ECCE 7.x RELEASE NOTES

Version 7.0—August 1, 2013
Version 6.4—August 22, 2012
Version 6.3—April 4, 2012
Version 6.2—December 16, 2011
Version 6.1—July 25, 2011

The intent of this page is to provide information specific to the 7.x and more recent 6.x versions of ECCE. Version 7.0 includes condensed phase reaction rate prediction based on NWChem support for Plane-wave Metadynamics calculations. Version 6.4 is the open source release of ECCE. Version 6.3 is the initial source code release of ECCE with an automated build script along with the first 64-bit platform binary distribution. Version 6.2 replaces password encryption with an in-memory cache of passwords. Version 6.1 supports building periodic systems and setting up NWChem Plane-Wave Density Functional Theory calculations plus more explicit control for password prompting. Version 7.0 notes, the most recent, have titles highlighted in **green text**.

RELEASE NOTES FOR PREVIOUS VERSIONS

Version 6.x Release Notes – August 22, 2012
Version 5.x Release Notes – March 10, 2009
Version 4.x Release Notes – December 27, 2007
Version 3.2.x Release Notes – April 5, 2006

WHAT'S NEW

Condensed Phase Reaction Rate Prediction

(7.0) The ECCE user interface now provides a task chaining or workflow user interface for setting up, running, and viewing the results of Metadynamics calculations that are supported by the existing NWChem Plane-wave module. New ECCE tools are the Solvation Editor and the Metadynamics Editor. Modified ECCE tools are the Organizer, Builder, Launcher, and Viewer. The following narrative and figures walk through the use of newly added ECCE capability for performing condensed phase reaction rate predictions. A small portion of this walkthrough covers existing ECCE features in order to provide context.

When ECCE is launched, the user is presented with the ECCE Authentication graphical user interface. After the user enters a password to authenticate to the ECCE data server, the ECCE Gateway is shown. The server stores existing input and output files, setup details, and output properties for all of the calculations for each user of a site install. The

Gateway provides access to several of the other ECCE applications and top-level functions like starting context sensitive web browser based online help and closing all applications for an ECCE session. Figure 1 shows the Gateway application window inset within the ECCE Organizer application. The Organizer, invoked from the Gateway, is the user's primary view onto the ECCE data server. Each user has their own top-level folder that contains all of their calculations collected into other folders (called projects in ECCE) they have created as well as studies, which contain the chained tasks as used for condensed phase reaction rate calculations among other purposes such as gas phase reaction rate calculations and molecular dynamics simulations. Each top-level user folder is only viewable by that user unless the user grants either read or read-write access for the purpose of collaborating with others. A common project named "share" is also available with global read-write access for all users of ECCE at a site. Any user can create new projects, studies, and calculations under the share project. In this walkthrough a project named "STTR" has been created under share in Figure 1. Selecting the "STTR" project by clicking on it, highlights the name and makes it the context for subsequent Organizer actions such as creating children objects and invoking tools.

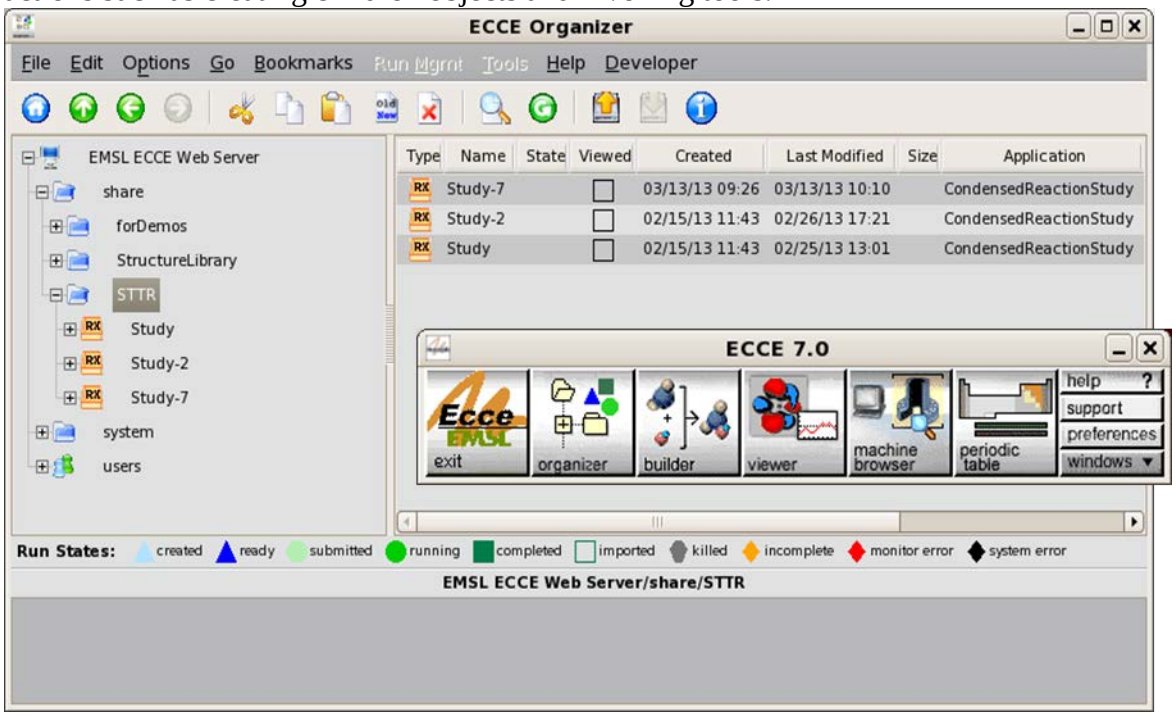

Figure 1. ECCE Gateway toolbar invoked from the command line and ECCE Organizer invoked from the Gateway. The Organizer has the "STTR" project selected in the left-hand pane as the context.

Figure 2 depicts the steps necessary for creating a condensed phase reaction study. From the File menu the "New Condensed Phase Reaction Study…" option is selected creating a new study under the "STTR" project. A study in ECCE allows a set of tasks or calculations to be connected together composing a workflow. The workflow has a hierarchical tree layout with parent and children tasks. Parent tasks feed their output as input to children tasks with ECCE knowing precisely what data to feed and how based on the parent and children task types. Multiple children can be created under a single parent task making branches in what can become quite sophisticated workflow trees, thus

allowing the user to explore alternative ways of determining reaction rates. This workflow study design has been used previously in ECCE initially for supporting NWChem molecular dynamics and more recently for the gas phase reaction rate prediction STTR. Significant enhancements were made to the ECCE Organizer in order to support condensed phase reaction rate workflows including adding support for new task types, allowing only valid sequences of tasks to be chained together and transferring the proper data between chained tasks. When a new Condensed Phase Reaction Study is created a Solvate task is automatically created as the top-level parent for any children tasks that the user will subsequently create. The purpose of the Solvate task is to define the chemical system of interest for that specific reaction rate study. By clicking within the border for the Solvate task in the right-hand workflow pane of the Organizer to set the context, the Solvation Editor application is invoked either by selecting "Solvation Editor…" from the Tools menu as shown in Figure 2 or from the right mouse button popup menu over the Solvate task.

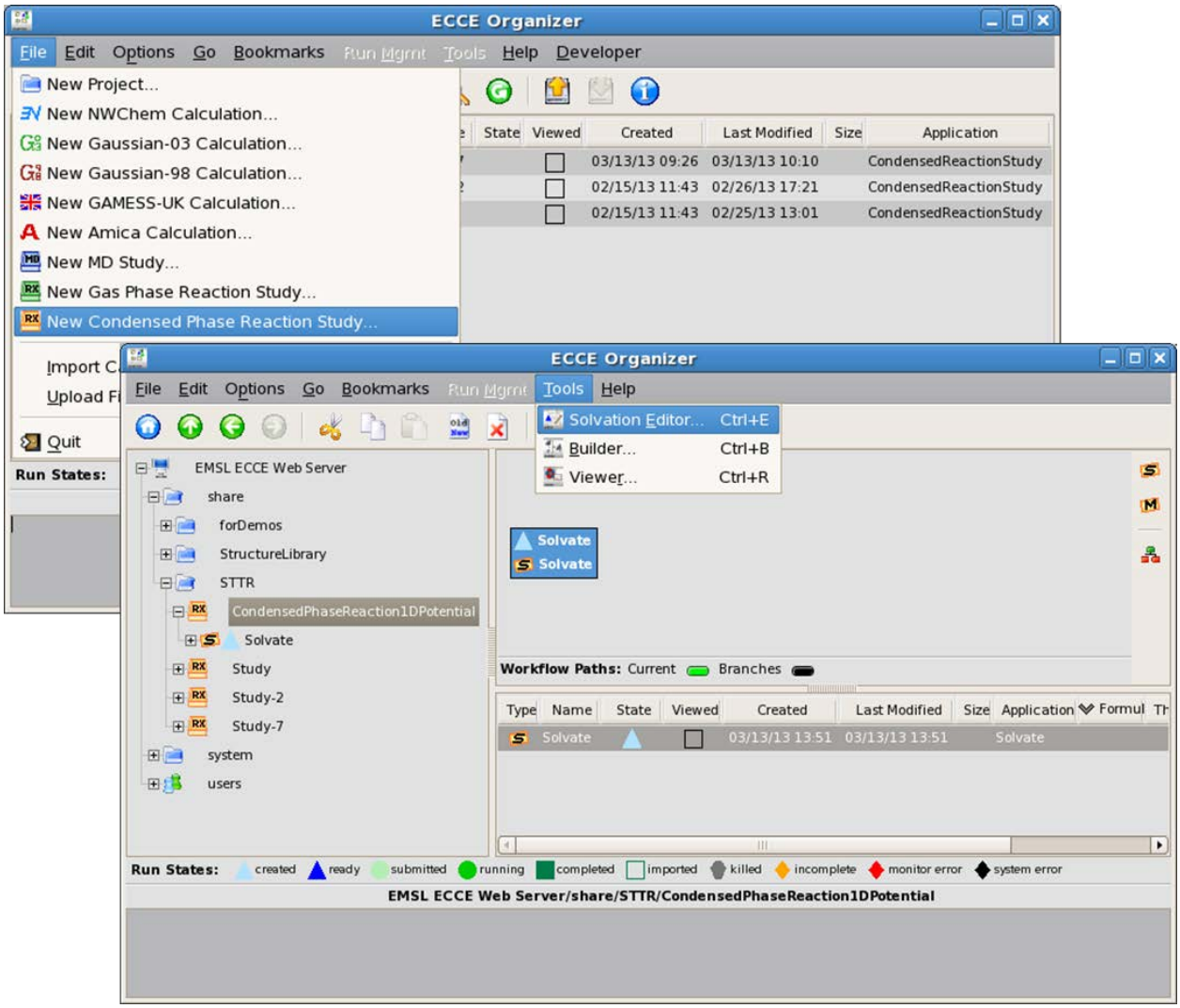

Figure 2. Creating a Condensed Phase Reaction Study in the Organizer (top-left screenshot). This automatically creates a parent Solvate task. The ECCE Solvation Editor application is invoked from the Organizer Tools menu (bottom-right screenshot).

The Solvation Editor application allows the user to specify the solute for the study and then solvate the structure based on settings specified in the application. Figure 3 shows the Solvation Editor as it initially comes up for a new condensed phase reaction study Solvate task. The first step is to build the solute by selecting the icon button labeled "builder" in the Solvation Editor. This invokes the ECCE Builder in the context of the Solvate task, as shown in Figure 4, so that what is built will be the solute after doing a save operation in the Builder. The Builder application is a sophisticated three-dimensional visualization and direct manipulation user interface with a wide variety of tools and features for creating and manipulating chemical structures such as periodic systems using symmetry building tools and residue-based biological systems using protein generation tools. For the purpose of creating condensed phase reaction solutes the user will typically either use the Builder to import a structure from a file in a format such as XYZ as a starting point and then likely modify it with Builder tools or build the structure from scratch. In building from scratch or modifying an imported structure, elements are selected in the Build panel (second panel from the top on the right-hand side of Figure 4) and then atoms of this type are added to empty bonding "nubs" of previously added atoms in the visualization workspace. The "Add H" button of the Build panel is used to automatically add Hydrogen atoms to all empty bonding nubs for the structure and then the broom icon is used to perform a basic force field clean operation adjusting bond lengths and angles over the structure. In Figure 4 a water molecule has been built as the solute with the final remaining step being to save the structure with the little floppy disk icon button at the bottom-left corner of the Builder.

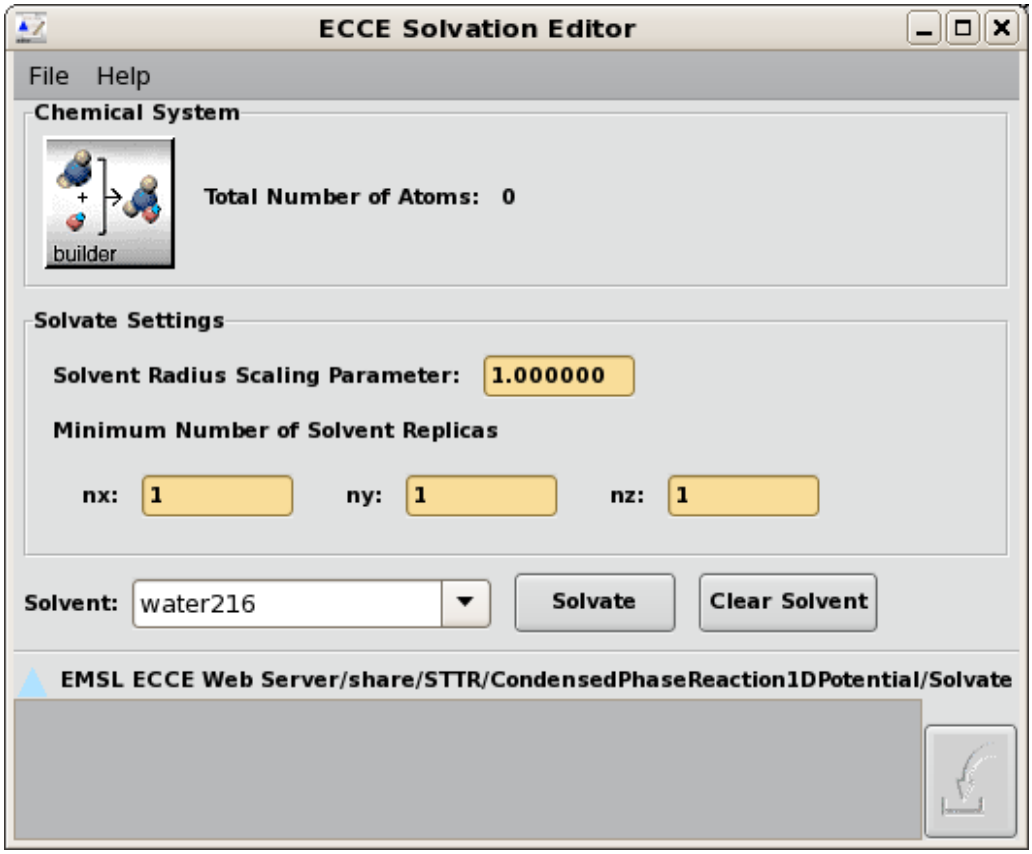

Figure 3. ECCE Solvation Editor as it comes up initially for a new condensed phase reaction study.

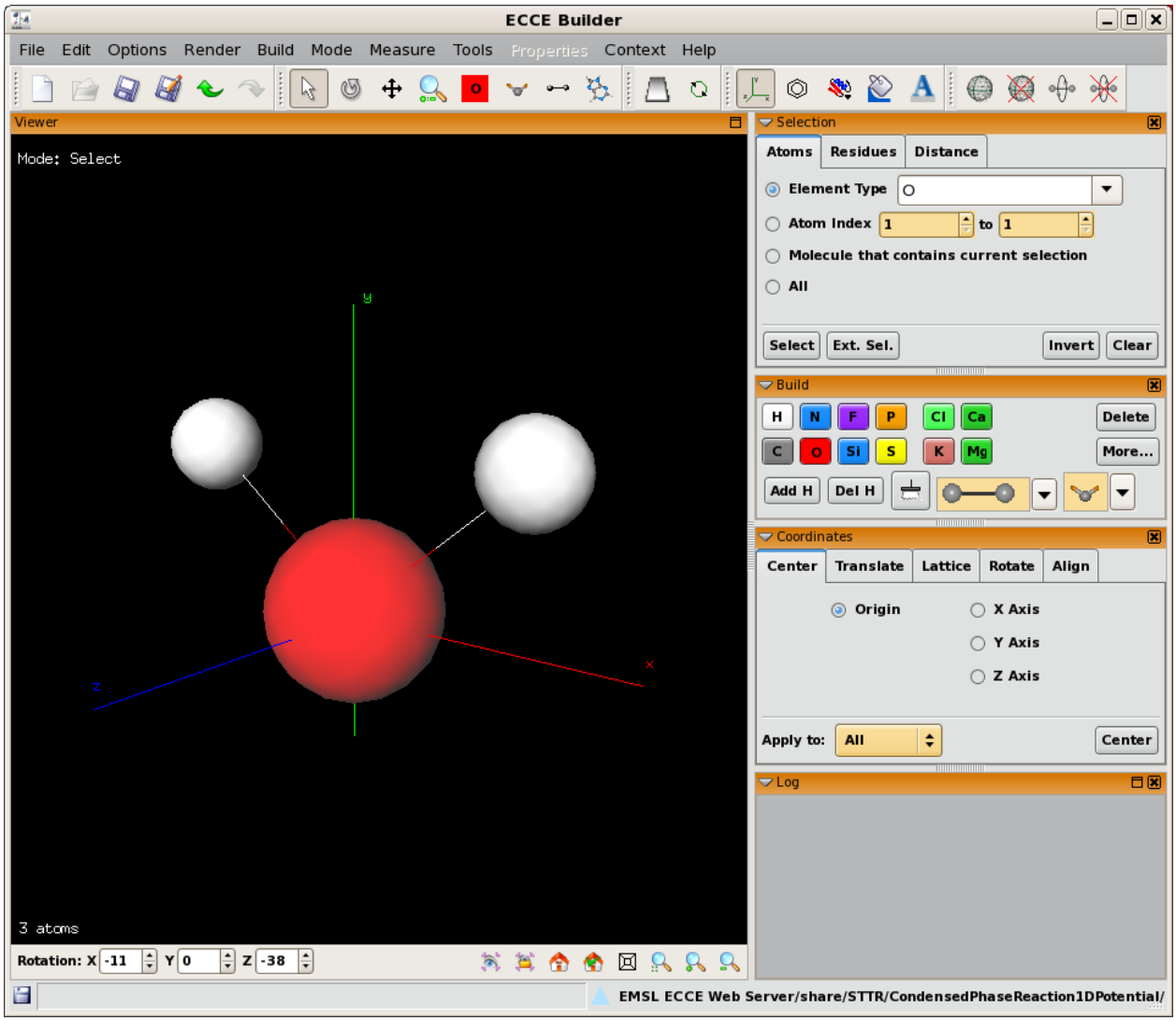

Figure 4. Creating a solute structure in the ECCE Builder invoked from the Solvation Editor.

