the desire to impose the minimum possible number of interactive prompts on users for logging into machines requiring one-time logins for job launching, monitoring, etc. Previously, for instance, a total of three remote connections (two remote shells and one remote copy) were created by ECCE to perform a job launch and initiate the monitoring process. These connections were all created invisible to the user since there was no need to interactively prompt for login information. With support for one-time login protocols, the job launch and monitor process is down to a single remote connection and thus a single interactive prompt to the user. Two new directives have been added to the $ECCE_HOME/siteconfig/CONFIG.<machine> file syntax: frontendMachine and frontendBypass. The frontendMachine directive is used to specify the full domain name of a "front-end" or "gateway" machine that is to be used to access the actual compute resource that is being registered. The frontendBypass directive is used when access to the compute resource via the machine specified by the frontendMachine directive is only required for users outside a network domain. The value of the frontendBypass directive is the name of the domain where users are not required to use the front-end machine. Please see $ECCE_HOME/siteconfig/CONFIG.mpp2 for an example usage of these two directives. The current ECCE remote communications protocol, which can be extended by the ECCE team as needed for external sites to support other machines requiring front-end or one-time login access, expects the remote shell prompt of "PASSCODE:" to determine when to interactively display a prompt dialog. Whenever this prompt is issued by a command line remote communications shell such as ssh, ECCE will display a GUI prompt dialog to collect this information from the user. Other remote shell prompts, such as "password:" along with a few variations thereof, will be automatically fed the password value that has been encrypted and saved by ECCE rather than interactively prompting the user for this information. Currently, only a single password for each compute resource can be saved with ECCE. This creates some restrictions on registering compute resources requiring a front-end machine or one-time logins. The ECCE team is

interested in hearing from external sites if these restrictions prohibit you from registering needed compute resources.

Running Local Java Install

(4.0.2) Due to some sites having difficulty getting ECCE to work with the version of the Java Runtime Environment (JRE) bundled with ECCE, changes were made to make it easier for these sites to bypass the ECCE distribution of JRE and use a locally installed version of Java instead. ECCE uses Java for the inter-application messaging that maintains consistency between applications when changes are made by the user or the ECCE software. Thus, if it appears that messaging is not working based on behavior of ECCE applications or Java-related warning/error messages are being issued to the shell window where ECCE was started, using a local version of Java may help resolve the problem. Changing the version of Java that is used by ECCE is done independently for the server and client ECCE software. For the server, which runs the JORAM Java Messaging Service, edit the start_ecce_server and start_ecce_message_server scripts in the ecce-utils directory under the ECCE top-level server install directory. Near the top of these files you will see the commented out statement "#setenv ECCE_LOCAL_JAVA". By uncommenting that statement (removing the "#" symbol), the ECCE JRE distribution will not be used when starting the message server. For ECCE client (application) software, individual users can choose to run a local Java version, or a site-level setting can be made applying to all users. The $ECCE_HOME/siteconfig/site_runtime file contains a new "ECCE_LOCAL_JAVA" key. Search for and uncomment this key if you wish to set a site-level default so all users will be using a local installation of Java. Alternatively, if problems with Java are tied to individual machines rather than all the machines at a site, each user can set the $ECCE_LOCAL_JAVA environment variable (such as in their .cshrc file) and override the site-level default. Finally, note that when choosing to use a local installation of Java for either server or client software, the path to the desired version must already be in $path or $PATH for the ECCE software to find it.

Itanium Processor Distribution of ECCE

(4.0.2) The ECCE 4.0.2 release includes a separate distribution for ia64 Intel Itanium processors running GLIBC 2.3 or 2.4 versions of Linux. Although the i686 processor distribution of ECCE will work on the ia64 processor, bundling a distribution of NWChem specifically built for ia64 was the reason for adding back the second Linux distribution. Besides improved performance running NWChem built for the 64-bit processor, using this version also eliminates warning messages being sent to the system log file. In fact, these system log warning messages also are issued when running the version of Java distributed with ECCE on the ia64 processor (whether running the ia64 or i686 distribution of ECCE). Thus, to completely eliminate warning messages from the system log generated by using ECCE, a local install of Java should be used (see the 4.0.2 release note related to running a local java install) in addition to the ia64 distribution of NWChem.

Apache Web Data Server Upgrade

(4.0.1) The Apache web server (http://www.apache.org/httpd), which serves as the data management system for ECCE, has been upgraded to Apache 2.0.59 for all platforms.

This release of Apache is principally a security release. The httpd.conf configuration file has also been modified to include the MaxRequestsPerChild directive with a setting of 100000. This directive limits the maximum number of requests that a given Apache httpd process will handle before voluntarily terminating and releasing any memory it has consumed. There is no impact to users of the Apache data server with these httpd processes terminating while ECCE is in use. Essentially this directive prevents an Apache process from consuming increasingly large amounts of memory. The default value for this directive is 0, which means that the Apache processes will never terminate. The ECCE team found that over a period of months, especially with the increased data management demands for supporting molecular dynamics, the memory consumed by the Apache httpd processes justified using this feature. This directive may be tailored to suit your site's requirements.

