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EMSL In Brief

Environmental Molecular Sciences Laboratory

EMSL Releases Ecce Version 4.0

A new version of the Extensible Computational Chemistry Environment software (Ecce) was released by software developers from the Environmental Molecular Sciences Laboratory (EMSL) and the Pacific Northwest National Laboratory (PNNL).



Ecce, part of the award-winning Molecular Science Software Suite (MS³), provides a sophisticated graphical user interface, scientific visualization tools, and the underlying data management framework that enable users to efficiently set up calculations and store, retrieve, and analyze the rapidly growing volumes of data produced by computational chemistry studies conducted using NWChem—DOE's premier computational chemistry software, which is also developed and maintained by MS³ software developers at EMSL and PNNL. The new Ecce Version 4.0 adds full end-to-end support for the molecular dynamics module in NWChem. Some of the many upgrades to Ecce include the following:

- The upgraded software provides NWChem molecular dynamics module support for the Prepare, Energy, Optimize, and Dynamics tasks, with user interfaces intuitively representing the full complement of options available to NWChem users who create molecular dynamics input decks by hand. Real-time visualization of trajectories and properties such as total energy, temperature, and pressure as they are calculated allows the user to determine whether simulations are proceeding as desired.
- To accommodate visualization and interactive editing of bio-molecules of 100,000 atoms and beyond, Ecce now uses a new molecular visualization toolkit, OpenMOIV, optimized by the Ecce team to efficiently handle these structures. This toolkit contains protein rendering techniques, including ribbons for backbone structures and cartoons depicting alpha helices and beta sheets.
- Distance, angle, and torsion measures set on atoms within trajectories can be captured over the course of a molecular dynamics simulation for additional analysis. Trajectory files are automatically compressed to save space on the Ecce data server, and sites may now preclude the storage of trajectories on the Ecce data server altogether if disk space is limited.
- The first major steps have been taken to migrate the Ecce software from a Linux/UNIX-only environment to support multiple platforms, including Microsoft Windows and Macintosh OS X.

For more information about Ecce Version 4.0, see the Ecce home page located at <http://ecce.pnl.gov> or contact Gary Black (email: gary.black@pnl.gov; phone: 509-375-2316).

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