After saving the solute structure in the Builder, the Solvation Editor application updates automatically to reflect the changes including the Builder icon being replaced with a thumbnail image of the solute. The other input fields on the Solvation Editor can be set prior to performing the solvate operation. The field labeled “Solvent:” is a dropdown menu listing the different solvent molecules and the number of molecules in the solvent box that will be applied. The default solvent configuration is “water216” meaning that a periodic configuration of 216 water molecules will be used to add solvent molecules in a box surrounding the solute. There is also a “water64” solvent configuration that can be selected to decrease the number of solvent molecules within the box. The specific solvent configurations that are included in the dropdown menu are based on files contained in a specific ECCE deployment directory. For an ECCE installation where the $ECCE_HOME variable is properly set to the top-level client installation directory the solvent configuration directory is $ECCE_HOME/data/client/solvents. The solvents in this directory are given in a simple XYZ file format where there is one solvent configuration per file with the file base name being the name of the configuration with an

extension of ".xyz". Thus, the solvent configuration file corresponding to "water216" is "water216.xyz". Users can easily add new solvents of interest in their work to their site installation of ECCE by creating new XYZ configuration files in this directory and the Solvation Editor will reflect any added solvents the next time it is invoked. The solvent radius scaling parameter is a scale factor that is used to determine whether a solvent molecule in the solvent configuration is too close to the solute molecule. If this happens, the solvent molecule is not included in the system. The cutoff criterion is to take all atoms on the solute and compare them to all atoms on the solvent molecule. If the sum of the Van der Waals radii of any pair of atoms times the radius scaling factor is larger than the distance between the two atoms, the solvent molecule is considered too close. The solvent radius scaling parameter can be used to increase (or decrease) the distance between the solute molecule and the surrounding solvent.

Figure 5 shows the state of the Solvation Editor after performing the solvate operation using the "water64" solvent. Hitting the "Solvate" button invokes the Builder if it is not already running and displays the solvated structure with the solvent molecules rendered as wireframe so the solute is easily visible. The thumbnail image for this newly solvated system replaces the previous solute-only structure in the Solvation Editor and the summary fields for total number of atoms and system dimensions are updated. The state of the task is set to "completed" indicated by the green square symbol near the bottom-left of the Solvation Editor (note that the full set of possible run states for a task are shown near the bottom of the Organizer as shown in Figure 1 and Figure 2). By completing the parent task it is now possible to perform any chained children tasks in the condensed phase reaction study. If desired, hitting the "Clear Solvent" button in the Solvation Editor removes all solvent molecules and restores just the solute, along with resetting the task state to "ready" to indicate a solvate operation needs to be performed before proceeding to chained tasks.

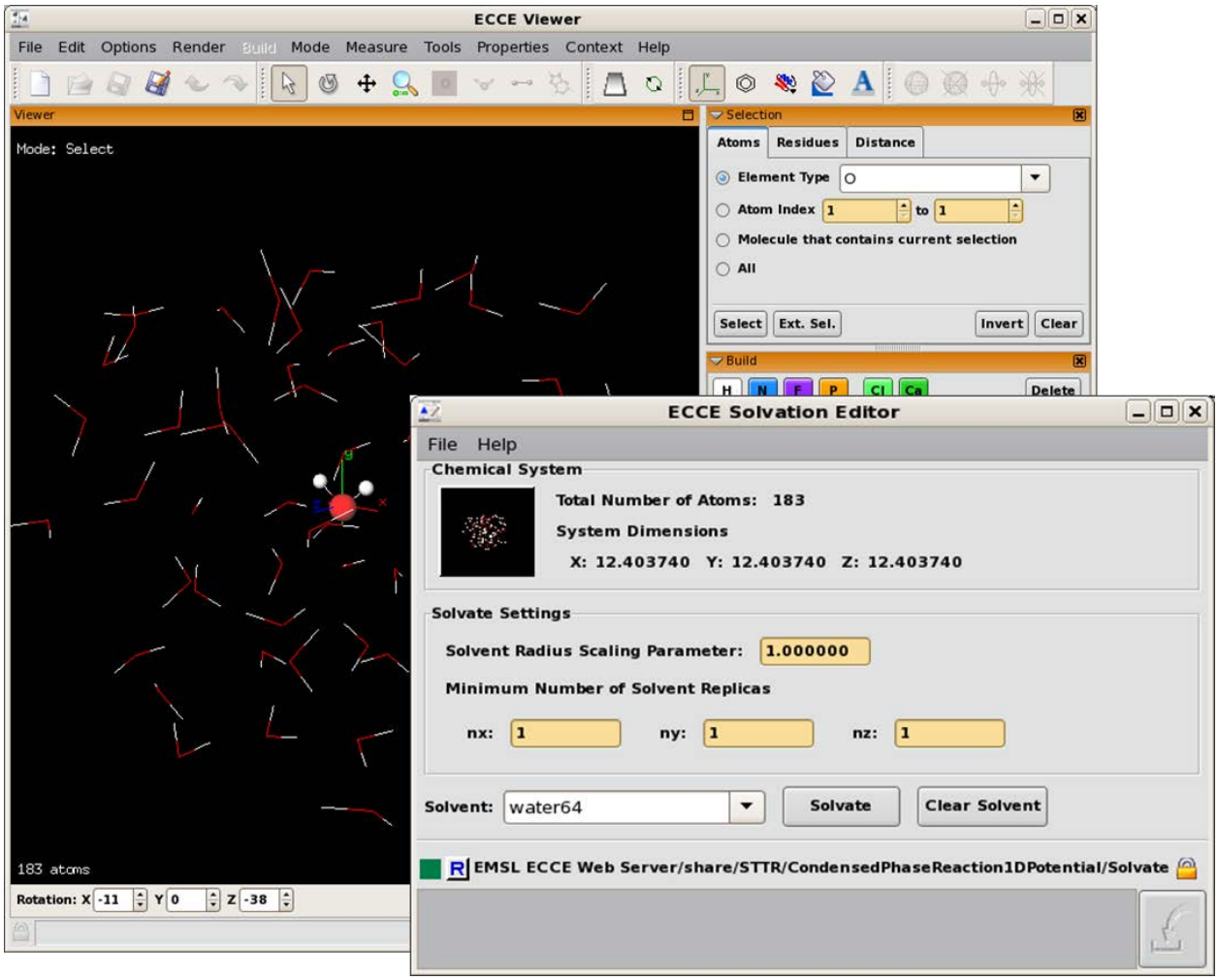

Figure 5. Hitting the Solvate button in the Solvation Editor brings up the Builder displaying the newly solvated system. Note that the Builder application is now labeled Viewer, which is a result of the task run state being "completed" indicating that the structure is read-only and cannot be changed directly within the Builder after solvation.

Figure 6 depicts a collage of three steps using the Organizer to create a Metadynamics task as a child of the previously created Solvate task. First, select the "New NWChem Metadynamics…" item from the File menu while the Solvate task is selected as the content in the workflow pane as shown in the top screenshot. This operation creates the Metadynamics task as a child of the Solvate task as shown in the middle screenshot. By selecting this newly created Metadynamics task using the left-hand tree view of the ECCE data server the right-hand pane will change from the workflow view for the entire study to being a task-specific view shown in the bottom screenshot. This task pane shows the tools available for that task with icon buttons to invoke each tool along with summary fields indicating progress in stepping through task setup and execution.

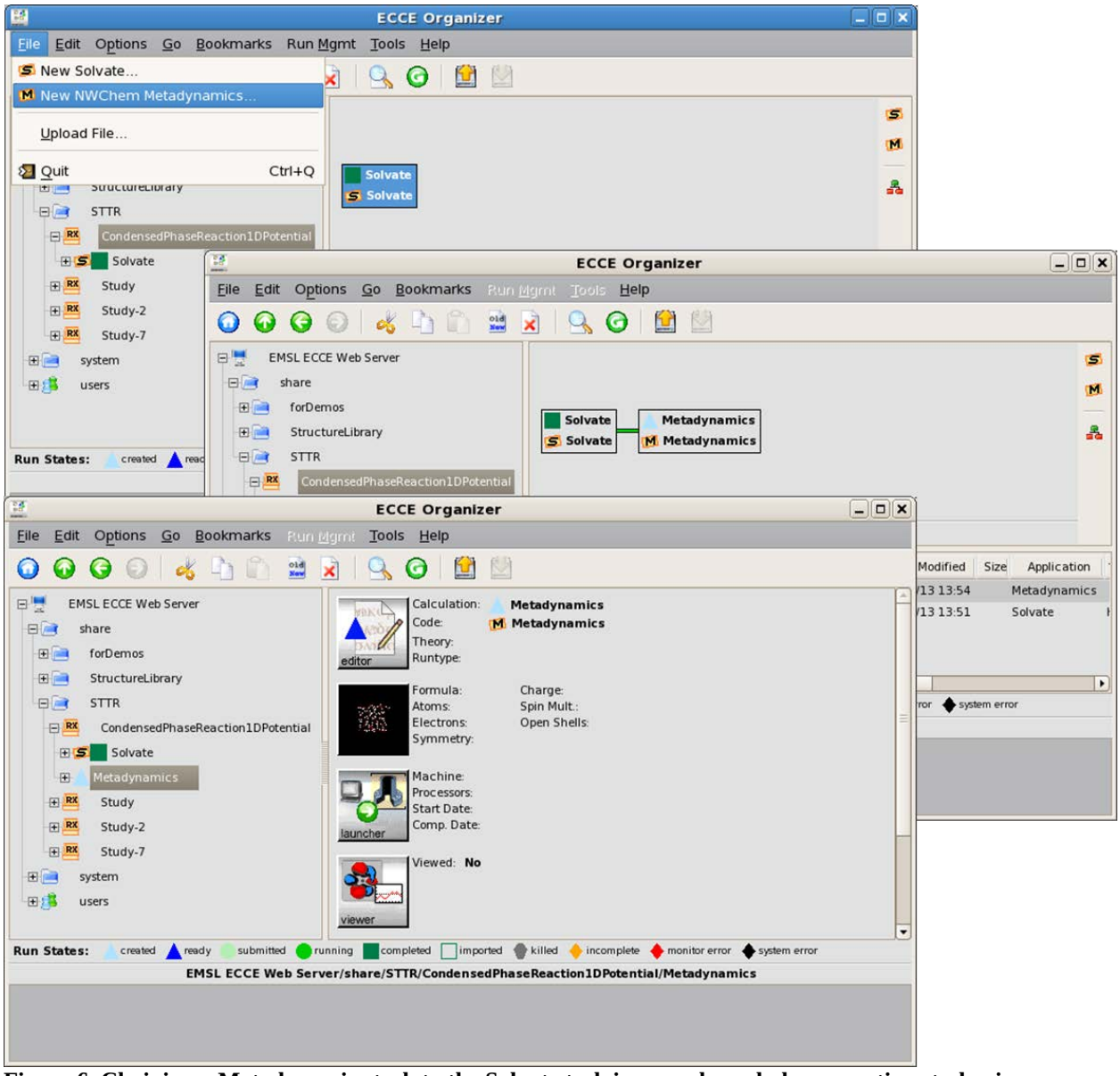

Figure 6. Chaining a Metadynamics task to the Solvate task in a condensed phase reaction study via the Organizer.

Hitting the icon button labeled “editor” in the bottom Organizer screenshot in Figure 6 invokes the Metadynamics Editor (the Metadynamics Editor is also accessible from the Organizer workflow pane analogous to how the Solvation Editor was invoked in Figure 2). Figure 7 shows the main window of the Metadynamics Editor before doing any task setup. The solvated chemical system is passed from the parent Solvate task to the Metadynamics task and thus its thumbnail image is shown along with the summary fields for the number of atoms and electrons. The chemical system charge and spin multiplicity can be set using dropdown menus in this area of the Metadynamics Editor main window. The Metadynamics Editor is a sophisticated user interface with a number of dialogs available from the main window for creating the input for an NWChem Plane-wave Metadynamics calculation. The interface is generic in the sense it allows different

variations of Metadynamics tasks to be created rather than single purpose such as calculating reaction rates. This allows user to perform energy minimization and system equilibration to initialize the metadynamics simulation. In this walkthrough an equilibration Metadynamics task is performed on the solvated system via a short simulation before adding a Metadynamics potential in a chained task and calculating reaction rates over an extended simulation. Several of the Metadynamics Editor dialogs will be described for this initial equilibration task and others will be described for subsequent tasks.

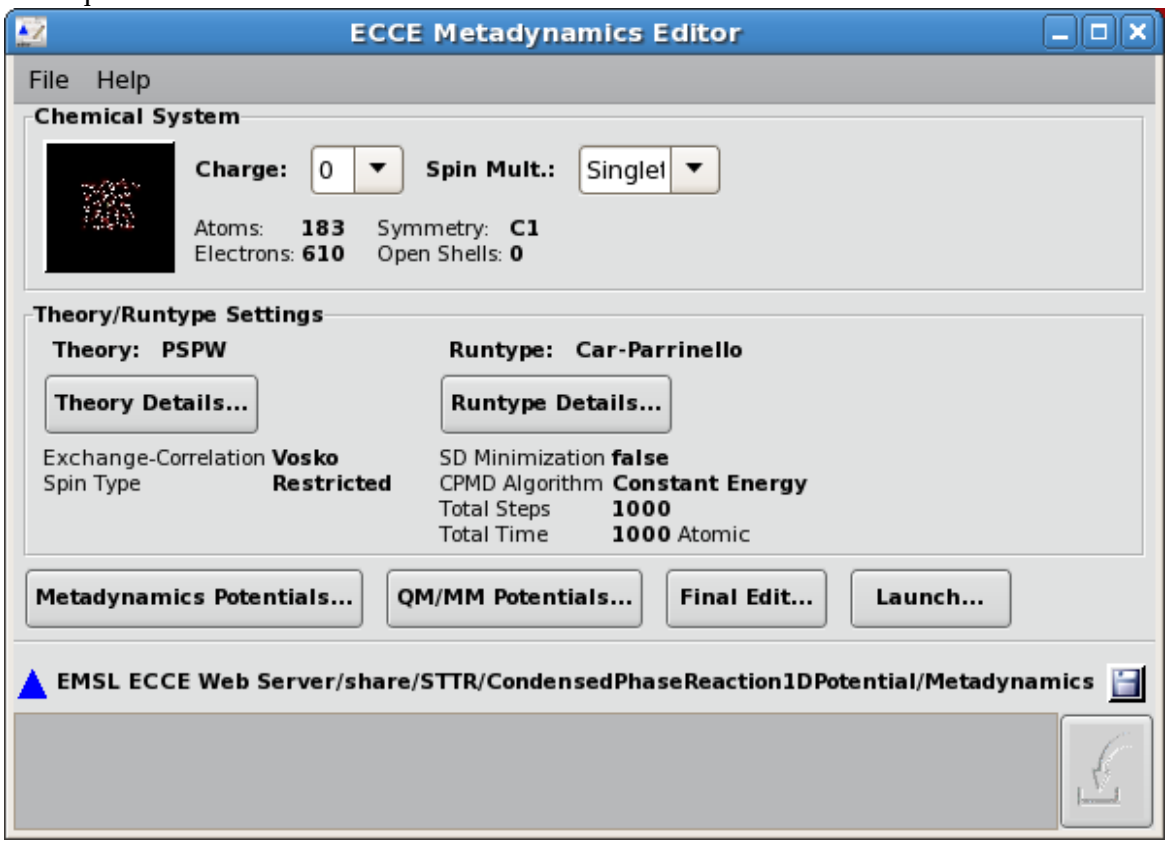

Figure 7. ECCE Metadynamics Editor as it comes up initially for a new Metadynamics task in a condensed phase reaction study.

The Metadynamics Editor Theory and Runtype Details dialogs are shown in Figure 8 and Figure 9, respectively. The Theory Details dialog is for setting the NWChem Plane-wave ("NWPW" block in the input file) specific parameters. The dialog initially displays all default values for running a Metadynamics task. Overriding a default adds that field to the NWChem input file whereas leaving the value as default omits it from the input file for readability. To facilitate the walkthrough many inputs are adjusted trading accuracy for faster simulation time. The exchange-correlation functional is being set to "pbe96" for performing the equilibration where the default is "Vosko" and the cutoff energy is being set to 10.0 Hartree. The Runtype Details dialog is for setting the Carr-Parinello block parameters that appear in the NWChem input file within the NWPW block. For this dialog the steepest descent minimization option was selected along with bumping down the simulation time via the outer iterations field (100 to 10), a CPMD algorithm of constant temperature was selected, and some Nose-Hoover settings were changed

including the electron period, ionic period, and ionic temperature. Note the Runtype Details dialog fields for total simulation steps and total simulation time. These fields are grayed out because they are read-only values calculated from other input fields—inner and outer iterations and time step.