Upgraded Java Open Reliable Asynchronous Messaging (JORAM)

(4.0.1) The JORAM server (http://joram.objectweb.org) has been upgraded to JORAM 4.3.21. This replaces the JORAM 3.1.0 server previously bundled with ECCE distributions. This was a major upgrade and required changes to some of the ECCE server scripts, the Java property file jndi.properties, and the ECCE server application responsible for registering message topics on server startup.

Platform Support

(4.0) ECCE 4.0 runs under Linux GNU C Library 2.3.x and 2.4 operating systems including Redhat Fedora Core 3, 4 and 5, plus Redhat Enterprise Linux Workstation 3 and 4. SGI IRIX 6.5 continues to be supported as well. ECCE 4.0 does not support GNU C Library 2.2 Linux operating systems, such as Redhat 7.x, since glibc 2.2 operating systems are several years outdated and we can no longer maintain it within EMSL. Support for Sun Solaris has also been dropped for ECCE 4.0 with the expectation it will eventually return with the full cross-platform release of ECCE.

Installing ECCE 4.0

(4.0) Those users familiar with installation and administration of ECCE v3.x will find that little has changed in this regard for ECCE 4.0. The upgrade feature can be used to migrate data from an ECCE 3.x installation to ECCE 4.0. This applies to both the application side information (machine registrations, etc.) and to data server side information (user calculations).

SGI Colormap Display Setting

(4.0) The default X Window System server display setting for the SGI platform may have an inadequate number of available colormap entries to support ECCE 4.0, which includes more detailed icons than previous releases. This may result in failure to start ECCE 4.0 applications if the following procedure for changing the visual display setting (as the root user) is not performed:

1) Use the “xdpyinfo” command to list available display settings
2) Select a visual id from the list of visuals returned by xdpyinfo. We recommend a visual using the “TrueColor” class and a depth of 24 planes. For this example, say that visual id 0x40 was selected

3) Append the "-visid" flag along with the selected visual id to the end of the command contained in the /var/X11/xdm/Xservers file. In this case, "-visid 0x40" would be appended (without quotes) to the end of the command in the Xservers file
4) Restart the X server by either executing the commands "/usr/gfx/stopgfx; /usr/gfx/startgfx" or rebooting the machine

WHAT'S FIXED

Gaussian Transition State Calculations

(4.5.1) A bug in ECCE generated Gaussian-03 and Gaussian-98 input files for calculations attempting to find a transition state structure has been fixed. Previously these calculations would fail to run correctly because the input file route card was missing the "noeigen" and "calcfc" keywords needed for transition state calculations. This fix is only applicable for the Geometry and GeoVib runtypes when the runtype details dialog parameter for finding a transition state structure is explicitly selected. This parameter has a default setting to find a minimum energy structure and the input file was correct in this case.

Builder Display Style Preference

(4.5.1) A bug in the initial Builder port to wxWidgets for ECCE 4.5 kept the user's preferred display style (Ball & Wire, Ball & Stick, etc.) from being remembered between invocations. The display style would come up as "Ball & Wire" regardless of what it was set to when the Builder was last run. The last set display style is now correctly saved as the user preference and restored as the current display style for subsequent Builder invocations.

Application Handling of Renaming Calculations

(4.0.2) When calculations, projects, MD studies, and MD tasks are renamed in the Organizer, other applications were not updating in response to the new name. This could easily result in applications crashing and job monitoring halting with no further property or state updates. This situation existed for the 4.0 and 4.0.1 releases of ECCE and applied to every application that works on calculations/tasks (Builder, Basis Set Tool, Calculation Editor, MD Task Editors, Launcher, and Calculation Viewer). The 4.0.2 release fixes this problem and now all applications should properly handle renamed objects by updating their state to be consistent with the new name.

Transient Data Display in Calculation Viewer

(4.0.1) Real time job monitoring of molecular dynamics simulations over many time steps exhibited two bugs where some data points might be duplicated in a property graph or table while others might be dropped. Both problems have been fixed in this release. In addition, the performance of the graphing has been improved for real time monitoring by appending new points rather than redrawing the entire graph, though using the histogram or auto correlation views on large numbers of data points will be slow.

Basis Set Polarization Type

(4.0.1) ECCE applications were incorrectly deriving the polarization type (i.e. spherical or cartesian) for a calculation's basis set. This would cause, among other problems, incorrect generation of molecular orbitals in the Calculation Viewer. This has been corrected.

Electrostatic Potential Output Parsing

(4.0.1) Parsing of data from ESP calculations has been fixed so that the additional output from the two-stage restrained ESP calculations is correctly accounted for. This output is only available for ESP calculations done using NWChem 5.0. If a restrained ESP calculation is done with no charge constraints, the two-stage calculation is reported under the heading RESP2, if a constrained and restrained calculation is performed, the new data is reported under the heading CRESP2.

Geometry Optimization Plus Vibration Symmetry Label Parsing

(4.0.1) A parsing error for NWChem Geometry Optimization plus Vibration (GeoVib) calculations has been fixed that was incorrectly setting the orbital symmetry labels in the Calculation Viewer to the completely symmetric representation, even if correct labels were being reported by NWChem. GeoVib calculations that are performed using automatic symmetry detection should now report the correct symmetry.

