Transforming Chemistry Education through Computational Science

An ongoing US National Science Foundation-funded project, the Institute for Chemistry Literacy through Computational Science (ICLCS), involves instructing rural Illinois high school chemistry teachers in the educational uses of computation. The project's training helps participants become educational leaders and change agents.

Chemistry research increasingly relies on computation, and even synthetic chemists use computation to guide their efforts. Because computational science is integral to chemistry research, chemistry education should reflect this.[1] Educators need to use technology that can transform the educational landscape, so they need support in incorporating new tools into their teaching.

Computation can help the student visualize,[2] for example, interactions between the atoms or molecules in a substance. The ability to "see" such phenomena helps them understand chemical principles and increases interest and enthusiasm.[3] Recent technological advances (such as the Web browser as a computing interface) have made powerful computational tools widely accessible. If teachers can use authentic research-grade computation in a pedagogically sound manner, we can harness students' interest in technology to motivate and improve the educational process.

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The availability of high-performance computing (HPC) means that a paradigm shift is overdue in our educational system, but the issue is how to implement the necessary changes. A US National Science Foundation (NSF)-funded project, the Institute for Chemistry Literacy through Computational Science (ICLCS; http://iclcs.uiuc.edu), uses a teacher-centered approach. This article provides an overview, chemistry content and computational tool details, example successes and challenges, and a description of a new computational workbench interface. With these tools and information, participants can become change agents and help drive the needed curriculum overhaul.

To help them in this endeavor, we've incorporated leadership training as a key aspect of the program. In this article, we report on the participants and their students' classroom experiences and discuss how petascale computing will impact educational uses of computational science and further promote scientific literacy.

Project Overview

The ICLCS is a partnership between the Department of Chemistry, the College of Medicine, and the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign (UIUC); A-C Central Community Unit School District #262; and the Regional Office of Education #38 in Illinois. The five-year ICLCS program, which is funded by the NSF Math Science Partnership program (www.nsf.gov/funding/pgm_summ.jsp?pims_id=5756), targets 110 high school chemistry teachers across rural Illinois (see Figure 1) to give them the competence and confidence to use computational tools and methods in their curriculum.

The ICLCS is hosting two cadres of high school teachers (which we refer to as "fellows"), who attend a two-week summer workshop each year for three years. Cadre 1 began training in the summer of 2007, and Cadre 2 will begin in 2008. Fellows also enroll in a three-credit hour graduate-level chemistry course during the academic year delivered through Moodle (http://moodle.org), an open source course development tool that supports the virtual learning community. Using a blended-learning approach, the fellows post reflections on their teaching, share materials, interact with faculty mentors, and attend online presentations to enhance their chemistry content knowledge. This virtual support network has proven to be one of the Institute's key features.

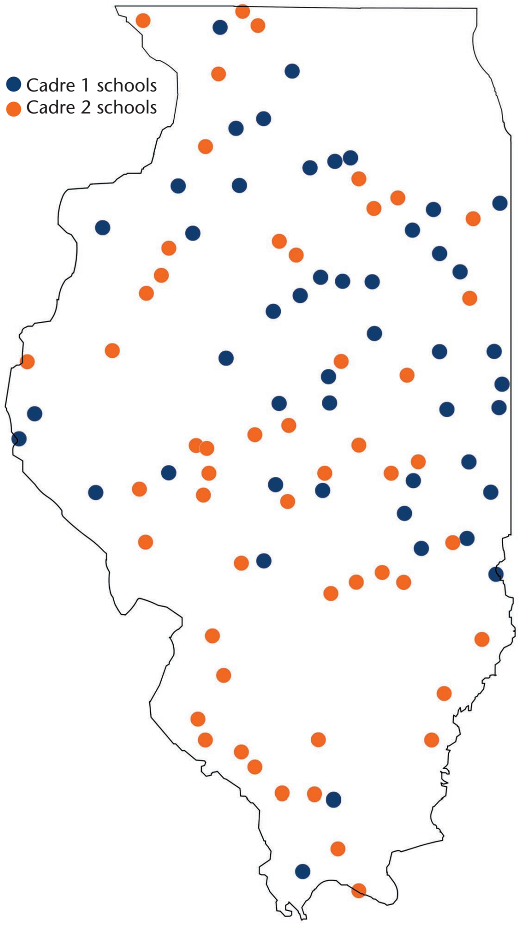

Figure 1. Distribution of Institute for Chemistry Literacy through Computational Science (ICLCS) high school teachers (or fellows). Cadre 1 began training in the summer of 2007, and Cadre 2 will begin in 2008.

Chemistry Content

Preceding the first summer workshop, the fellows completed a survey that asked which chemical concepts they and their students needed help with. Based on the answers, the ICLCS staff used the resources in the Computational Science Education Reference Desk (CSERD; www.shodor.org/refdesk/) to identify the tools that could address these needs.[4] We designed instructional tutorials using these tools for the summer workshop. Because all the fellows will return for three summer workshops, we divided the materials into those to be used in the first summer (individual molecular properties) and the second summer (collective properties of molecules). The content of the third summer workshop will be determined at a later date.