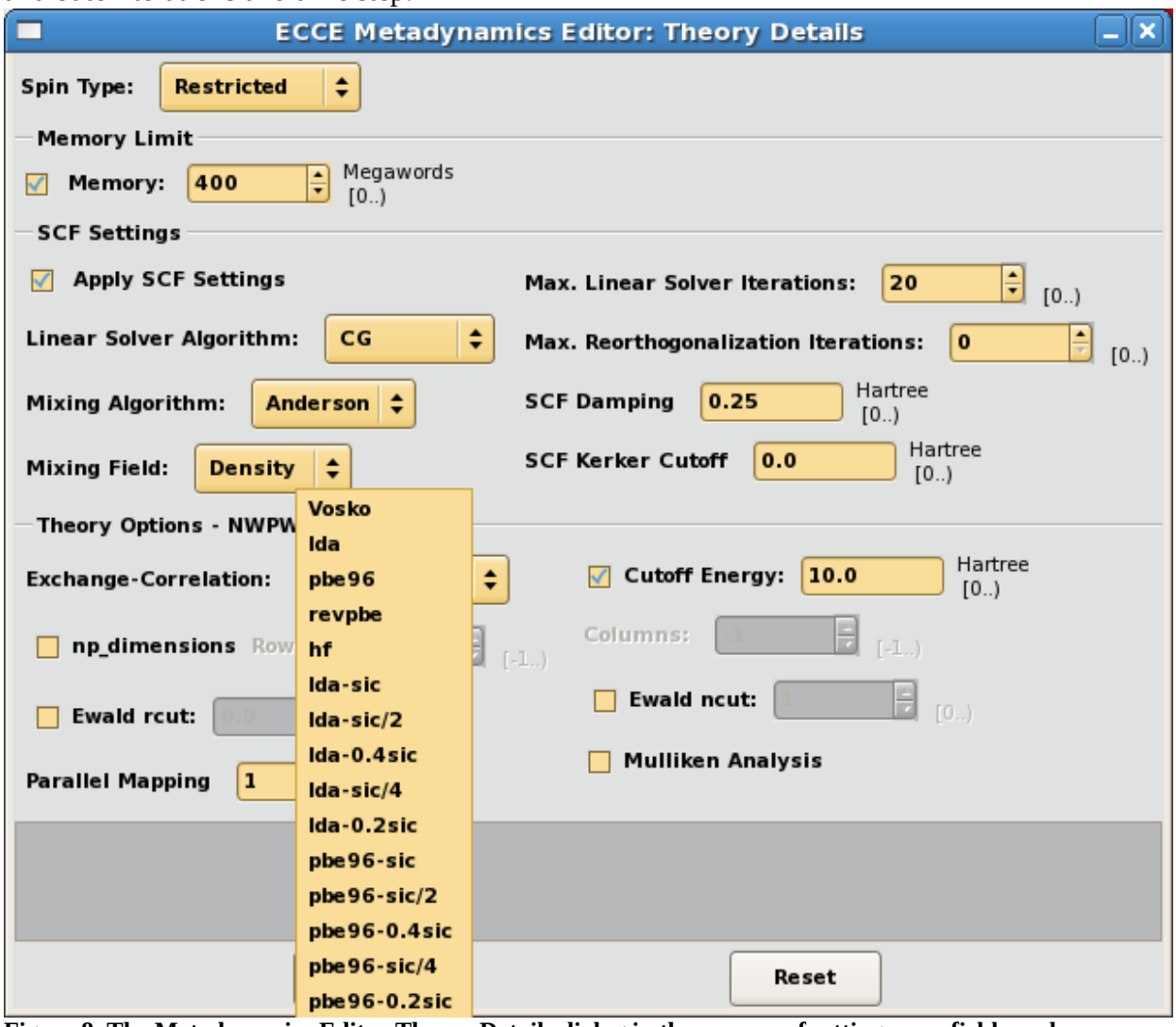

Figure 8. The Metadynamics Editor Theory Details dialog in the process of setting some fields such as the exchange-correlation functional for performing equilibration.

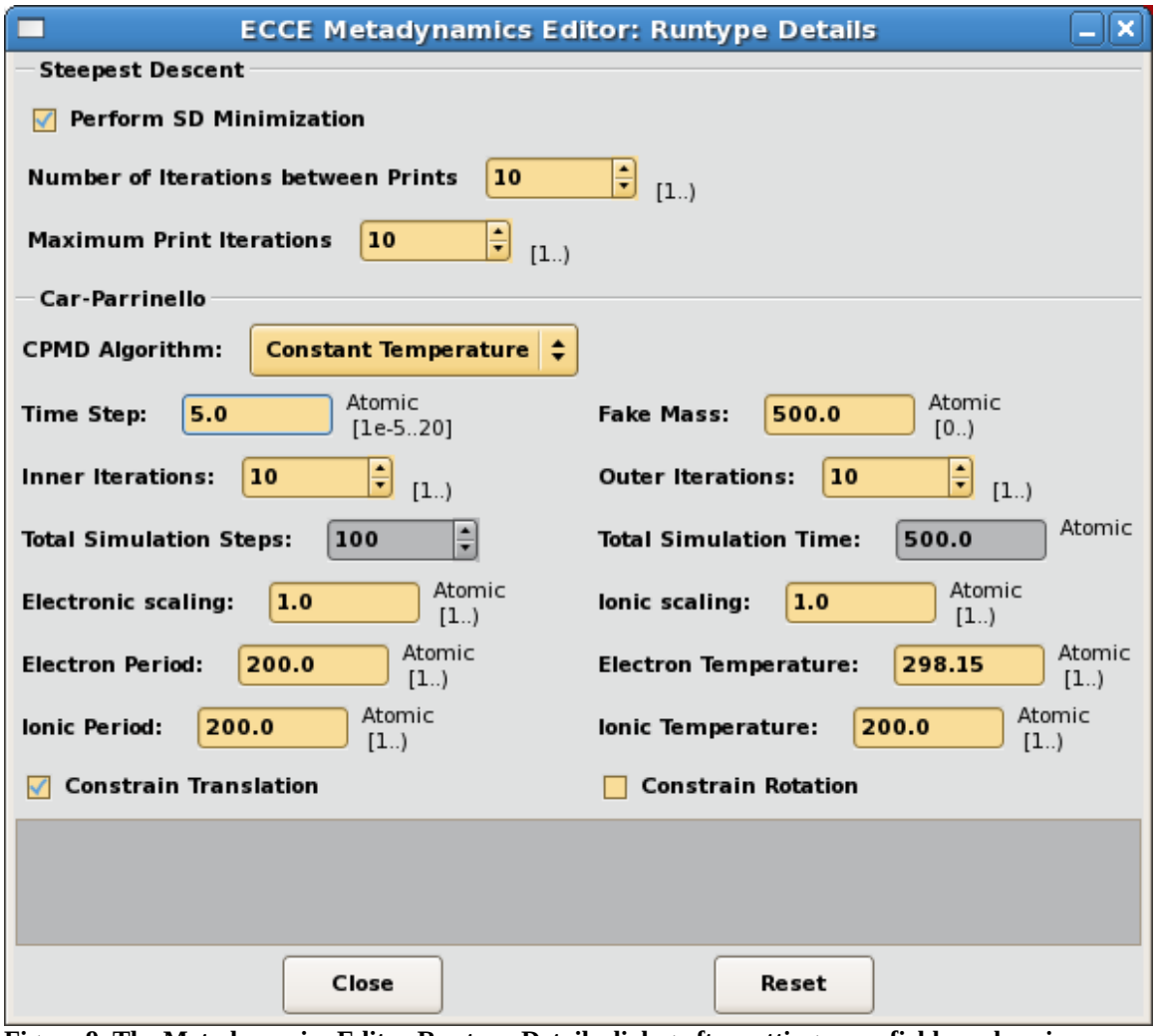

Figure 9. The Metadynamics Editor Runtype Details dialog after setting some fields such as inner and outer iterations for performing equilibration.

Ab initio molecular dynamics is performed by moving molecules subject to the forces defined by a potential energy function. ECCE provides support for QM/MM potentials, which couples the plane-wave density functional theory describing the solute (QM) to the classical potential of the solvent (MM). The solvent is treated classically because of the large savings in computational time. It is also possible to model the full system or a few additional solvent molecules using QM for cases where the solvent reacts with the solute. The last settings that are needed before running the equilibration task are under the QM/MM Potentials dialog as shown in Figure 10. This dialog is used for setting the classical potential terms describing the interactions between atoms on the solute and solvent, as well as interactions between different solvent atoms. These potentials are based on the solute and solvent atom types in the solvated system. These terms all default to zero until they are explicitly set through this dialog. For the equilibration the "Use Shake Constraints" option is set along with values for Sigma and Epsilon for the solute and solvent atoms and finally the solvent atom pseudo-potential terms. The "Use Shake Constraints" option currently only applies to solvent atoms with three atoms (e.g. water). For larger solvents, this option is not available and angle and bend potentials will

have to be supplied for the entire solvent molecule. Figure 11 is the Metadynamics Editor main window after making these changes via the Theory Details, Runtype Details, and QM/MM Potentials dialogs. Note the summary fields below the Theory and Runtype Details buttons showing the values of the most important parameters including the calculated field values for total simulation steps and time.

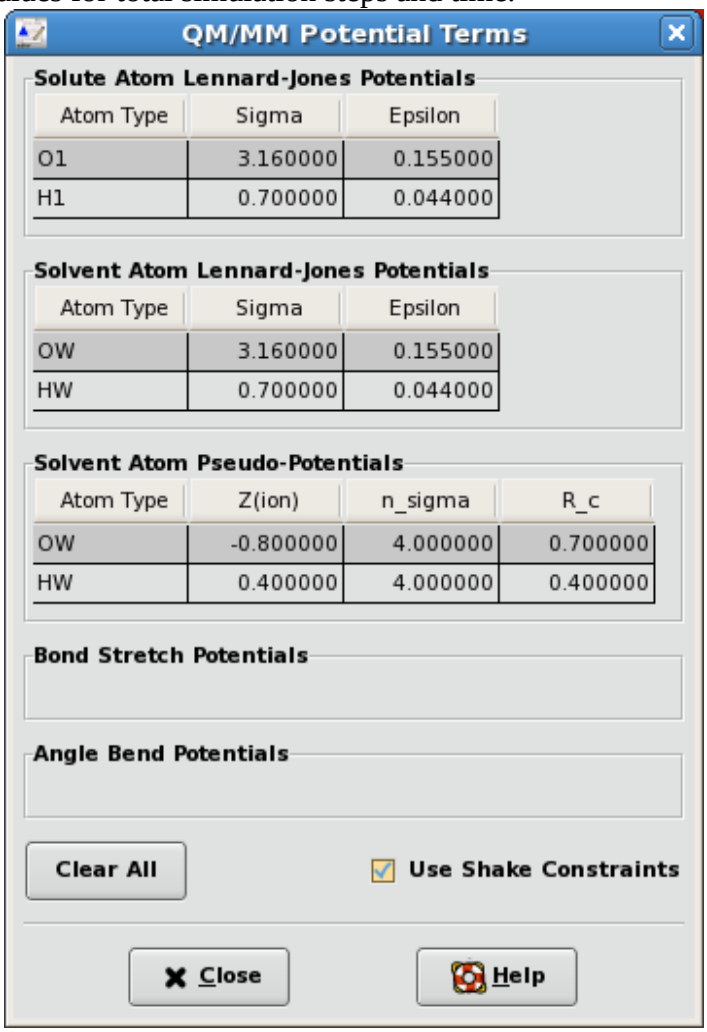

Figure 10. The Metadynamics Editor QM/MM Potentials dialog after setting potential terms for equilibration.

The "Final Edit…" button on the Metadynamics Editor invokes a text editor with the NWChem input file generated based on the current settings of the Metadynamics Editor including the solvated chemical system, main window charge and spin multiplicity fields, and all the associated dialog window settings previously described. Figure 12 is the NWChem input file as displayed by the final edit feature for the equilibration task. Most of the chemical system is scrolled out of view so that the more interesting parameters can be seen. The purpose of the final edit feature is for users who understand the underlying NWChem input file format to be able to make any additional changes to the input file not supported through the ECCE user interface. There are always some features of computational chemistry codes that are rarely used and it makes sense to only allow

experts to tweak those directly in the input file rather than adding confusing fields to the ECCE user interface.

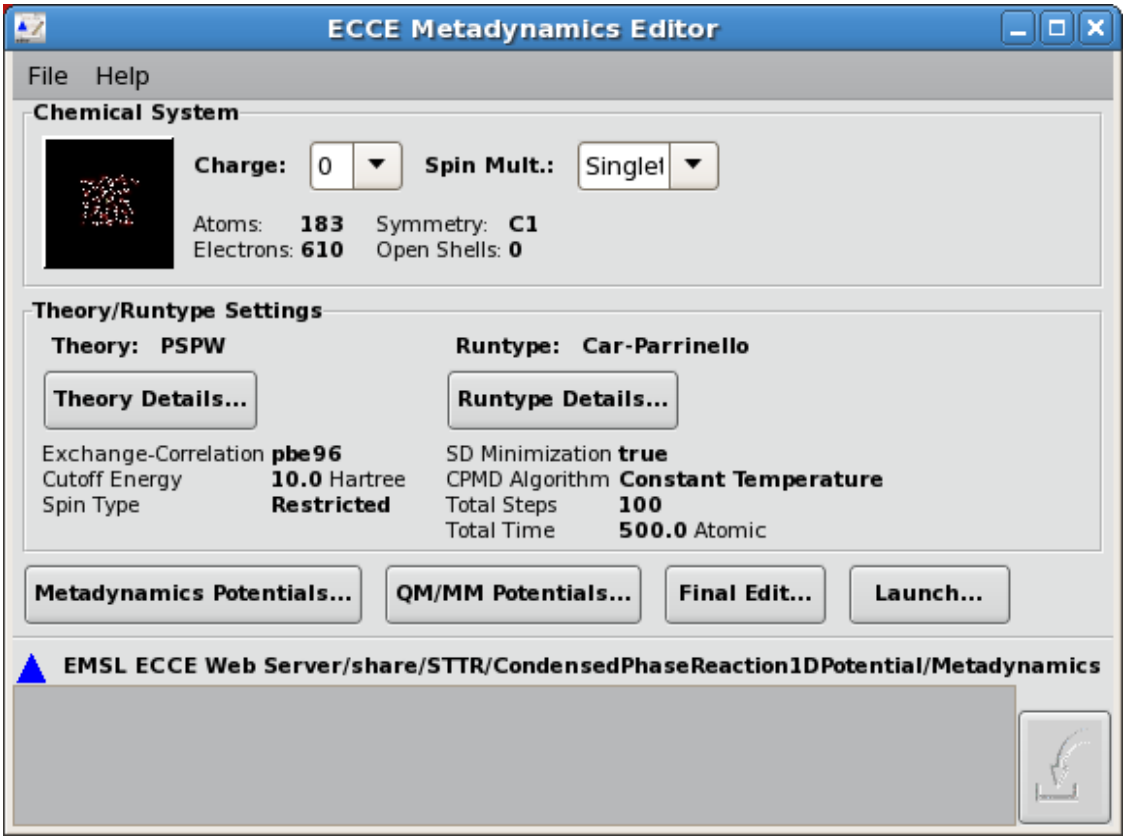

Figure 11. The Metadynamics Editor with updated summary fields for the theory and runtype settings for equilibration.

With the setup for the equilibration task complete, the ECCE Launcher is used to select the target compute host for running the job, set host-dependent parameters such as the number of processors to use, and to submit the job. Although the Launcher user interface was not changed, a number of underlying changes were made to the Launcher application to support running Metadynamics tasks. Figure 13 shows the Launcher for the just launched equilibration task after hitting the button labeled “Launch”. Note that the multiline message area at the bottom of the Launcher lists the last few steps of the job launch process with earlier steps having scrolled out of view. If one of these steps had failed a message would have appeared in this area and the launch would have aborted with the job remaining in the ready (darker blue triangle) state. For running jobs, the Launcher supports a variety of computational resources from single CPU workstations on up to massively parallel clusters and supercomputers. ECCE knows how to interface with several batch queue schedulers (e.g. OpenPBS, SGE, LSF, NQE, NQS, LoadLeveler) in addition to running jobs on hosts that don’t use scheduling software. Depending upon the type of computational resource and the batch scheduler it runs the Launcher will present different fields for the user to set for each launch. The host used for running the equilibration task in the walkthrough is a basic Linux workstation and thus a minimal Launcher interface is shown. For more powerful computational resources

there would additionally be fields for parameters like the name of the queue to use, time and memory limits for the job, and the number of nodes to run on along with the total number of processors.

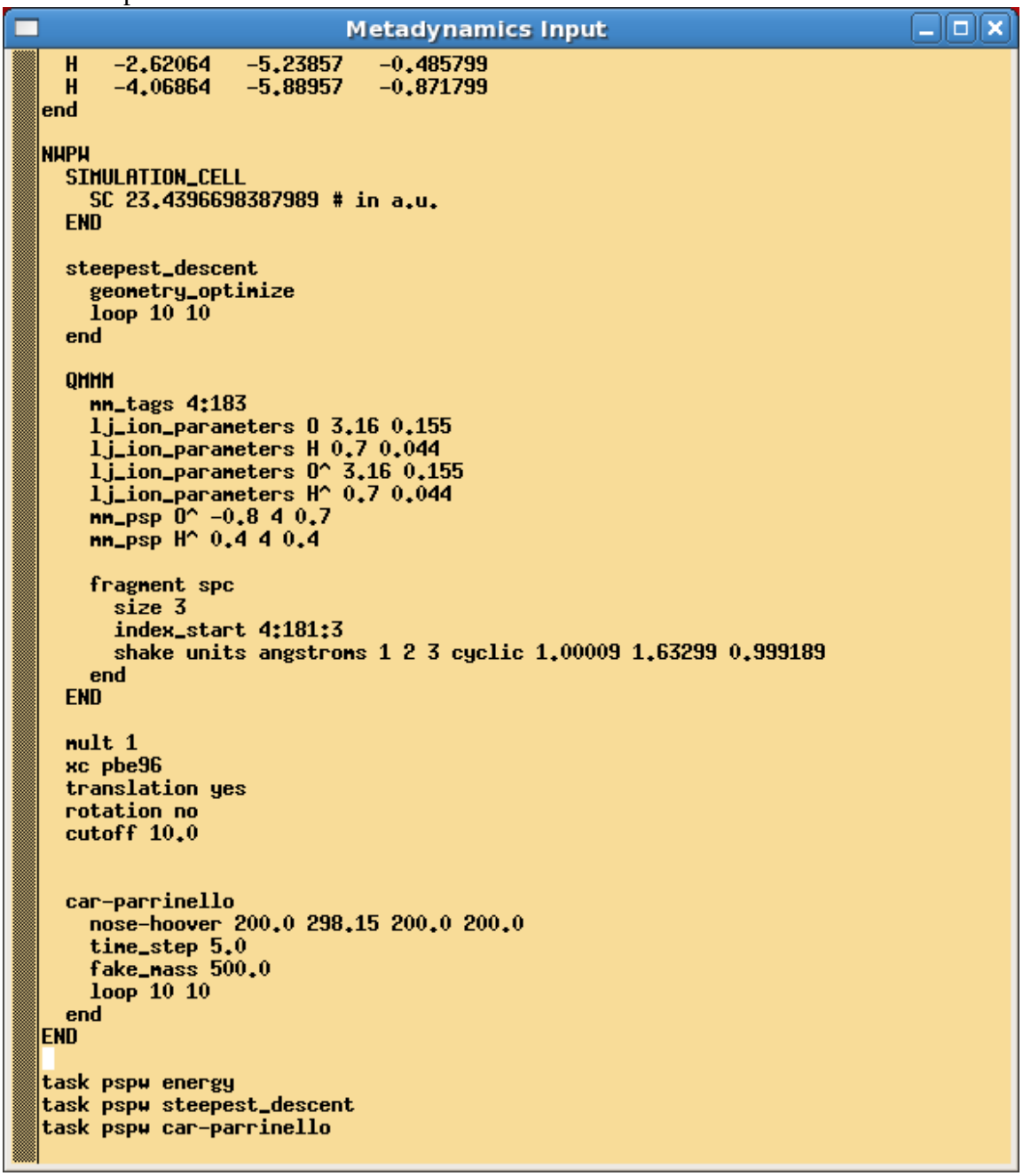

Figure 12. The Metadynamics Editor Final Edit window showing the NWChem input file for equilibration.

