



### Computational Chemistry: From the Minors to the Majors

Robert Gotwals stood in front of his high school chemistry class in 1987, pouring the contents of a test tube into a beaker to create a chemical reaction. When he asked his students to describe the reaction that had just occurred, none could answer his question.

As a trained chemist whose teaching career began over 15 years ago, Gotwals was frustrated that he couldn't illustrate molecular interactions to his students via test tube. He also knew the only way to really show them what reaction was occurring was by using software to simulate these interactions. "I wanted to expose them (students) early on to this very important approach to how science is being done in this generation," he said.

Known generally as computational science, Gotwals was referring to the process of using a computer to simulate and understand scientific phenomena. Computational Science aims to richly mimic, albeit in software, occurrences that cannot be observed. Some examples include things that happen too quickly (a chemical reaction) or too slowly (global warming or evolution), as well as things that are too big (the galaxy) or too small (changes on the molecular level). Such occurrences can be studied by scientists directly by using a computer to evaluate the underlying mathematics.

Gotwals' specific field of inquiry is computational chemistry, which uses the grad-level mathematics of quantum mechanics (physics + chemistry) and is commonly used in pharmacology for drug design. In this realm, the benefits extend beyond the classroom since experiments are performed inside a computer, therefore reducing testing costs and, in some cases, minimizing the need for animal testing.

While computational chemistry introduces a higher level of teaching chemical concepts in the classroom, software and the high-performance computers required to run them are expensive, sometimes equating to a school's annual budget. In addition, there was a missing layer for teaching purposes, one that would enable ease of use for both teachers and students to manipulate the mathematical software.

In his continued quest to bring computational chemistry into his classroom, Gotwals discovered a product called WebMO that surfaced out of Hope College in early 2000. This product provided an interface to some of the more powerful open-source simulators that were being created by university researchers. With its user-friendly layout, WebMO allows users to build their molecules using a molecular editor with pull-down menus. More importantly, WebMO serves as a "front-end" to several types of research-grade quantum chemistry software packages, such as Gaussian 03, GAMESS, and MOPAC. All in, the interface and its corresponding quantum codes created a "portal" for students to easily select molecules and conduct calculations, or "jobs," to illustrate molecular changes. It was the final component of the perfect computational chemistry teaching tool, facilitating ease of use for both teachers and students. Gotwals' vision of bringing computational science to the classroom was finally viable; now all that was needed was funding to bring it to the classroom.

With the help of some grant money from the Burroughs Wellcome Fund and the North Carolina Mathematics, Science and Technology Center in Research Triangle Park, North Carolina, Gotwals was able to realize his vision. Combined with his negotiation skills and the generosity of commercial software providers with an appreciation for higher education, Gotwals raised enough funding to acquire a single computer server where he

installed WebMO for students at the North Carolina School of Science and Math (NCSSM), a public, residential school for high school juniors and seniors with a curriculum centered around science and math, where he is a full-time faculty member.

In the late spring of 2006, Gotwals was ready to employ his tool in the classroom and offered a Medicinal Chemistry seminar to the students of NCSSM. Brittany Fotsch was a senior and in the twilight of her high school career when she heard about the class. Already carrying a strong passion for chemistry, she wanted to take her knowledge to the next level and heard computational chemistry could help her get there.

Fotsch's friends couldn't believe she signed up for an additional class at the end of her senior year, but she described herself as a "kid in a candy store." She learned how to run jobs on the server and, through the user-friendly WebMO interface, could select molecules and run specific computations on them. "It's a perfect intermediate step before going up to the majors of Computational Chemistry. It's great for teaching and helps high school students make the transition into using larger servers," Fotsch said.

In early 2007, with funding provided by the Cisco Learning Institute, Gotwals teamed up with Dr. Steven Armentrout, CEO of Parabon® Computation, who is also an ardent supporter of Computational Science. The two sought to elevate the existing performance capability of the NCSSM system from one server, which could perform poorly under heavy use, to a distributed solution that employs potentially thousands of computers across the Internet. Using Frontier®, Parabon's grid computing platform, the idle capacity of networked computers is harnessed to deliver supercomputing power to the desktop of anyone who needs it. Parabon engineers built a grid portal that runs WebMO, but instead of running simulations locally, it distributes them to the computers of participating classrooms.

Students in North Carolina have been the first to use the new service, which is hosted at the Global Grid Exchange® in Fairmont, West Virginia (<http://cli.GlobalGridExchange.com/>), but the idea is much bigger than this. Gotwals and Armentrout intend to extend the program nationally, but they now face the challenge of getting the word out to schools across the country to take advantage of it. "Depending on your audience, you can scale the tool. Teachers have the ability to run their show; you don't have to understand all the underlying mathematics – you can include this or not include it, depending on level of audience," Gotwals said.

Their endeavor is also a strong complement to the American Competitiveness Initiative (ACI), an enterprise announced in the 2006 State of the Union address by the President of the United States (<http://www.whitehouse.gov/stateoftheunion/2006/aci/>). ACI recognizes the importance of a well-educated and capable workforce and the importance of investing in programs that perpetuate this. In this case, bringing computational chemistry into the high school classroom directly complements this initiative by investing in the tools available for students to achieve higher levels of computational science.

Bringing computational chemistry into classrooms around the country is a challenge worthy of pursuit, as evidenced by Steven Lin, Gotwals' former student at NCSSM. Lin took Gotwals' computational chemistry class starting November 2005. He will matriculate at UNC Chapel Hill this fall and attributes his success to the concepts he learned in the class. Lin claims, "If hadn't learned those concepts, I wouldn't have gotten this far."

How can you support the advancement of education and support the American Competitiveness Initiative? Gotwals can tell you – adopt computational chemistry in your classroom. "There are teachers and students out there who are ready and waiting for this level of chemistry education and we have the curriculum and computational tools to help them engage. I look forward to hearing from them."

To learn more about the Cisco Learning Institute, visit [www.CiscoLearning.org](http://www.CiscoLearning.org)

To learn more about Parabon® Computation, visit [www.Parabon.com](http://www.Parabon.com)

To learn more about how the computational chemistry server could be used in your community or classroom, contact Bob Gotwals at [gotwals@ncssm.edu](mailto:gotwals@ncssm.edu).