At the initial summer workshop, the fellows spent the first week learning various tools with scaffolded, hands-on exercises. In the second week, they self-organized into teams based on specific areas of interest and began developing classroom modules using the tools. At the workshop conclusion, each team presented the results of their work-in-progress to their peers. The module work focused on topics such as acids and bases, equilibrium, stoichiometry, molecular geometry, kinetics, chemical bonding, quantum mechanics and atomic theory, and biological molecules.

The fellows are currently enrolled in a distance-learning course where they continue to work in teams facilitated by the ICLCS Moodle and the Access Grid (www.accessgrid.org). The course project for each team is a paper on the year's work in a format suitable for submission to an education journal.

At the first workshop, the fellows were interested to hear about chemistry knowledge expectations for incoming freshman. They were surprised to learn that UIUC doesn't assume a great deal of content knowledge. We shared with them the results of a study at UIUC in which we found no statistical difference in grade distribution between students with one or two years of high school chemistry. This suggests that learning outcomes do not depend on the amount of material students are exposed to, but the methods used to expose them to it. The methods used in the classroom help define what it means to learn and understand chemistry. These discussions were a smooth segue into introducing computational science as a tool to increase student interest in and understanding of chemical principles.

Computational Content

In designing the computational chemistry portion of the two-week workshop, the plan was to use free, widely available software; provide time for module development; and address the disparity in computer proficiency. We should note that computational chemistry, in the context of this project, means using computer technology to effectively demonstrate and teach chemical principles. We view molecular modeling, thought by many to be synonymous with computational chemistry, as a specific type of computation.

We designed the exercises to foster expertise in software use through building molecules, performing geometry optimizations, measuring bond distances and angles, determining energies, and viewing surfaces.

The training began with an overview of the methods used in molecular modeling followed by a hands-on exercise introducing WebMO (www.webmo.net), a server-based GUI to computational chemistry programs such as the Molecular Orbital Package (http://openmopac.net), the General Atomic and Molecular Electronic Structure System (www.msg.chem.iastate.edu/gamess/), and Gaussian (www.gaussian.com). Fellows access WebMO through a Web browser on a Java-enabled computer, and it lets them draw, set-up jobs, view results, and perform visualizations and computations. We designed the exercises to foster expertise in software use through building molecules; performing geometry optimizations; measuring bond distances and angles; determining energies; and viewing surfaces such as molecular orbitals, electron densities, and electrostatic potentials (see www.bsw-uiuc.net/moodle/Tutinfo.php).

We also introduced the participants to CSERD. After they worked through an Excel tutorial that reviewed the basics, they used CSERD sites to generate data that they then analyzed using Excel. For example, they used an ideal gas law simulation to collect volume data as the number of gas particles, particle velocity, or the system pressure were changed (www.phy.ntnu.edu.tw/ntnujava/index.php?topic=25). This method helps learners discover several important gas laws in active learning fashion, which research has shown to be a more effective educational method.[5] They also used the Virtual Lab Simulator (www.chemcollective.org/vlab/vlab.php) to generate pH titration data, which they graphed in Excel to more accurately locate the endpoint.

Although students need hands-on laboratory experience, costs and safety concerns limit access. The combination of applets for data generation and subsequent analysis using Excel expands the types of laboratory experiences offered. Technology thus helps level the playing field between schools that have resources for extensive, wet laboratory experimentation and those that don't.

Another tool we introduced was the ChemSketch Freeware available from Advanced Chemistry Development (www.acdlabs.com/download/chemsk.html). Using this tool, students can construct molecules and (assuming a feasible structure) use the software to name the molecule. They can practice both the concept of valence (the number of bonds an atom can form) and molecular nomenclature. The structure is easily transferred to the 3D viewer, and a geometry optimization (using simplified molecular mechanics) can be performed. The fellows also learned about investigating display modes, cutting and pasting images between various programs, and so on.

Computational Science Student Workbench

Our sister NCSA project, the Biology Student Workbench (http://bsw-uiuc.net/), has now added chemistry to its content. The tutorials are in an optimum configuration for efficient online navigation among the three major components of the educational environment: the instructional scaffold (lesson), relevant Web materials, and the computational tools. The key is an interface constructed of Java and Frames within a Web browser that uses two frames. The upper frame contains tabs to the tutorial, Wikipedia, CSERD, Google Scholar, and so forth. Some terms in the tutorial are in hypertext. Mousing over the hypertext provides a pop-up window with more information.[6] Words that aren't in hypertext are linked to answers.com, letting us provide a quick reference for every term in the lesson.

One tutorial provides instruction in using the WebMO interface. The instructions can be immediately implemented by scrolling down to the tool interface, located in the lower frame. This behaves exactly like the raw interface to the computational tool, but detailed instructions are just a quick drag on the scroll bar away. One of the time-consuming steps to learning new materials and skills is the time taken to navigate between access paths to different resources—the lesson scaffold, background material, and relevant computational tools. By minimizing that time, our interface eliminates a source of inefficiency and keeps the learners (fellows and students) on task.