As part of the job launch sequence of steps performed by the Launcher an ECCE job monitoring script is invoked on the computational host immediately after the job is submitted. This job monitoring script performs two functions. First it monitors the state of the job (submitted, running, completed, or one of several job failure states) as reported via the job state icon in the bottom-left corner of most applications such as the

Metadynamics Editor and Launcher or in the left-hand pane tree view in the Organizer. Note in the Launcher shown in Figure 13 that the job state is “running” based on the key in Figure 1. The second ECCE job monitoring script function is parsing output property data of interest from the running calculation output file(s) and triggering the parsing of these properties, storing them on the ECCE data server, and notifying other applications they are available, notably the ECCE Viewer. What properties are parsed and how to parse them is part of the code registration process in ECCE. For supporting the NWChem Plane-wave Metadynamics task a variety of output data is parsed including plots of different energies over geometry and wave steps in order to create plots. Figure 14 shows two Viewer screen shots displaying output from the equilibration task. In this case the job has completed, but an important feature of ECCE job monitoring is that most properties are parsed and available in the Viewer as soon as they are written to the running output file rather than just on job completion. This allows progress to be easily evaluated often saving valuable high performance computer time by aborting a job that has gone astray.

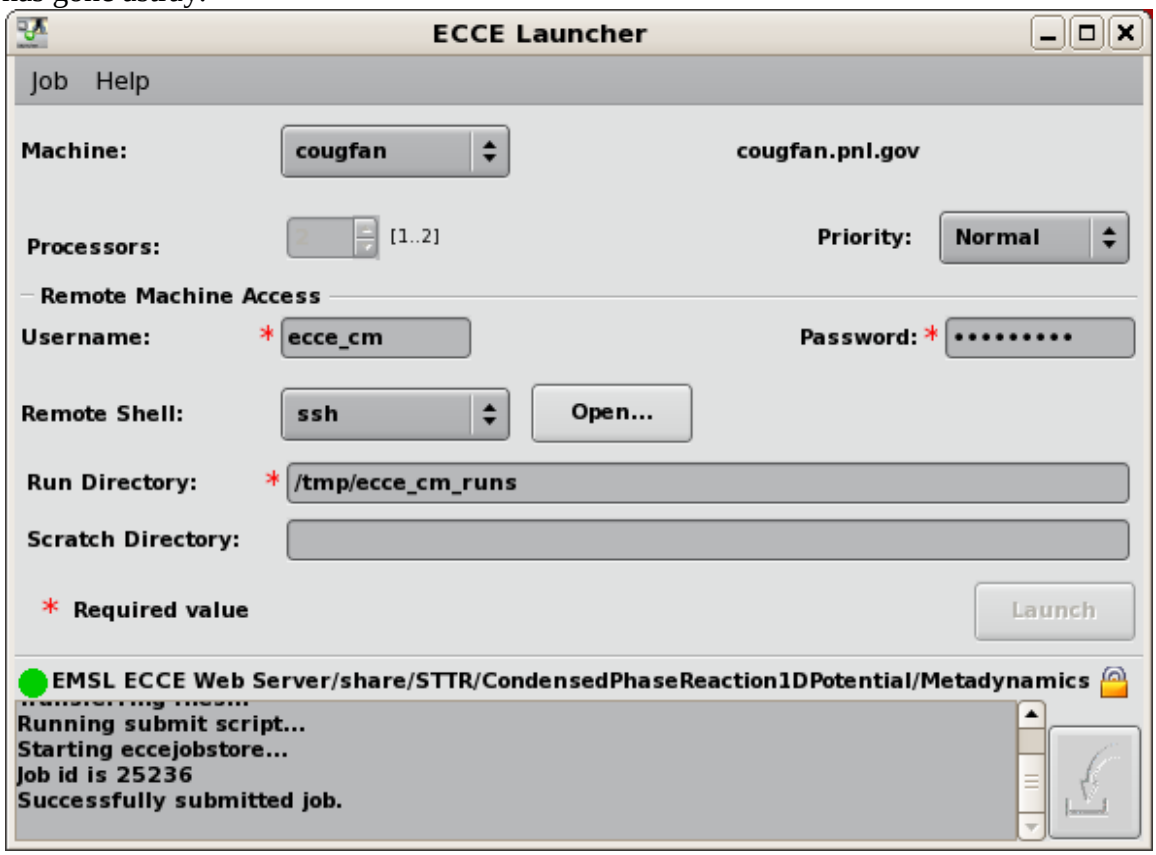

Figure 13. The ECCE Launcher application showing a successful launch for the equilibration task.

The top Organizer screenshot in Figure 14 shows the list of properties that can be selected from a menu for the “Geometry Step Plots” property panel. In this case the ion kinetic vector is plotted. Partially hidden behind the properties menu is the “Wave Step Plots” property panel that is similar to the “Geometry Step Plots” panel other than the list of properties available. The bottom Organizer screenshot is plotting the potential energy vector for “Geometry Step Plots” panel. Above that plot in the bottom screenshot the electron kinetic vector is being plotted over the geometry step for the “Geometry Trace”

property panel. In addition to a simple plot, geometry trace properties also store a geometry configuration for the entire chemical system at each step. These geometry configurations can be animated by rendering each one in the main Viewer visualization workspace in sequence with a configurable time delay between each step. The play, stop, step, rewind, etc. icon buttons in the "Geometry Trace" property panel control animation as well as stepping through configurations explicitly for finer control. With such a small number of steps for this equilibration task the animation is neither very interesting nor meaningful compared to a longer simulation as will be performed next.

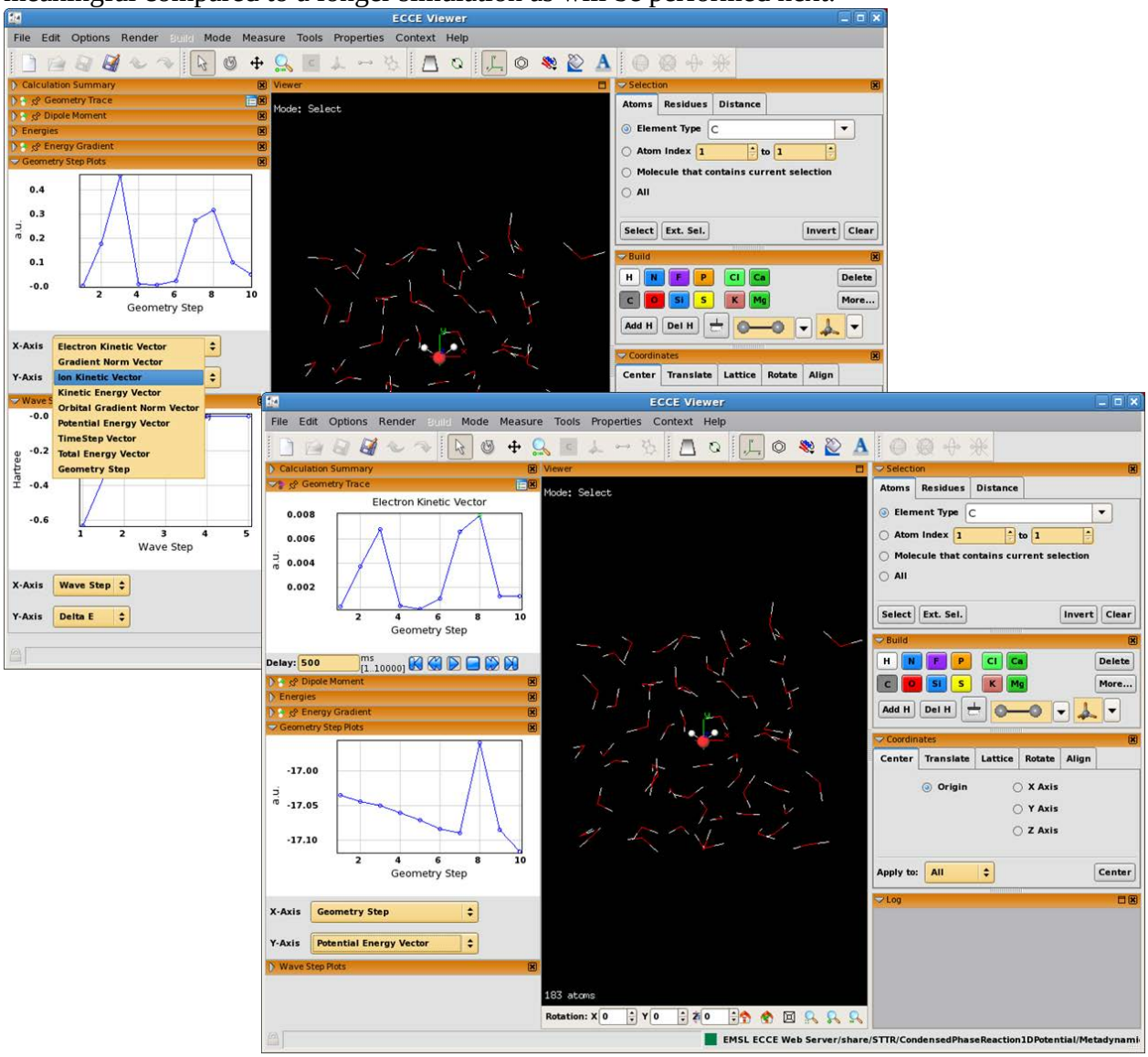

Figure 14. ECCE Viewer showing output properties from the completed equilibration task. These same properties would be viewable (with fewer steps shown) for a running task.

With the equilibration of the solvated structure complete the reaction rate determining Metadynamics task can be performed. Figure 15 shows a newly created Metadynamics task chained to the existing equilibration task in the Organizer. The new task is created by selecting the equilibration task in the Organizer and then either selecting "New NWChem Metadynamics…" from the File menu (see Figure 6) or by hitting the orange-

bordered flag icon with the “M” to the right of the Organizer workflow pane (similar flag icons are available for every type of study in ECCE as a quick means to create workflow tasks). When two Metadynamics tasks are chained together in a study ECCE transfers the necessary parent task files and changes the child task NWChem input file to perform a task restart operation picking up where the parent task ended, which in this case is the equilibrated condensed phase structure. Among other files the NWChem runtime database file is transferred for chained tasks as well as removing the chemical system definition in the input file (as it represents the starting chemical structure and the equilibrated one needed is contained in the NWChem runtime database file).

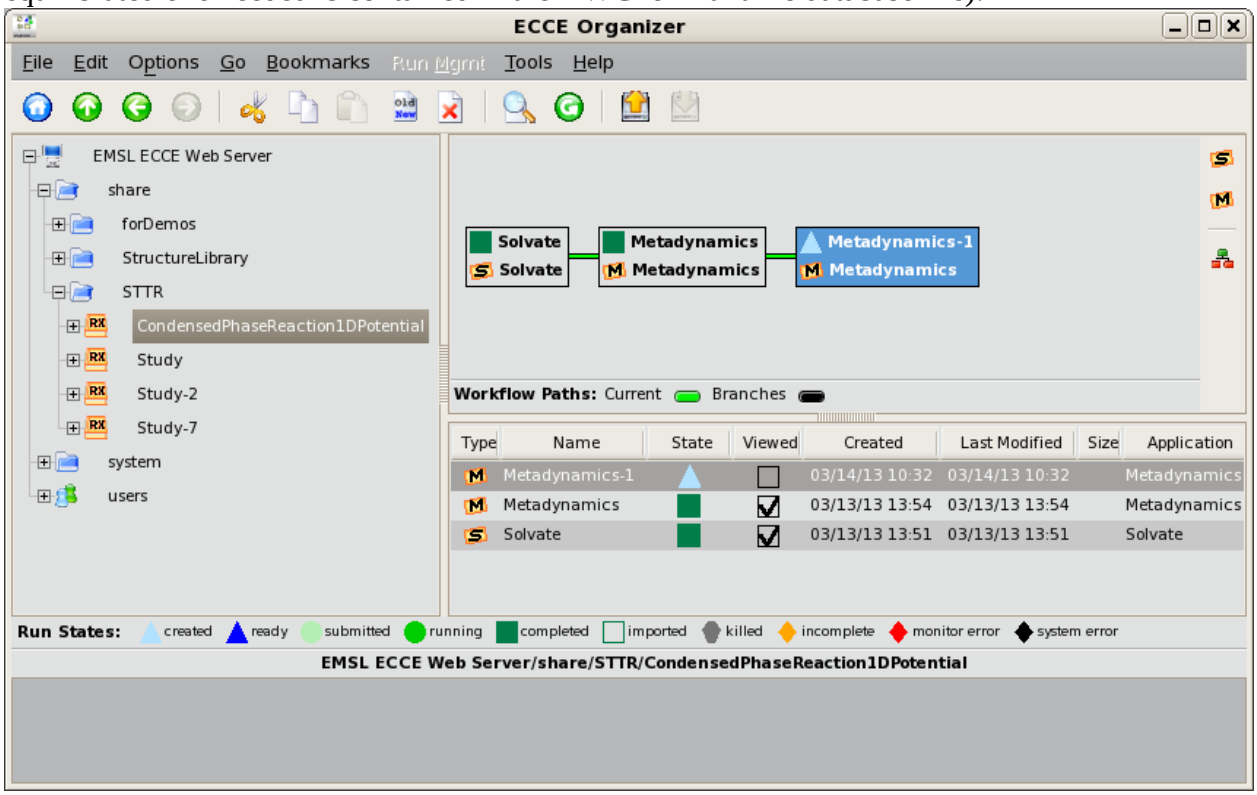

Figure 15. Chaining a new Metadynamics task to the original Metadynamics equilibration task in the Organizer.

In order for the new Metadynamics task to calculate reaction rates the duration of the simulation is increased and a metadynamics potential term is added. Figure 16 shows the Metadynamics Editor main window and the Runtype Details dialog. The outer iterations value in the details dialog is bumped up to 150 giving a total of 1500 steps. In Figure 17 the Metadynamics Potentials dialog is shown along with the Builder. The Builder is used to select the atoms the potential applies to. Hitting the left mouse button over atoms in the Builder visualization workspace area (Shift key for multiple atom selection) highlights (in purple) and selects atoms. Two atoms are selected to create a bond potential term and three atoms for an angle potential. Hitting the Add Potential button on the Metadynamics Potentials dialog retrieves the atoms selected in the Builder to add the appropriate potential term. For a bond potential term values for W and Sigma in atomic units are entered for the newly added potential. The final column for the new potential, Relative Error, is calculated by ECCE rather than entered by the user to provide a metric for the accuracy of the reaction rates that will be calculated based on simulation output.

W and Sigma are the height and width of the Gaussian functions used to construct the free energy surface. Their values affect the accuracy of the calculated surface. The relative accuracy between the new settings and the default setting is displayed to help users visualize how modified settings compare in accuracy to the defaults.