Molecular Dynamics Job Monitoring on EMSL HP Itanium Linux Cluster mpp2

(4.0.1) Real time monitoring of molecular dynamics property and trajectory data for mpp2.emsl.pnl.gov has been fixed. The design of the NWChem molecular dynamics module mandates that both .prp property files and .trj trajectory files be generated in the directory where NWChem is run. For mpp2, this is on the compute nodes under the high performance /scratch local file system. This hardwired design in NWChem necessitated several changes to the design of ECCE job monitoring, which previously depended on all files that are monitored in real time being written to the calculation run directory. The end result of these changes are that the job monitoring perl script, eccejobmonitor, now runs on the head compute node for mpp2 job launches and has direct access to the /scratch property and trajectory files. The previous design only supported real-time monitoring of a single "non-batched" property file and did not display trajectories until after the calculation had completed. The new design display properties and trajectories as they are calculated both for batch file sequences as well as non-batched files.

Organizer Tree View Resource Type Representations

(4.0.1) The Organizer under certain conditions would incorrectly represent the type of a resource in its left-hand tree view. For example, a molecular dynamics task might have been shown as a project folder. This would cause the Organizer to display an incorrect set of operations for the resource when selected. Also, for the example described above, selecting the parent MD study would cause the Organizer to crash. This has been corrected.

Organizer Context Panel Focus

(4.0.1) The Organizer would easily lose the selection focus in the right hand context panel during refresh operations such as processing state changes for resources being displayed in the panel. This resulted in the user needing to continually re-select the resource within the context panel to perform operations from menus on the resource. This has mercifully been fixed.

Copying Folders Between ECCE Data Servers in Organizer

(4.0.1) A bug was discovered with copying a project under the “Share” folder from one ECCE data server to another. The project folder causing the bug to be manifested had been modified using the Organizer "Change Access Control" dialog to grant other ECCE users read and/or write privileges on the folder and its contents. This has been fixed.

Organizer Duplicate/Copy of Running Calculations

(4.0.1) When duplicating or copying calculations that are in the running state within the Organizer, the state was being set as “running” for the newly created calculation instead of being set to the “ready” state. These duplicated/copied calculations are now correctly set and displayed in the “ready” state.

Organizer Change Access Control

(4.0.1) The Organizer “Change Access Control…” Edit menu item was not enabled when selecting the user’s top-level home project folder. The “Change Access Control…” menu item is now properly enabled for all folders owned by a user including their home folder.

Organizer and Calculation Viewer Shell in Run Directory

(4.0.1) The Organizer and Calculation Viewer “Shell in Calculation Run Directory…” menu items now bring up an xterm window even when neither the run directory for the calculation nor the base run directory exist. Previously an xterm window would not come up in this instance and a cryptic error message was issued. The xterm that comes up now will be in the user’s home directory on the host where the job was run.

Calculation Viewer Display Style Preference

(4.0.1) The Calculation Viewer will now correctly save and restore the user’s last display style setting between invocations. Previously the display style was being set back to the “Ball and Wire” option each time Calculation Viewer was started. This fix makes the Calculation Viewer operation consistent with the Molecule Builder, which has always saved and restored the user’s last display setting between invocations.

Calculation Viewer Auto Normalize During Trajectory Animations

(4.0.1) In the Calculation Viewer Trajectory property panel, when animating a trajectory, the “Auto Normalize Display” toggle in the Options menu is now checked between each step to see if the system should be re-centered.

Builder and Calculation Viewer Print Dialog

(4.0.1) The underlying command used to generate the printer list for the Builder and Calculation Viewer Print dialogs has been enhanced to be compatible with more formats of the /etc/printcap file than were previously supported.

SITE ADMINISTRATOR WHAT'S FIXED

Apache Server Compression Module

(4.0.1) A memory leak type bug was discovered and fixed within the Apache filter module, Server Side Compression (SS_COMPRESSION).

Message Server Startup Script

(4.0.1) The start_ecce_message_server script aborted with a shell script error when the message server was already running when the script was invoked. The problem was related to the UNIX netstat command not being issued properly when attempting to check for busy ports. Now the start_ecce_message_server script correctly reports a busy port and gracefully exits when the server is already running. This same issue had been fixed in a previous ECCE release for the start_ecce_server and start_ecce_data_server scripts.

WHAT'S BROKEN

Raising Application Windows in Stacking Order

(4.0.1) With newer releases of the Linux KDE window manager including the version which ships with Red Hat Enterprise Linux Workstation 4, there is now a concept referred to as "focus stealing policy". By setting this preference as too high (strict) of a value, the ECCE functionality that raises an application's windows in the stacking order and un-iconifying application windows will no longer work. This functionality is accessible through the "windows" menu in the bottom right corner of the Gateway application. It is recommended that users relax their setting for the focus stealing policy within their window manager preferences outside ECCE if they find this to be a problem. This issue may also exist with Linux window managers other than KDE such as GNOME, although this has not been verified.