



EMSL Software to be Deployed for First-Ever Educational Use

For the first time, EMSL's Extensible Computational Chemistry Environment—or Ecce—will be formally used in a classroom setting by an institution for educational purposes.

Matthew Asplund, Assistant Professor of Chemistry at Brigham Young University, has persuaded the faculty of BYU's Chemistry Department to forego their current chemistry software and implement Ecce—a problem-solving environment for computational chemistry—in their physical chemistry lab classes. About 100 chemistry and biochemistry majors will benefit from the use of Ecce during the fall and winter semesters.

“We have a large supercomputer complex at BYU, and using Ecce lets us leverage those machines to allow students to perform higher-level calculations than with our previous software,” says Asplund. “One of our goals is to have the students calculate a moderate-sized molecule with a bunch of basis sets to show that variational theory really does work.”

Asplund also cites Ecce's user friendliness and no cost as drivers for incorporating Ecce into BYU's curriculum.

Ecce provides a sophisticated graphical user interface, scientific visualization tools, and the underlying data management framework that enable scientists to efficiently set up calculations and store, retrieve, and analyze data produced by computational chemistry studies. The software has been downloaded by more than 400 sites with multiple users at each site.

“Users of Ecce range from grade school children who 'build' molecules, to the graduate level where students are beginning to explore atomic-level bonding, to professors who have incorporated Ecce into their research programs to set up problems, visualize results, and store solutions,” says PNNL Computational Scientist Gary Black, an original developer of Ecce.

One thing that makes Ecce unique from other software packages is its comprehensive capabilities that take users from the beginning stages of the problem-solving process through the analysis stages.

For more information about Ecce, contact Theresa Windus (509-376-4529) or Gary Black (509-375-2316).

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