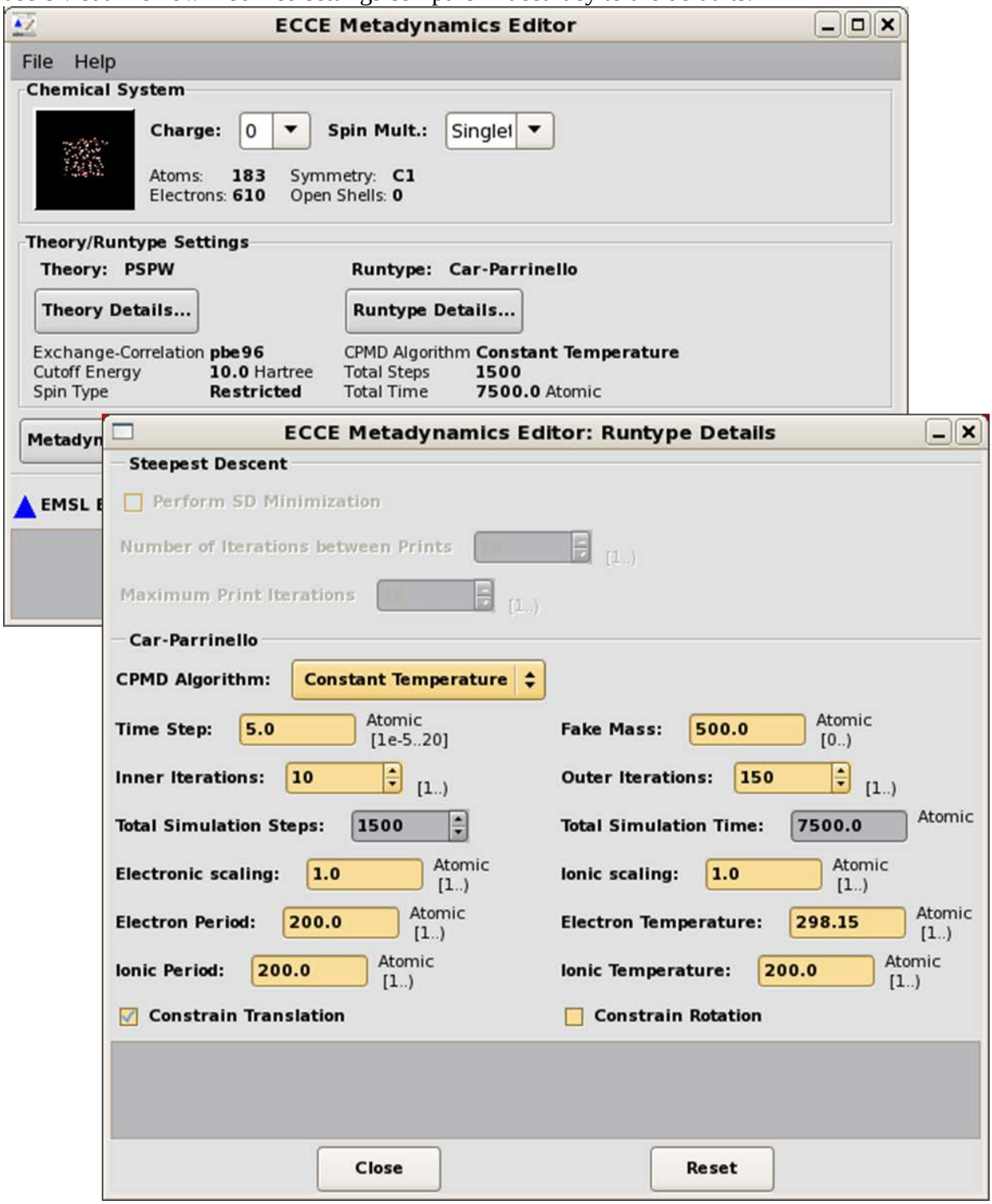

Figure 16. Metadynamics Editor and Runtype Details dialog for the new chained Metadynamics task.

Figure 18 is the Metadynamics Editor Final Edit window showing the NWChem input file for the chained simulation including the bond potential term. Note the entire input file now fits on one screen due to the absence of the geometry block (derived from the NWChem runtime database file for a chained task), the use of the NWChem restart directive on the first line, the change to the loop directive in the car-parrinello block, and the metadynamics block defining the bond potential inside the Plane-wave NWPW block.

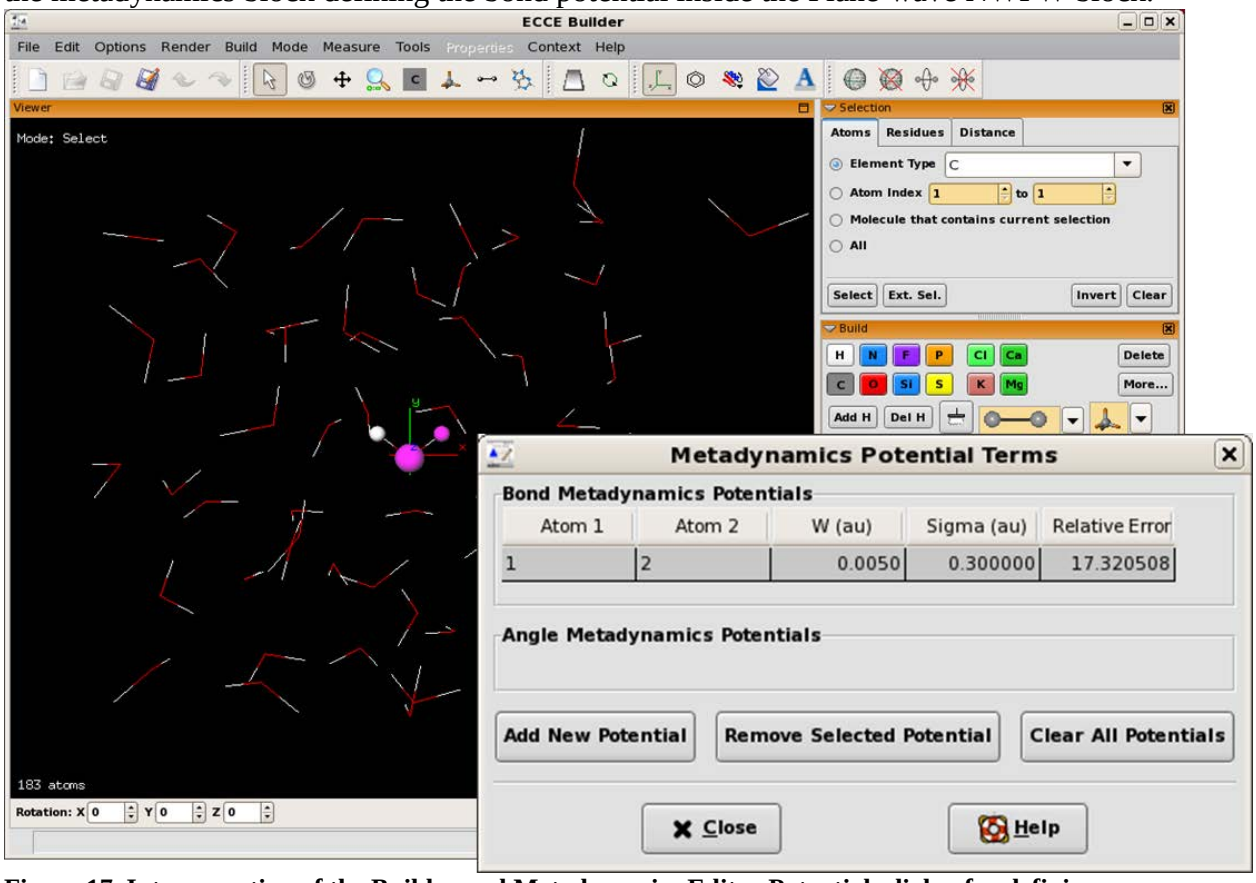

Figure 17. Interoperation of the Builder and Metadynamics Editor Potentials dialog for defining potential terms.

After running the simulation the Viewer is shown displaying output properties in Figure 19. The one property panel added that is new since the previous equilibration task is the top one labeled "1D Metadynamics Potential". A plot of Free Energy vs. Position is at the top of this panel along with associated properties below it such as the position and value of the free energy minimums and maximums along with the average simulation temperature. The final value output in this panel is the predicted reaction rate constant that is calculated by ECCE. The Metadynamics Potential panel reports the location of the maximum and minimum values of the free energy curves as well as the free energy at those locations. The calculation of the reaction rate is also based on those values, plus the measured value of the temperature. The location of the minimum and maximum can be adjusted by the user, along with the value of the temperature and the calculated reaction rate will be automatically updated. Note in the visualization workspace in Figure 19 that a Hydrogen atom on the solvent has dissociated from the water solute near the end of the

simulation as a result of the bond metadynamics potential (the desired result). The Geometry Trace property panel that is open at the bottom of the Viewer is used to animate the trajectory showing the solute dissociation. The interface allows the user to predict that rate constant between any two points along the free energy curve at any temperature. Setting the maximum position to 10 returns the bond disassociation free energy.

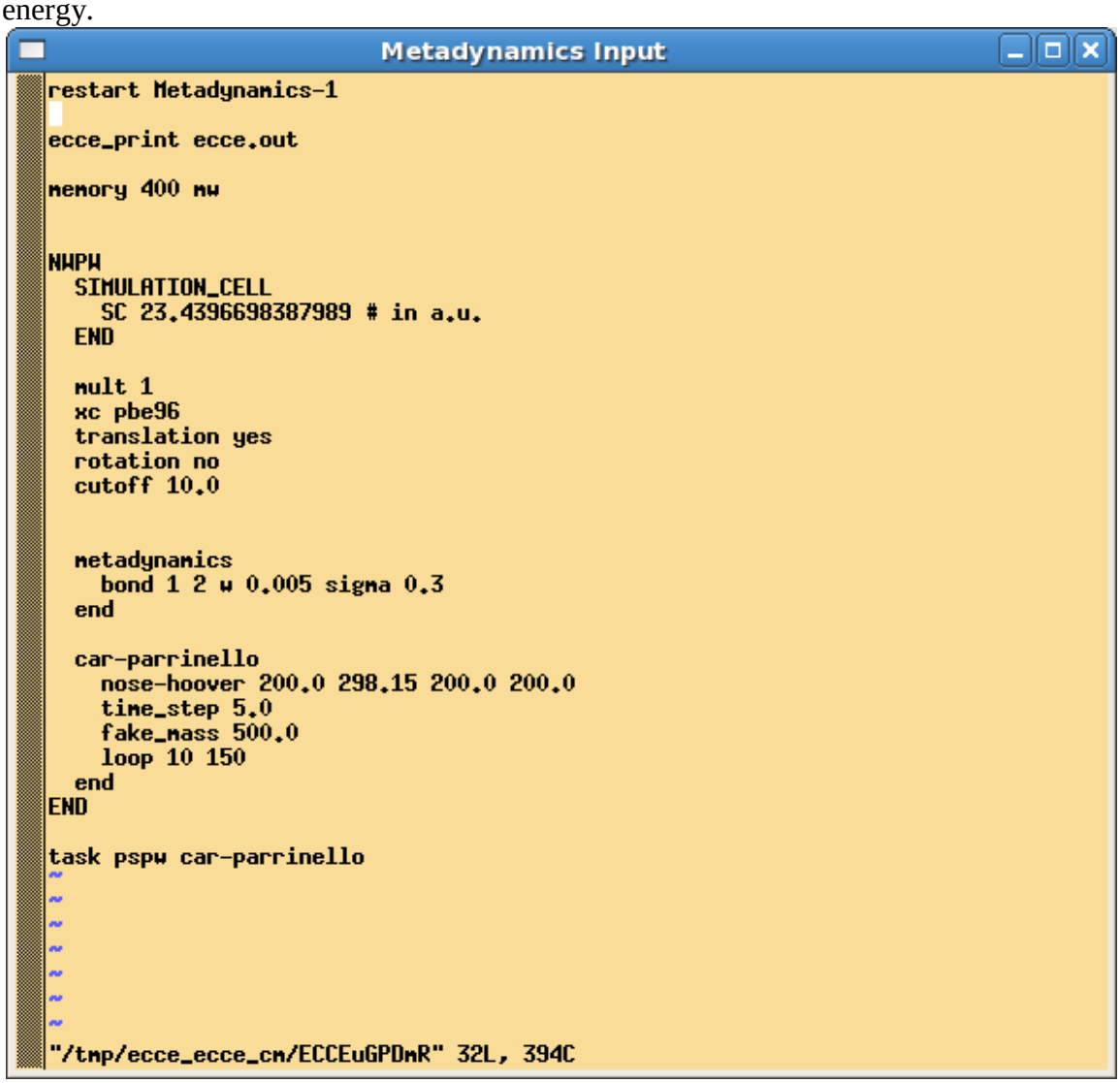

Figure 18. The Final Edit window for the chained Metadynamics task with the bond potential term added.

Because plots are critical to the interpretation of results of computational chemistry studies and often included in formal publications (along with ECCE 3D visualizations) additional features have been added to ECCE to support them. Figure 20 shows the same Free Energy vs. Position plot as in the Viewer property panel using an ECCE option (from the right mouse button menu over the plot in the Viewer) to display it in a separate window. This allows the plot to be resized to better discern results as well as do a screen capture for publication/presentation. The top-left screen capture is the entire plot while the bottom-right screen capture is zoomed in to a small area contained within the plot for

even finer resolution. This is accomplished using another ECCE feature to lasso a region of the plot with the mouse and redraw it in the full window.

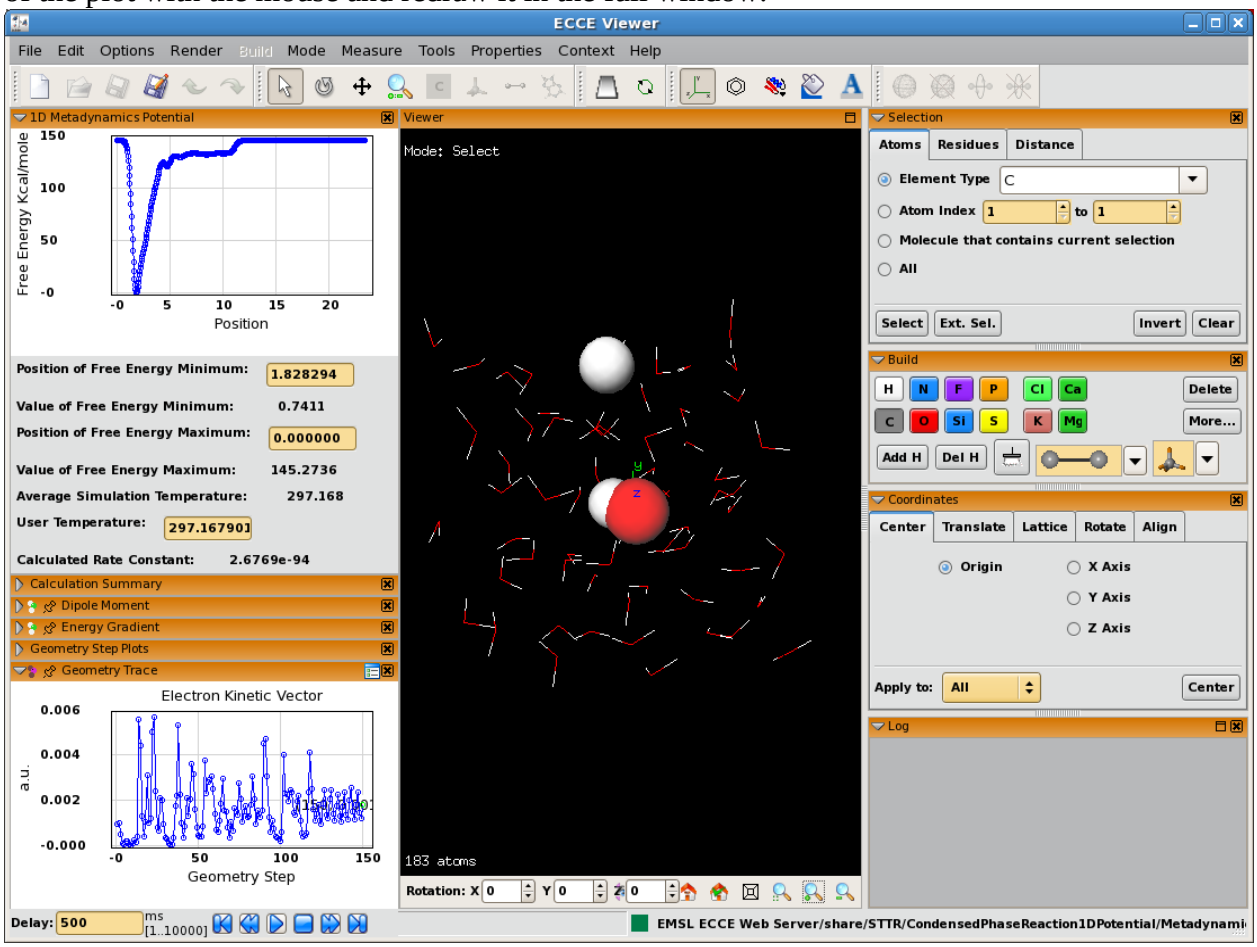

Figure 19. ECCE Viewer output from the Metadynamics simulation with the bond potential term.

Figure 21 shows a newly added branched task off the first equilibration Metadynamics task. This is also a Metadynamics task, this time renamed to EqProps (default names were used for all previously created tasks). Task branching allows investigation of alternatives—going back to a previous point in the workflow and starting from there without having to discard previous work. In this case a longer simulation will be run after the equilibration without adding any potential terms. The plots resulting from this simulation won't have the perturbation from being driven by strong metadynamics potentials. Figure 22 shows the setup for the EqProps task in the Metadynamics Editor. A total of 1000 steps will be run by again adjusting the outer iterations value. Figure 23 shows the results of running this simulation without the metadynamics potential with the Geometry Step Plots panel plotting the Total Energy Vector and the Geometry Trace panel plotting the Electron Kinetic Vector. Plots, such as these, are not only useful for quantitative analysis but help verify that the simulation is running properly. The figure shows oscillations in the total energy consistent with overly strong coupling to the constant temperature algorithm, which is the result of changing the defaults to decrease simulation time for a quick software demonstration.

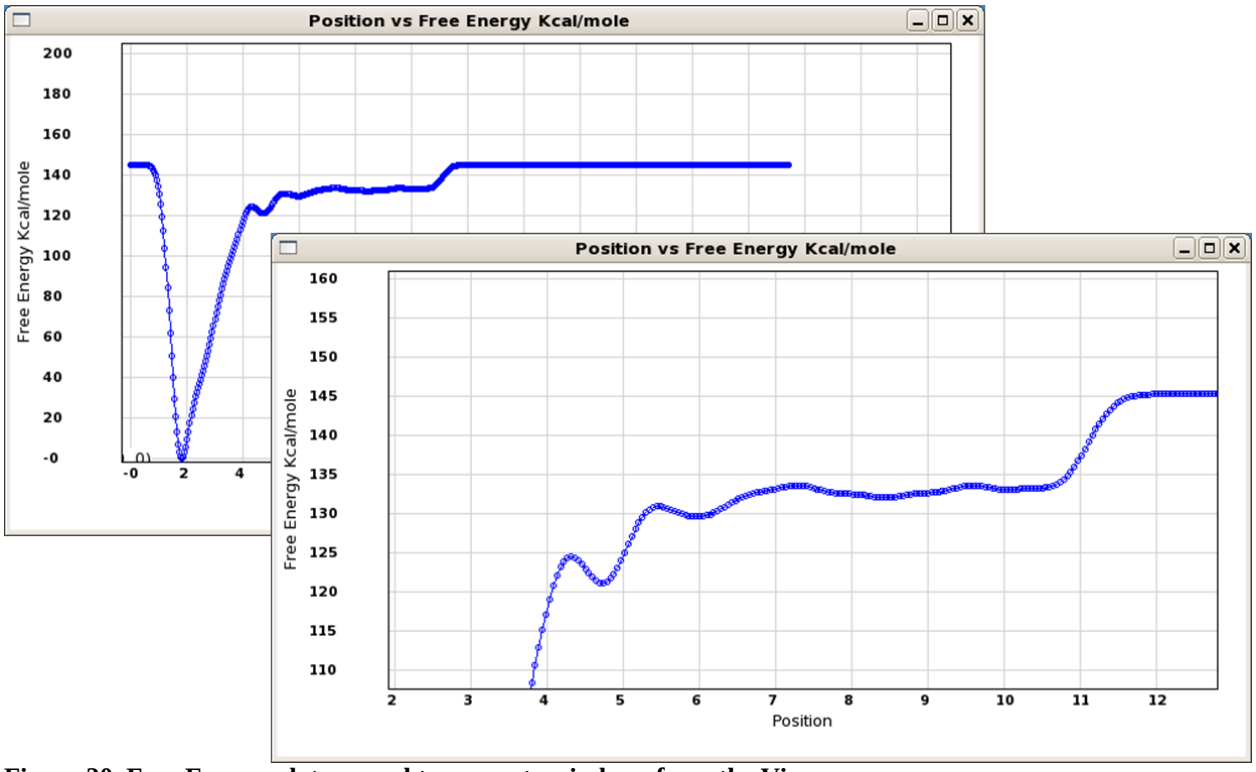

Figure 20. Free Energy plots moved to separate windows from the Viewer.