Leadership Training and Project Sustainability

Over the course of the project, the fellows will engage in a series of activities to help them progress from personal awareness to peer leadership to becoming leaders in the educational community. Fellows are already assuming leadership roles such as training and mentoring other teachers and by presenting their work at local, regional, and national meetings. The Institute will continually support the fellows in their efforts to publish their materials and student outcomes. Leadership training is essential for the project's long-term sustainability. We expect many of the ICLCS fellows to become change agents and help drive the needed reform of the high school chemistry curriculum in the years to come.

The final summer workshop for Cadre 2 will be in the summer of 2010. All the tools and associated tutorials introduced in this project to date are available online (www.bsw-uiuc.net/moodle/workbench.php), and we'll also make future developments available. The fellows have begun module development, supported by the virtual Moodle environment, and many will continue this after the project ends. The best modules will be placed on the Web, accessible to all teachers. We hope that the module collection will eventually cover all aspects of high school chemistry where computation can improve the educational process.

Classroom Experiences

After the first workshop, the fellows began incorporating computation into their classrooms. A critical goal of the ICLCS is to increase their competence and confidence with computation. This has fueled their passion to update their courses. It's become clear, however, that some fellows require examples of exactly how to effectively use computation. We've therefore arranged demonstrations by successful fellows to show how to expand current activities and make them more effective using computation.

The addition of computation has been well received by students. The top benefit reported is that computation lets students "see" the phenomenon being taught. Rodger Baldwin, a teacher of Clinton High School says,

> Chemistry is a tough subject because it has one foot in the abstract world and the other in the phenomena observed in the real world. Students can have a real problem with all these "imaginary" particles, mental "models" of the atom, strange chemical symbols, and complicated stoichiometric and logarithmic calculations. My students will have a great chance to connect the macroscopic, hands-on world of wet chemistry to the sub-microscopic world of charges and forces and motions of atoms and molecules.

Technology-savvy students quickly learn to use the tools in meaningful ways. One fellow pointed out, "I wish I could catch on to using computational tools as quickly as my students do." Fellows also realize that the entertainment aspect of the technology can be used as an effective educational approach: "We are able to show abstract ideas in a way that is educational as well as entertaining. Entertaining our students is not a priority. However, providing interactive materials can engage students and promote learning." Using computation has the added benefit of honing students' computer literacy, which will be important whether they continue to the university or enter the workforce upon graduation.

Computation is also a universal language that helps reach diverse populations. Sheila Stephens, at the Illinois School for the Deaf, teaches chemistry to deaf students for whom English is a second or even third language. She says, "With my students, the more visual aids we offer, the better their degree of understanding. I can bridge this visualization to both American Sign Language and English. Computation is a great bridge that I have relied on for years. ICLCS is affording me

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the opportunities to expand in that area. Computation, yes, is a universal language."

Fellows have already garnered interest of regional and community newspapers. The ICLCS has been highlighted in publications of the Illinois Farm Bureau[7] and the Association of Illinois Rural and Small Schools.[8] An article in the *Mattoon Journal Gazette* highlighted Jim Sparks for using computation in his classroom to aid in students' conceptual understanding and to provide laboratory practice in a "consequence-free setting."[9] It said use of classroom laptops "skyrocketed this year following Sparks' involvement with the [ICLCS] project." In a *Paris Beacon News* article,[10] Brett Block of Paris High School credits the ICLCS with helping her prepare students to continue their chemistry education. According to Block, "College professors often expect incoming students to have knowledge of software that was previously not available to many rural schools, including Paris High School. Now, PHS students will use the software in high school and should be better prepared when they enter college."

In the near future, the education community we serve will have access to large computing resources. Beginning this year, NCSA will devote 1 percent of the computing resources under its control to education. Presently, this means there is access to just less than 2 teraflops of processing power. A large increase in this capacity will occur when the recently announced Blue Waters petascale machine comes online in 2011 (www.nsf.gov/news/news_summ.jsp?cntn_id=109850&org=OCI&from=news). This date coincides with the conclusion of the ICLCS project. Through this project, we hope to help teachers and students across the nation exploit Blue Waters for chemistry education by providing them with meaningful and ready access to education-adapted computing tools of the sort that have been essential in chemistry research. We have recently initiated work with the Concord Consortium[3] to begin designing educational materials that will take advantage of Blue Waters.

Some students currently entering high school will become scientists making important discoveries with future large-scale computing systems. Computational models can motivate students to become interested in and better understand the mathematical foundations used to create and explore such models. Understanding the mathematics leads to improved quantitative reasoning ability, which is the basis of all science. As systems such as Blue Waters let us create ever more sophisticated and detailed models, we must begin to use computation throughout the educational process so that tomorrow's scientists will have the skills they need to fully take advantage of future computer technology.

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