

Computational Chemistry Comes to North Carolina

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In 1929, the Nobel Prize winning scientist P.A.M. Dirac wrote “the underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too

complicated to be soluble.” Dirac was correct in this statement; the mathematical principles needed to solve problems in chemistry are known, yet solving these equations proves to be daunting for even the most brilliant members of the scientific community, let alone typical high school chemistry students. However, today, almost 80 years later, computational chemistry provides the tools to solve even the most complicated chemistry equations, placing it at the forefront of many areas of chemistry research.



The Shodor Education Foundation, Inc, a “national resource in computational science education” based in Durham, NC, has been a leader in computational chemistry education for its entire existence. Its “Computational Chemistry for Chemistry Educators” summer program for university chemistry faculty, offered through the National Computational Science Institute (NCSI) is probably the most popular NCSI offering. For a number of years, Shodor has been teaching “Explorations in Computational Chemistry” through the SUCCEED program and as a seminar offering at the North Carolina School of Science and Mathematics.

Now, thanks in part to a \$12,000 grant from the Burroughs Wellcome Fund and the North Carolina Center for Science, Mathematics, and Technology, Shodor is able to provide North Carolina secondary students and teachers with free access to a high performance chemistry computational laboratory. Shodor has established the “North Carolina High School Computational Chemistry Server”, a research-grade computational resource for performing a wide variety of molecular calculations. The resource is available free of charge to all secondary students and teachers in North Carolina, and features three of the most powerful computational chemistry software programs: Gaussian, GAMESS (General Atomic and Molecular Electron Structure System), and MOPAC (Molecular Orbital PACKage). Through a Web-based interface known as WebMO, users can build molecules, submit calculation requests, and view their results in a user-friendly Web interface.

Choose Computational Engine

Status	Engine	Description
student	<input checked="" type="radio"/> GameSS	Ab initio and semi-empirical calculations
Unlimited	<input type="radio"/> Gaussian	Ab initio and semi-empirical calculations
Unlimited	<input type="radio"/> Mopac	Semi-empirical calculations

0 jobs

Progress

- Job manager
- Build molecule
- **Choose engine**

Choose the desired computational engine from those installed.

- Job options
- Submit job

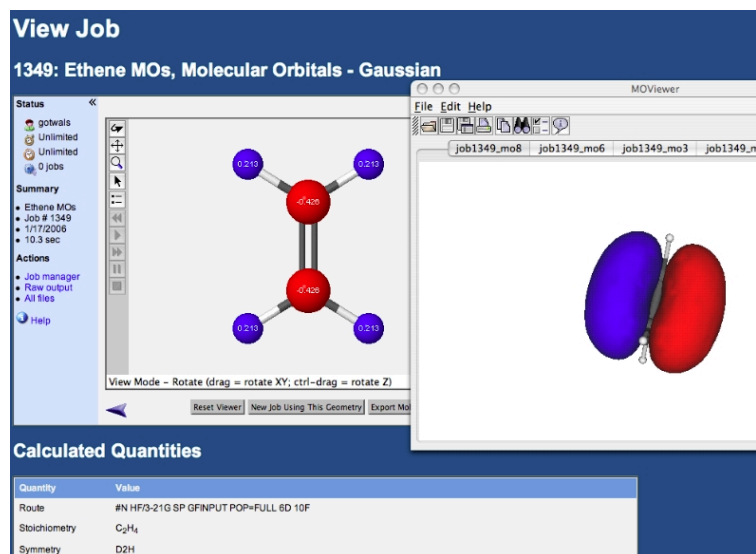
Help

Select Server:

We envision the server being used in two distinct ways, what we refer to as the “associative law of computational chemistry education”. This law can be diagrammed in this manner:

Computational (chemistry education)

By this we mean the following: we believe that teachers can teach the chemistry content they are already teaching (and that content they are expected to teach as a part of the NCSCOS) through the use of computational methods. For example, most chemistry students struggle with the concepts of atomic and molecular structure, especially in terms of orbitals, hybridization, and bonding. These concepts can be taught in a highly interactive and visual manner using computational techniques. We are also interested, however, in students learning about computational chemistry as a discipline. The National Science Foundation (NSF) and other leaders in science education have described computational methods as being a critical skill needed for today's scientific challenges. As such, we want our students to see computing as it is used to understand and solve problems, and we want our students to understand computation as its own field of study.



As such, there are two ways for the server to be used. The first is a teacher-directed approach. Teachers can request free classroom accounts. With a classroom account, a teacher can have his or her entire class do a laboratory exercise using the computational chemistry server. Typically, classroom accounts are provided with two time limits. The first time limit is on the time allocated to do a single calculation. The second time limit is for total time. We typically allocate a 4-minute per job limit and a 20-minute total time limit. As an example, suppose you wish your students to calculate the vibrational frequencies of the water molecule. This calculation takes about 26 seconds, well below the 4-minute per job level. Once the student does this, they have 19 minutes and 34 seconds of time left. If,

however, they try to compute the vibrational frequencies of a large molecule, the job will not complete in less than 4 minutes. Most calculations that a teacher might want his or her students to do will run in under 4 minutes, and the 20 minute total time limit gives the student a little bit of extra time to try other things.

The second method by which the server can be used is with a student account. Individual students can submit a proposal for a research project, and time will be allocated in support of that project. The projects do not need to be too formal: for example, a student might just want to try an extension to something they did in class. They do, however, have to submit a request for time. Larger projects, such as for science fairs or for entering into local, regional, state, and/or national competitions, are strongly encouraged. Staff scientists at Shodor can provide some mentoring and other technical support for student work.

We encourage students and educators to visit this resource at <http://www.shodor.org/chemistry>.

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