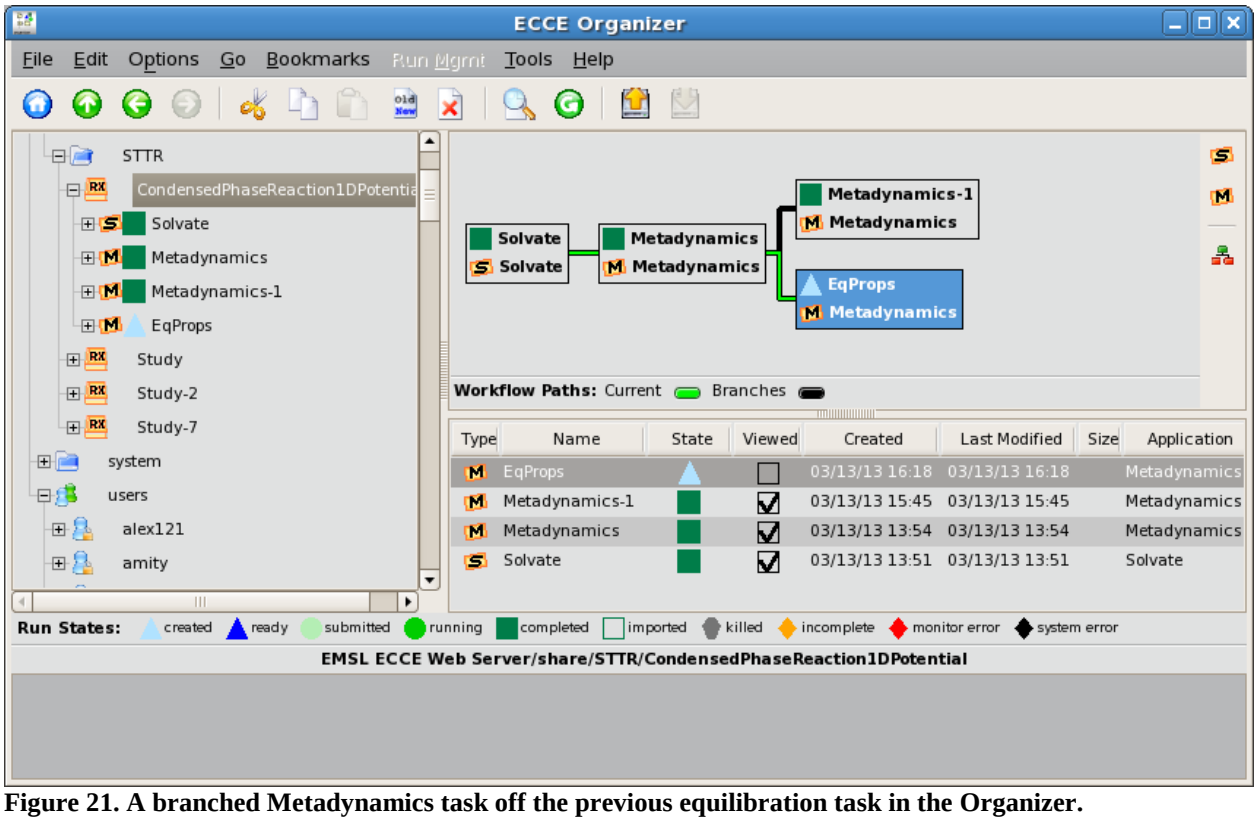

Figure 21. A branched Metadynamics task off the previous equilibration task in the Organizer.

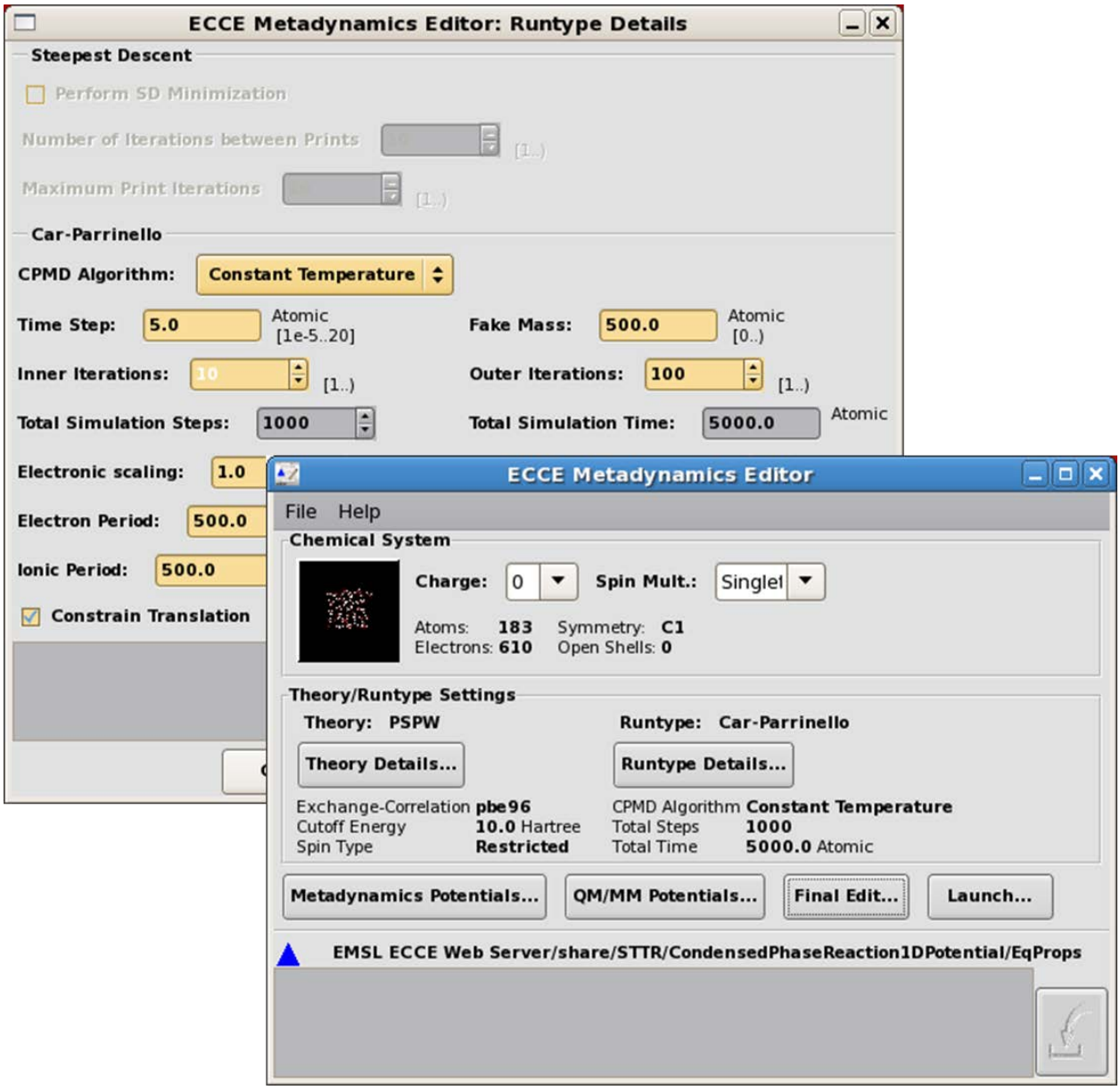

Figure 22. EqProps Metadynamics task setup in the Metadynamics Editor.

The last task as part of the walkthrough will add a second metadynamics potential. Figure 24 shows a running Metadynamics task in the Organizer with the corresponding Metadynamics Potential dialog (parent Metadynamics Editor window not shown). A newly created study has been used for this reaction rate calculation, although the previous workflow study could have also been used by creating a third branched task off the equilibration task. ECCE supports copy and paste of full studies as well as individual calculations and projects containing other objects. Thus a brand new study named CondensedPhaseReaction2DPotential can be created by copying the original CondensedPhaseReaction1DPotential study and then deleting the two tasks chained to the equilibration task in the new study.

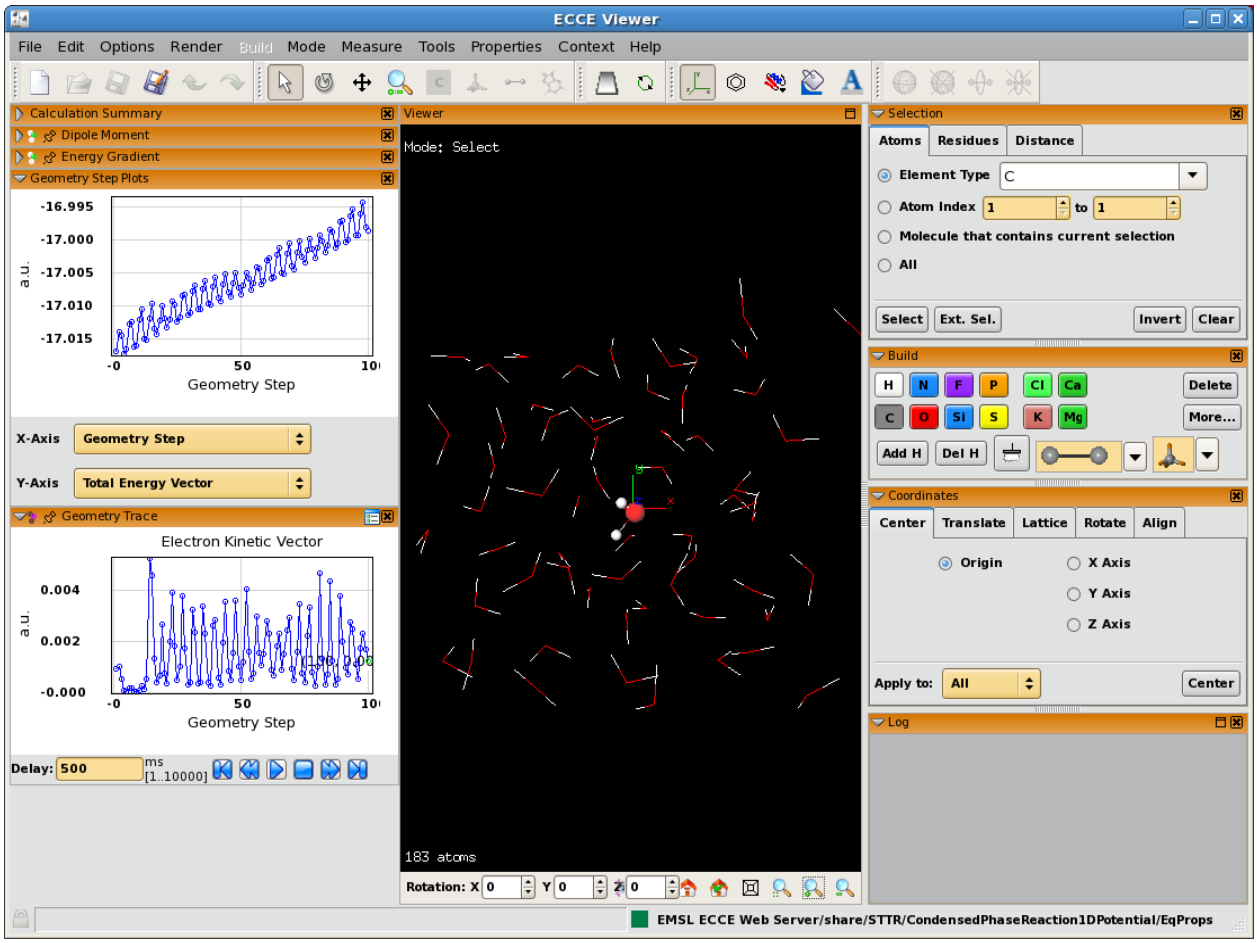

Figure 23. EqProps Metadynamics task output displayed in the Viewer.

From the Metadynamics Potential dialog in Figure 22 note that the W value in the bond potential term has been changed from the 1D metadynamics potential task and then a new angle potential term has been added along with adding W and Sigma values for this new potential. The Relative Error outputs report a large increase in error (multiples of 77 and 5.5) given the new setting. This is the accuracy cost associated with the change from the defaults and thus only qualitative results are expected. Figure 25 shows the Viewer displaying output properties from this 2D Metadynamics tasks. Note the first property panel is labeled "2D Metadynamics Potential". A simple XY plot of Free Energy is not possible for a 2D potential so only output scalar values are shown. These include both the X and Y coordinates at the free energy minimum and maximum values with the corresponding free energy minimum and maximum values, the average simulation temperature, and the predicted rate constant calculated by ECCE. The Geometry Step Plots panel is currently showing the Total Energy Vector. The rate constant is calculated using the same approach as that used for the 1D potential, except that in this case the free energy minimum and maximum are based on the behavior of two coordinates, not one.

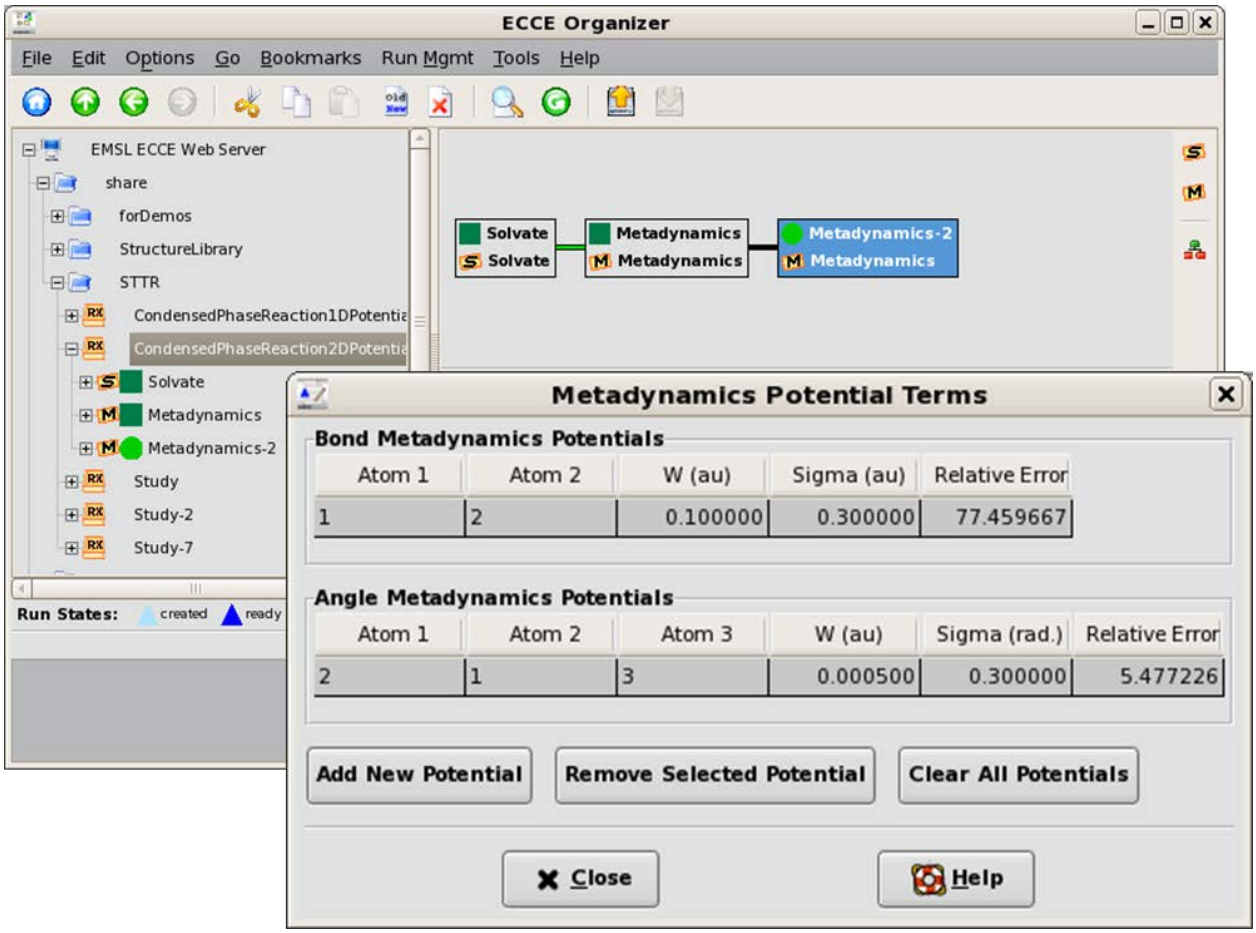

Figure 24. A new 2D Metadynamics study in the Organizer (foreground). Both a bond and angle metadynamics potential are specified in the Metadynamics Potential Terms dialog (background) of the Metadynamics Editor (not shown) for the Metadynamics task shown in the running state.

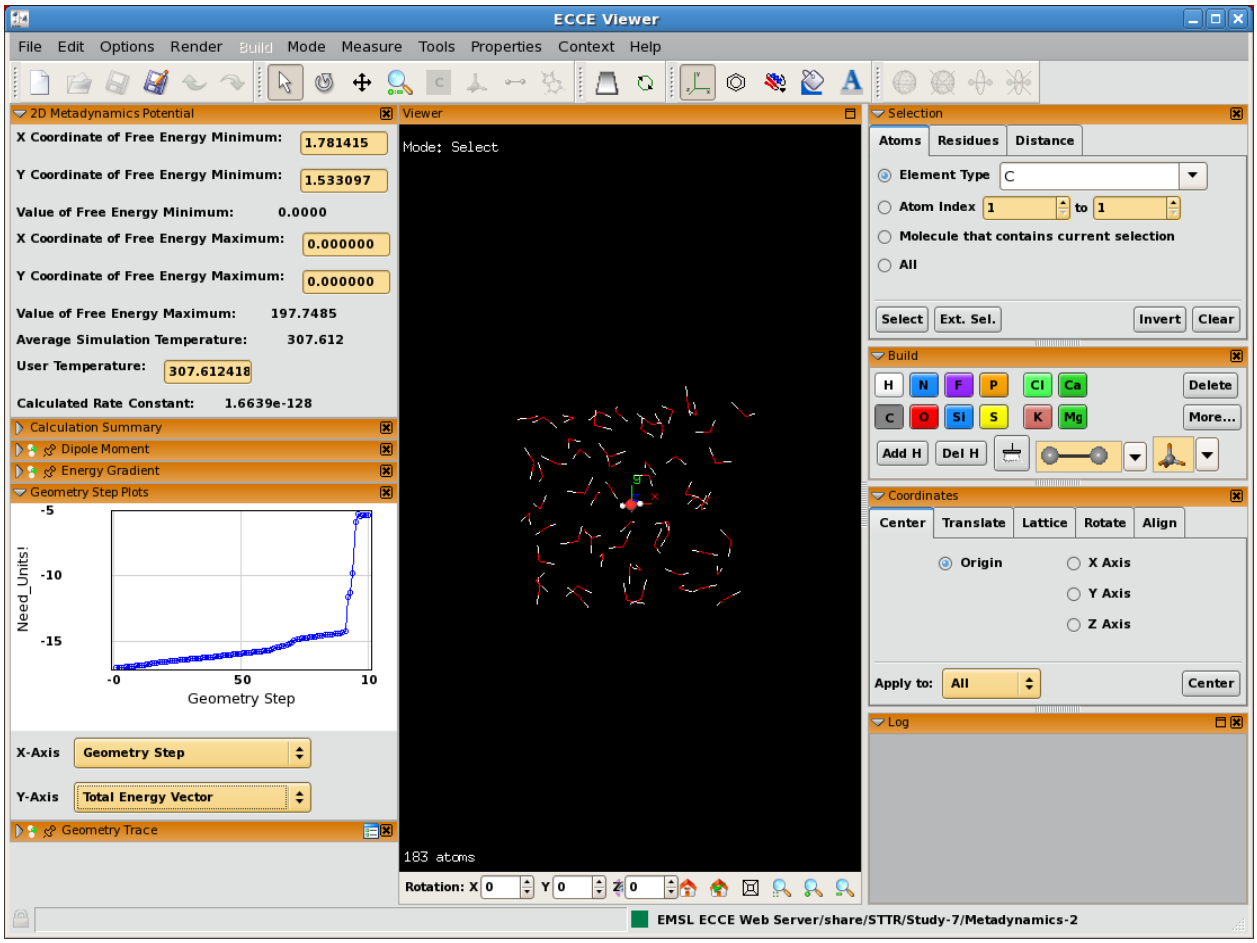

Figure 25. Completed 2D Metadynamics task output in the Viewer.

NWChem 6.3 Bundled

(7.0) The latest production NWChem release 6.3 has been bundled with ECCE 7.0. This is the version that will be used when calculations are run on the host where the ECCE application software is installed. ECCE bundles NWChem as a matter of convenience for those evaluating either ECCE or NWChem with the intent that users running the software for research/production purposes will install NWChem separately on higher performance hardware using platform specific NWChem compilation settings. Previous ECCE releases included both 32- and 64-bit distributions of both ECCE and NWChem. With ECCE 7.0 only 64-bit distributions of both are supported. Note that the NWChem 6.3 binary distribution bundled with ECCE is a generic compilation for Linux workstations using the GNU gfortran compiler with only the use of MPI for message passing as a non-default compilation setting. The build/build_details.doc file of the ECCE source code distribution describes the exact NWChem 6.3 compilation settings used.

New ECP Orbital Basis Sets

(7.0) The split valence, triple zeta valence and quadruple zeta valence balanced basis sets by Wegend and Alrichs (Phys. Chem. Chem. Phys, 2005, 7, 3297-3305) have been added to ECCE 7.0. These basis sets cover all elements from H to Rn (excluding the

lanthanides), and employ deliberately small effective core potentials for atoms Rb to Rn. The basis sets include polarization functions denoted by p and pp suffixes, with the pp modified sets being intended for correlated methods and the p modified sets are meant for DFT computations.

Basis Set Exponent and Coefficient Precision

(7.0) Previous ECCE releases limited the precision of basis set exponents and coefficients in NWChem input files to 6 digits after the decimal when the "Use Exponents & Coefficients" checkbox was selected in the ECCE NWChem Editor. With ECCE 7.0 the precision has been set to 12 digits after the decimal. This has increased the accuracy of results to better match that calculated with NWChem using built-in basis set library names. Besides the newly added ECP basis sets described in the preceding release note, existing ECCE basis sets have used a maximum of 8 digits after the decimal with the full 12 digits only being used for the new basis sets.

New Basis Set Administration Scripts

(7.0) A pair of Python scripts have been contributed to ECCE 7.0 simplifying the process of adding new basis sets for use with the Basis Set Tool application. These scripts are named gbsDescriber and gbsNWChemConverter. Invoking these from the command line provides usage documentation, and the gbs.README file provides a worked example. If you add new basis sets to your local deployment of ECCE that you believe would be of benefit to the broader user community, please consider contributing them back for inclusion into a future ECCE release. Post to the ECCE support forum of the NWChem wiki at http://www.nwchem-sw.org/index.php/Special:AWCforum/sf/id11/General_ECCE_Topics.html if you are interested in contributing to the ECCE open source release.

NWChem COSMO Solvation Model Solvent Radius

(7.0) A solvent radius input field has been added to the NWChem theory details dialog for use with the COSMO solvation model. This input field corresponds to the "rsolv" directive within the "cosmo" block of an NWChem input file. The default solvent radius value is 0.5 Angstrom.

Open Source Release

(6.4) ECCE is now available as open source software under the terms of the same Educational Community License (ECL) 2.0 used by NWChem. This eliminates the need to sign an EMSL software use agreement and download the software via the EMSL User Portal. Both binary and source code distributions of ECCE can now be downloaded from the ECCE website at http://ecce.pnl.gov/using/download.shtml. ECCE distributions will also be made available from the NWChem wiki at http://www.nwchem-sw.org Other than open source availability and bundling the latest NWChem 6.1.1, the ECCE 6.4 release is otherwise equivalent to the 6.3 release. Because source code is now available the ECCE team is interested in hearing about any enhancements or fixes to ECCE made by the user community and encourages those be contributed back for inclusion in ECCE core distributions. Please contact the ECCE team using the NWChem wiki ECCE forums at http://www.nwchem-

sw.org/index.php/Special:AWCforum/sc/id4/ECCE:_Extensible_Computational_Chemistry_Environment.html if you wish to contribute.

Source Code Release

(6.3) An ECCE source code distribution is available for the first time. This allows sites to compile ECCE natively on both 32- or 64-bit Linux platforms. A build script automates the process of compiling ECCE including checking for the existence and compatible versions of compilers and other packages needed to build and run ECCE, automating builds of third party software ECCE requires, and compiling ECCE core code. ECCE builds have been tested on a variety of Linux operating systems including 32- and 64-bit releases of Debian 6.0.4, Ubuntu 11.10, OpenSUSE 12.1, Red Hat 5.7, and Mint 12. Build guidance such as the names of prerequisite software packages to install for each of these operating systems is provided. The ECCE source code distribution bundles compatible versions of the third party packages used by ECCE such as the Xerces XML parser, the wxWidgets and wxPython GUI toolkits, and the Apache HTTP server. The README file in the build subdirectory of the source code distribution describes how to use the build_ecce to automate the entire build process and operating system specific guidance. For those having problems compiling the third party software used by ECCE or wishing to try newer versions, details for manually building the third party packages are given in the build_details.doc file in the same directory.

64-bit Binary Distribution

(6.3) A native 64-bit platform binary distribution is now provided in addition the 32-bit distribution that had been the only one available. While both the 32- and 64-bit binary distributions of ECCE are built under the Red Hat Enterprise Linux 5.7 operating system they include operating system dependent shared libraries that allow them to be run on Linux operating systems from many other vendors. The majority of sites do not need to build ECCE from the source code distribution unless they prefer to do so. The quickest way to get up and going with ECCE is to first install the appropriate binary distribution based on whether it's a 32-bit or 64-bit platform and then test various ECCE applications. If any issues are found then go back and build ECCE from the source code distribution. In addition to the 64-bit ECCE binary distribution being available, the compilers used to build the ECCE binary distributions as well as the versions of the third party software used such as the wxWidgets GUI toolkit and Xerces XML parser have been upgraded to newer releases. The ECCE 6.2 and prior versions used the GNU C++ (g++) 3.2.3 compiler while the 6.3 binary distributions use the 4.1.2 compiler that is native with Red Hat 5.7 where the distributions are built. Note that ECCE source code has been built and tested with the newer g++ 4.x releases including g++ 4.6.

Virtual Machine Distribution

(6.3) The virtual machine distribution of ECCE allows users with only Windows or Mac OS X platforms available to them to run ECCE. However, the VMware distribution of ECCE 6.0 is obsolete and was therefore removed from the download area. Since the ECCE 6.0 release three years ago virtual machine technology has improved dramatically. It is now a much more straightforward process to use these products than when this native VMware distribution of ECCE 6.0 was created. Due to having more flexible no

cost products and its less commercial nature, the ECCE team recommends the use of VirtualBox (http://www.virtualbox.org) although VMware (http://www.vmware.com) remains a well-supported alternative. The previous ECCE 6.0 VMware distribution bundled the CentOS Linux operating system because of its small size and similarity to the Red Hat operating system which was the only operating system where ECCE was compiled prior to the 6.3 release. But, with the added flexibility of both the ECCE 64-bit binary distribution and the ECCE source code distribution any constraints on what Linux operating system can be installed as a virtual machine have been eliminated. From extensive development and testing prior to the ECCE 6.3 source code release the ECCE team recommends Debian, Mint, and Ubuntu for robust and stable Linux operating systems (see the build/README file of the ECCE source code distribution for more details). But, if your facility mandates or favors a different vendor (e.g. OpenSUSE, Red Hat) ECCE is also fully compatible with those operating systems. After installing a virtual machine product like VirtualBox or VMware and then a Linux operating system on a newly created virtual machine, it is a simple matter to install either an ECCE binary distribution or to build ECCE from the source code distribution on the Linux virtual machine. There is no distinction between installing ECCE on a native/local Linux operating system and one running on a virtual machine. One special note is that typically the BIOS settings for a Windows or Linux host do not allow 64-bit virtual machines to be installed even on 64-bit platforms (it isn't possible to install 64-bit virtual machines on 32-bit hosts) without changing default BIOS settings. Simple Google searches will reveal what BIOS changes need to be made to allow 64-bit virtual machines.

Password Caching Redesign

(6.2) Encryption of passwords to file has been eliminated in preparation for the open source release of ECCE in 2012. An in-memory cache of passwords is now kept by ECCE applications for both compute hosts and data servers. The memory cache is synchronized between existing and newly started applications so that a password will only be prompted for a single time when it is first needed by any ECCE application (e.g. Job Launcher, Machine Browser, and Organizer). The Gateway toolbar now prompts for the data server password rather than the ECCE login password (aka encryption key). The ECCE login password (encryption key) prompt dialog previously displayed when first starting ECCE has been eliminated, although the new password prompt dialogs have adopted the same look with the ECCE logo and PNNL/EMSL branding. Because the default administrator configuration of ECCE automatically creates data server accounts for new users when starting ECCE for the first time and this data server password is auto-generated, many users won't know their current data server password. Thus, before running ECCE 6.2 users will need to look up their data server password with the instructions provided in the following release note. New users are now allowed to select their own data server password (6 characters minimum) the first time they run ECCE. Using the "Change…" button on the data server password dialog existing users can change their password to something more easily remembered than the auto-generated password. The Job Launcher and Machine Browser applications still have compute host password entry fields, but if the user does not enter a password in this field a separate password prompt dialog will be displayed when a login is attempted. These prompt dialogs will also appear when accessing an account on a remote host from an application

that does not have a password field such as starting remote shells from the Organizer. Of course if the compute host password for this account has previously been prompted for in the same ECCE session such as to launch a job, the password cache will be used by the Organizer and no prompt is displayed.

Lookup Data Server Password

(6.2) ECCE requires users to enter their data server password at startup to access their calculations via the Organizer and other applications. Because the data server password was most likely auto-generated and then encrypted without the user needing to know or remember password, most users will need to retrieve their existing data server password. This can be done without an ECCE administrator resetting the password via the ecce_htpasswd server utility script by running ECCE 6.0 or 6.1 (the capability to lookup data server passwords has been eliminated in ECCE 6.2). For this reason it is recommended that sites make both the new and previous ECCE installation available to users for a period until users are able to retrieve their data server passwords from the previous installation. ECCE administrators should see the "SITE ADMINISTRATOR WHAT'S NEW" release note on installing ECCE 6.2 for details. Here are the steps for users to lookup their data server password:

- Start ECCE 6.0 or 6.1 (will require sourcing the proper runtime_setup file if already setup to run 6.2 by default)
- Enter the encryption key at the login dialog but do not hit return or "OK" as would normally be done to bring up the Gateway toolbar
- Hit the "More…" button
- Hit the newly shown "Lookup Data Server Password" button and the password will be displayed in a popup dialog assuming the correct encryption key was entered
- Write down this password unless you can remember it
- Close the password lookup dialog and select "Quit" from the login dialog for ECCE 6.0/6.1 (note that due to the upgrade to the 6.2 server, ECCE 6.0/6.1 is no longer functional except for looking up passwords)
- Start ECCE 6.2 (will require sourcing the proper runtime_setup file if running from the same window where ECCE 6.0/6.1 was just run)
- The prompt dialog displayed immediately will be for this data server password, not the encryption key prompted for by previous ECCE releases
- Enter the data server password retrieved from ECCE 6.0/6.1
- At this time or a future ECCE session it is recommended that the data server password be changed (6 character minimum) to something that is more easily remembered than the auto-generated one since it will be entered every time ECCE is started

Preferences Directory Rename

(6.2) The .ECCE4 user preferences directory that lives in each user's home directory has been renamed to .ECCE. Given the password caching changes, this was a good time to tackle this long overdue bit of cleanup. Over the years a number of preference files associated with previous ECCE releases have been deprecated but still exist in .ECCE4 directories. The preference directory rename starts everyone again with fresh preference

files—none are copied from the .ECCE4 directory. Since encrypted passwords are no longer saved to preference directory files the most noticeable change for most users will be losing their previous window sizes and locations. Other miscellaneous preference settings will also be set back to defaults, but should be easy for users to restore such as through the Gateway toolbar preferences dialog. Users who don't anticipate needing to run prior releases can remove their old ~/.ECCE4 preferences directory after transitioning to ECCE 6.2.

Password Prompting Options

(6.1) Figure 26 shows the Login dialog for ECCE 6.1. Of note are the newly added checkboxes labeled "Save encryption key" and "Save machine passwords". The settings for these options determine when passwords are prompted for by ECCE and thus what is cached on disk to eliminate password prompts selectively, completely, or not at all. Prior to ECCE 6.1 machine passwords, i.e. those needed to access remote machines and submit computational jobs, were always saved, although in encrypted form. This is still the default option for ECCE 6.1 although there is now an option to not save machine passwords and prompt for them each time they are needed. Thus the "Save machine passwords" checkbox is provided for sites and users who have security concerns about storing any passwords to local disk regardless of the encryption applied to them. The "Save encryption key" checkbox controls whether the ECCE Login dialog itself is needed. By choosing to save the encryption key (the default is not to save it), ECCE will bypass the Login dialog asking for the encryption key completely and simply start the ECCE Gateway toolbar. In order for this option to take effect the correct encryption key must be entered when the option is first selected on the dialog. By choosing both to save the encryption key and save machine passwords ECCE won't prompt for any passwords throughout a session other than to initially configure a machine to launch jobs by supplying a valid username/password combination and assuming any username/password combinations used remain valid. Of course "one-time login" type passwords still require prompting regardless of these checkbox settings. By saving neither the encryption key nor machine passwords ECCE will not cache any passwords to disk within or between sessions. ECCE uses an open source 64-bit block cipher encryption algorithm named Blowfish with the encryption key being selected by the user the first time ECCE is run (and changed via the "More…" button options on the Login dialog after that). Because of the underlying Blowfish algorithm and the encryption key itself not being saved on disk unless the "Save encryption key" option is selected, this is an exceptionally strong encryption for machine passwords (the ECCE data server password is also encrypted in the same way) despite being saved to disk in encrypted form. The new checkboxes have been added for those sites/users that either prefer a little extra convenience of not entering an encryption key to start ECCE or need to insure ECCE always prompts rather than maintaining even strongly encrypted passwords. Note that in order to reset the "Save encryption key" option to once again prompt for the key after it is set to not prompt, the "preferences" button on the Gateway toolbar is used to call up a dialog that also contains these two new checkboxes.

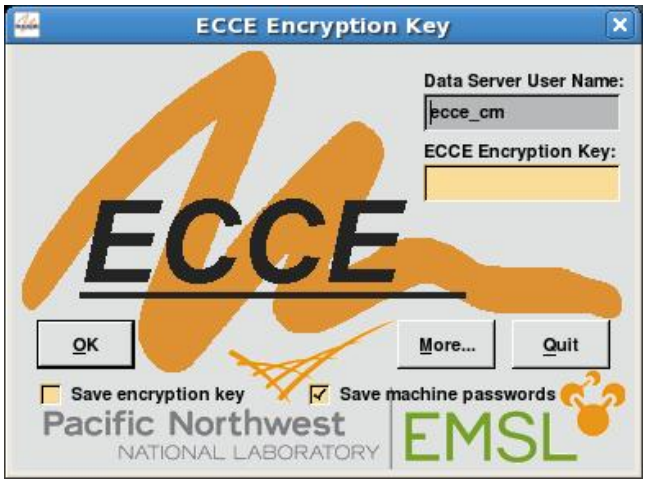

Figure 26. ECCE Login dialog

Periodic System Builder

(6.1) Figure 27 shows the Builder in ECCE 6.1 having imported a CAR file format periodic system. The new Periodic Builder toolkit is at the top of the right-side frame of the Builder in the figure. When loading chemical systems into the Builder using the "Import Chemical System…" item under the File menu, CAR format is now listed in the import dialog. The Periodic Builder toolkit will be shown automatically when a CAR file is imported and is otherwise available from the Tools menu. The "Cell Type" dropdown menu in the Periodic Builder toolkit allows the unit cell to be defined either by the lengths "a, b, c" and angles "alpha, beta, gamma" or by the lattice vectors "a1, a2, a3". These values can be input by the user at the start of an editing session or they will automatically be set if the user imports a CAR format file. The "Lock" checkbox fixes the coordinates of atoms during any change to the lattice cell definition with the aforementioned fields. If "Lock" is unchecked the atom coordinates will be transformed along with any changes to the lattice cell. The "Center Lattice" checkbox causes the lattice to be centered based on atom coordinate extents with any change to the cell definition. The display of the lattice unit cell can be toggled on and off with the "Show Lattice" checkbox. The "Fold" button will automatically shift atoms by an appropriate periodic distance so that all atoms in the system are inside the unit cell. The resulting structure is equivalent to the starting structure, in a periodic sense. The "Equiv. Rectangle" button can be used to create a unit cell with the same volume as the original unit cell but with all cell angles as 90 degrees. Note that this does not necessarily result in an equivalent lattice. For example, this operation applied to a standard unit cell of a 2D lattice of equilateral triangles will result in a different lattice. However, if this operation is applied to a 2x2 super-lattice of the standard unit cell, the resulting lattice is equivalent to the original triangular lattice. New unit cells can be built using the "Super Lattice" button.

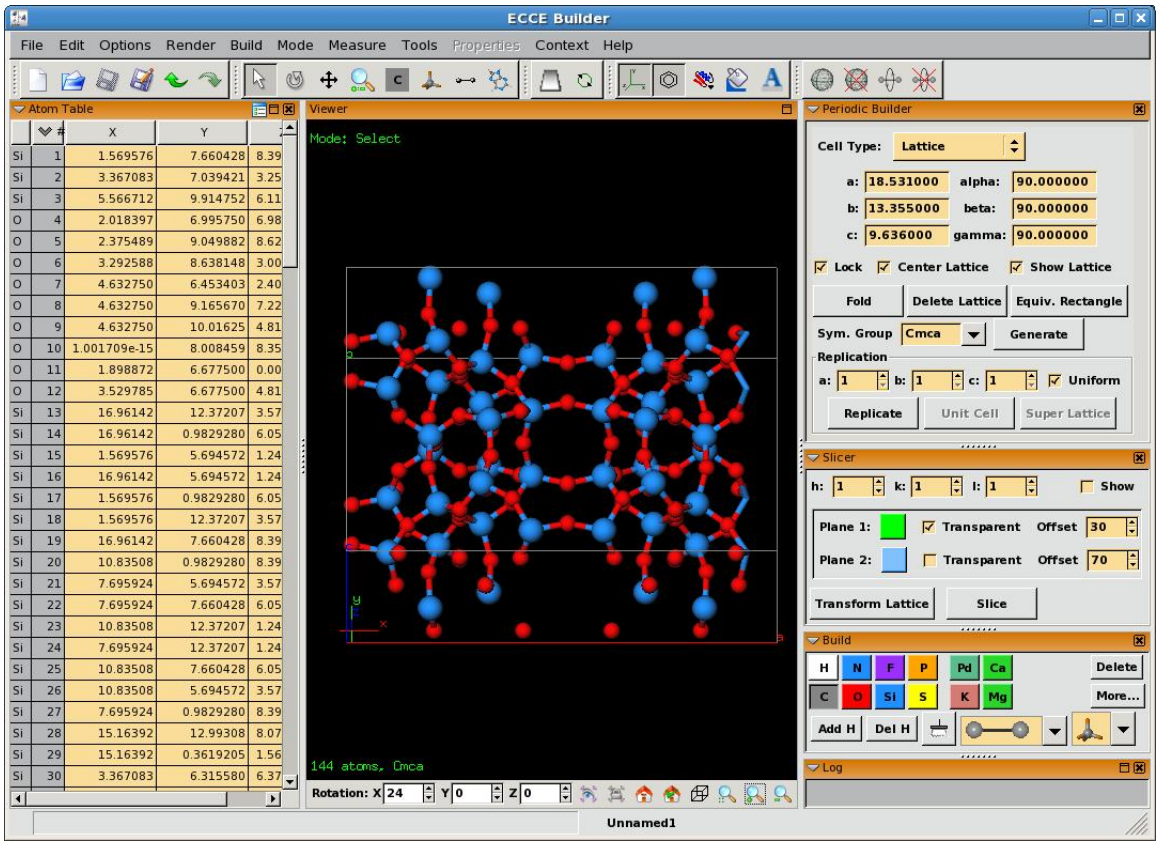

Figure 27. ECCE Builder for periodic systems

If the system is imported from a CAR format file, the symmetry group is automatically set to whatever group was specified in the CAR file. The user can also specify the symmetry group manually. After adding the unique atoms, the full lattice can be generated by pressing the "Generate" button. Visualizations of multiple unit cells can be created using the "Replicate" functionality. The number of cells in each lattice direction can be specified in the three type-in fields labeled "a", "b", and "c". If the "Uniform" checkbox is selected, then all three directions will have the same number of boxes; if it is unchecked, then each axis can have a unique number of boxes. After specifying the number of boxes, pressing the "Replicate" button will generate an image with multiple unit cells. Pressing the "Unit Cell" button will return to the original unit cell. If you want to convert the multiple unit cells into a larger single unit cell, this can be done by pressing the "Super Lattice" button. Note that once a multi-cell system has been converted into a super-lattice cell, it cannot be converted back to the original unit cell.

A second toolkit that is designed to help users manipulate periodic systems is the Slicer, shown below the Periodic Builder toolkit in Figure 27. This toolkit allows users to visualize different crystal planes, slice the system based on these crystal planes, and transform the unit cell so that a desired crystal plane in the original system lies along the 001 direction of the new system. The three type-in fields "h", "k", and "l" are the integer components of the vector defining the crystal plane. If the box labeled "Show" is checked, these planes will show in the workspace. The properties of each plane, including their color, transparency, and location can be manipulated with the fields after

the “Plane 1” and “Plane 2” labels. The offset is the relative displacement of the plane (ranging in values from 0 to 100) from the farthest corner or edge of the unit cell. The “Slice” button will remove all atoms from the system that are exterior to the space contained between the two planes. Note that “Slice” only works on the unit cell. To slice a multi-cell system, it first needs to be converted to a single cell using “Super Lattice”. The “Transform” button will transform the original unit cell so that the lattice specified by h, k, and l values is now the 001 vector of the transformed system. This is useful for creating configurations where a desired crystal plane is one of the faces of the unit cell. Note that this transformation does not necessarily conserve the number of atoms. The transformed cell will generally be larger and contain more atoms than the original cell. That lattices represented by both unit cells will be identical though.

NWChem Plane-Wave Density Functional Theory (NWPW) Calculations

(6.1) Figure 28 shows the Calculation Editor Theory Details dialog for the NWChem Plane-Wave Density Functional Theory (aka NWPW) PSPW theory. ECCE GUIs for setting up both PSPW and Band NWPW calculations are now available. The NWPW module PSPW theory additionally includes support for the Car-Parrinello runtype through its own Runtype Details dialog as shown in Figure 29. NWPW calculation support is tightly woven with the periodic system building capability in the Builder that is also new in ECCE 6.1. Note that when selecting either PSPW or Band as the theory for an NWPW calculation in the Calculation Editor that basis set selection is disabled. ECCE Viewer support for plotting a number of per geometry step properties for NWPW and in particular Car-Parrinello calculations has also been added. Figure 30 shows the ECCE Viewer displaying the Geometry Trace and Wave Step Plot properties for a PSPW Car-Parrinello run.

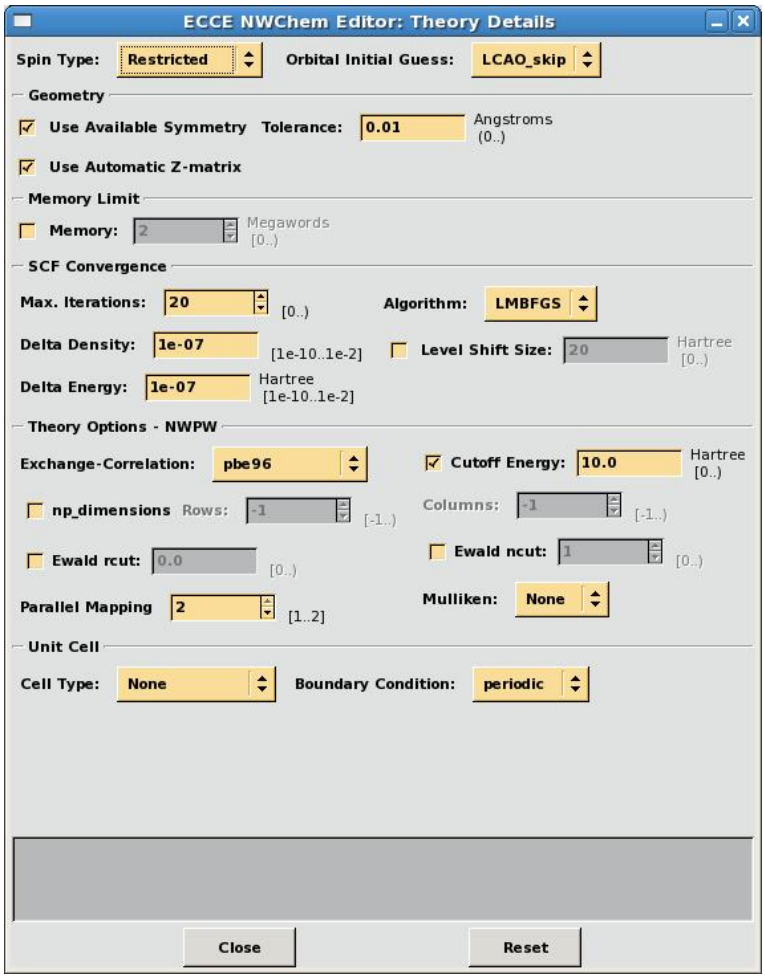

Figure 28. NWPW PSPW Theory Details dialog

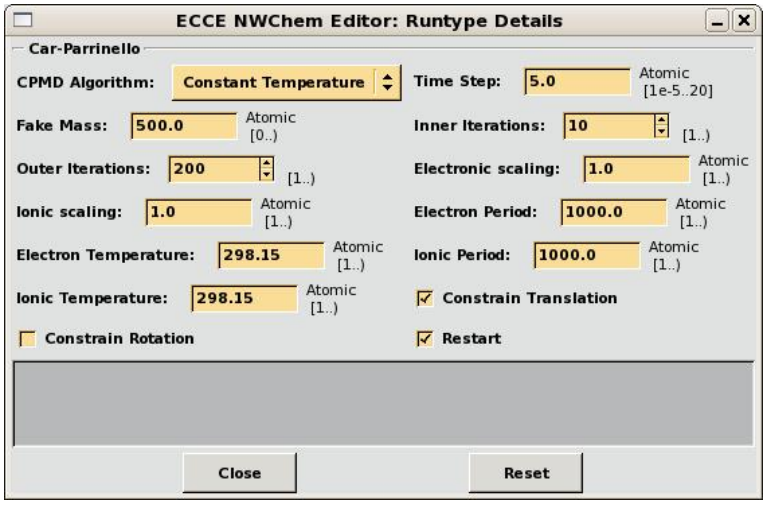

Figure 29. NWPW Car-Parrinello Runtype Details dialog

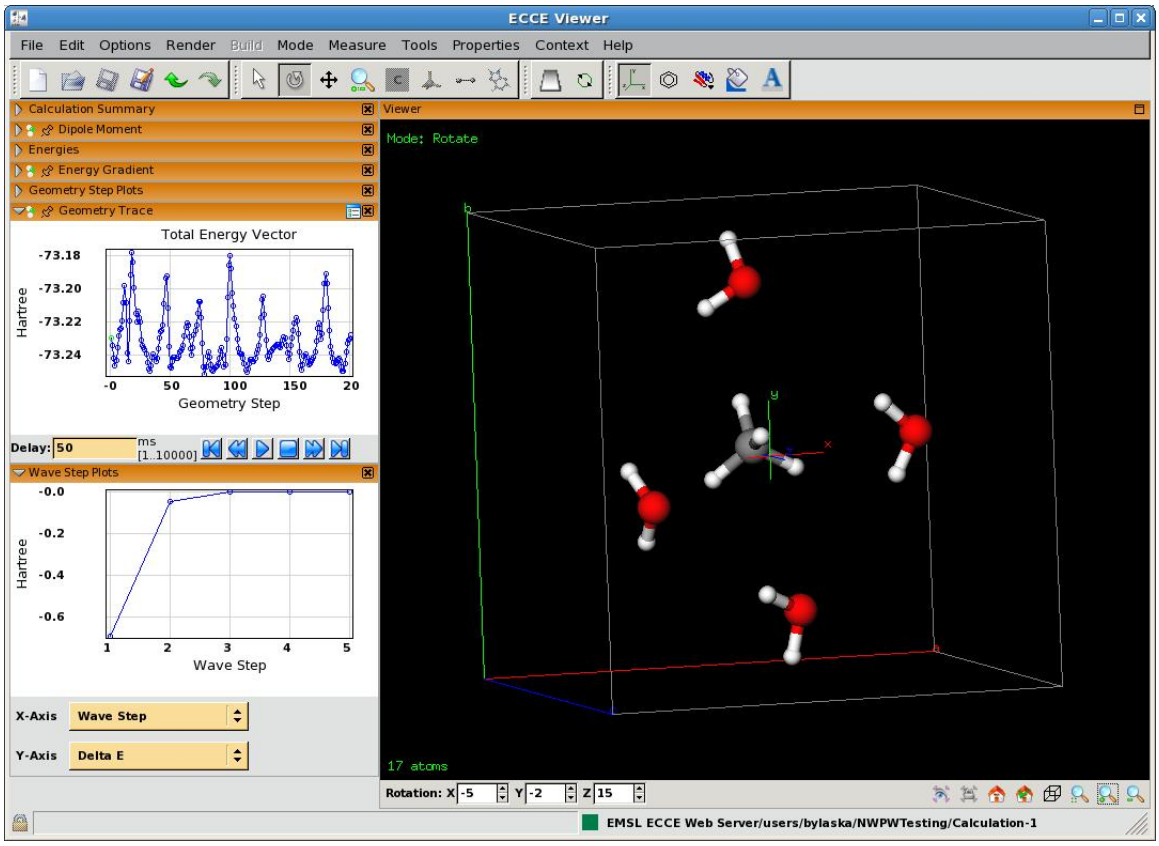

Figure 30. ECCE Viewer showing NWPW PSPW Car-Parrinello results

SITE ADMINISTRATOR WHAT'S NEW

Upgrade of Apache HTTPD

(7.0) The Apache HTTPD server (see http://httpd.apache.org) used for the ECCE data server has been upgraded from release 2.2.22 to 2.2.25. This version of the source code distribution of HTTPD is bundled with the ECCE source code distribution and ECCE binary distributions have this version of HTTPD built and ready to run after ECCE is installed. Along with the HTTPD server being updated, the CGI perl module, CGI.pm, needed by HTTPD has also been upgraded to version 3.63.

Prerequisite Software Check

(6.3) The ECCE binary distribution installation script now includes a check for prerequisite software needed to run ECCE such as the java runtime environment, python and perl scripting languages, and the underlying Gtk user interface toolkit. If the package is found then a check for an ECCE compatible version is performed. This prerequisite software check is a new menu item available from the main installation menu and thus the previous item numbers have changed. These checks are analogous to those done for building ECCE from the source code distribution via the build_ecce script except that checks are only made for software needed to run ECCE instead of software needed both to run and build ECCE. Therefore if the binary distribution of ECCE being installed has

been built from source code on the current platform there is no need to perform the prerequisite software check when installing.

Installing ECCE 6.2

(6.2) Because ECCE 6.2 requires users to enter their data server password and most existing users will not know this password (it is not the same as the ECCE login password or encryption key that was entered on startup prior to ECCE 6.2), it is recommended that sites run both ECCE 6.2 and their existing ECCE 6.0 or 6.1 concurrently. This is possible because the default ECCE server ports for the Apache HTTPD data server and Apache ActiveMQ message server have been changed allowing a 6.2 ECCE server to run concurrently with a 6.0/6.1 server on the same host. To be able to run both the old and new ECCE either a "Full upgrade" (option 2) or "Server upgrade" (option 6) should be selected at the main installation menu. This will allow users to lookup their existing data server password using ECCE 6.0/6.1 and then use the password to gain access to ECCE 6.2. Note that because of the upgrade process user calculation data will no longer be accessible from ECCE 6.0/6.1 so this old version is functional only for retrieving passwords (hitting "OK" on the login dialog yields an error dialog about the server not having user data and the Gateway toolbar will not be displayed). After some period of time at the discretion of the site administrator the 6.0/6.1 server can be shutdown. At this time any users who didn't retrieve their data server password will need their password reset by contacting the site administrator before running ECCE 6.2. If the site administrator doesn't want to run concurrent ECCE servers then the ECCE 6.0/6.1 server can be shut down immediately when installing ECCE 6.2 and all users will need to have their data server password reset with the new passwords being communicated to users before they can run 6.2. The ecce_htpasswd utility script in the ecce-utils directory under the top-level ECCE server directory is used to reset data server passwords. Simply run ecce_htpasswd as the same user who installed ECCE (for write permissions) with the username as the only command line argument. The new password will then be prompted for by ecce_htpasswd.