Proposal
Associated Colleges of the South
Teaching with Technology Fellowship

Title: Developing Molecular Simulations based courses in General Chemistry.

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1. Background

The effects of computer technology in the General Chemistry curriculum over the last years are obvious; one needs only to examine a typical freshman textbook to see the flashy pictures gracing the pages and the movie-filled CD's sealed to the back cover. While these tools have indubitably improved the learning experience for many students, they are not the most exciting development that is possible with the here-to-fore unimagined level of computing power available to students.

Chemists, physicists, and more recently, biologists, have developed and used freely available research-quality programs that can simulate *in real time* not only the molecules studied by freshmen students in general chemistry, but also large *clusters of molecules*. We emphasize these last two points because, while not immediately obvious, they represent a "quantum leap" in pedagogical technology. We also point out that with the level of computing power available to students is such that students can study large scale molecular systems *on the fly* which would have required weeks of supercomputing when their parents were in school.

One of the most difficult concepts for chemistry students to grasp is that the molecules they see drawn in their books interact with each other to lead to the chemical reactions and properties and they witness in the lab. Molecular simulations allow them to view a molecule, allow it to interact with another, and see what happens after they collide. They no longer have to take the Professor's word that A reacts with B to make C. They can make it happen themselves. On a larger scale they can look at, say, 200 molecules at once and see what happens when you take their temperature from freezing to 2000 degrees. Again, they can do this on their laptops.

This is a step up from the typical CD's included with textbooks; on those CD's, a student views movies that were pre-made under certain conditions. A student using molecular modeling can change any parameters of the simulation and re-run it to see what happens if they change the temperature, or change the volume, or add an impurity.

This proposal is for the development of a platform students may use to interface with freely available molecular modeling software to perform designed exercises which illustrate chemical principles. Right now the bottleneck to widespread use of these programs is the fact that they are developed for research, not for ease of use. A simple interface designed exclusively for education rather then research will allow students access to the same powerful software used by scientists. One such interface exists at the current time but is a proprietary commercial product with a large price tag and very limited ability, that is, it is not research quality software. The interface I propose to develop can be distributed freely along with the underlying software

2. Description

The Tinker Molecular Modeling / Molecular Dynamics suite of programs is offered freely to the scientific community[1]. This is a powerful set of programs used by many scientists for research in mostly biological areas. The drawback to this program for educational use is that its interface is non-intuitive and downright difficult for students. Recently an excellent Graphical User Interface (GUI) has been developed for Tinker (Force Field Explorer[2]). While this has proven a very useful tool for research, it still requires a working knowledge of molecular dynamics to run. I plan to develop a similar GUI which eliminates jargon and provides a simple to understand "black box" for student use. A student would be able to open the program and enter the general type of exercise he wants to perform. The program would the offer the user some simple choices such as number of molecules, temperature, and volume, and then run the molecular simulations, providing output in the form of a real-time movie of the simulation and plots of molecular properties that change during the course of the simulation. The student could then go back, change whatever parameters he/she wishes, and re-run to see the effects. Basically it would replace the static pictures in textbooks or the pre-ordained movies on the CD's.

In simple terms we propose to:

- Develop a simple freeware GUI to interface with Tinker using Java.
- Design "units" corresponding to general chemistry lessons which may be illustrated by molecular dynamics.
- Make "workbooks" within the GUI that correspond to each "unit."

3. Timeline

I propose to complete the initial design of the GUI and at least three to four example "units" during the summer of 2005. I estimate it will take approximately 1 month to 6 weeks to complete the GUI. This somewhat short timespan for development is based on the fact that the research GUI for Tinker is available as source code, and so building off of this technology we should be able to eliminate a lot of the preliminary work and focus on what will basically be a redesign of the GUI for education. After this is complete, I believe it will take another 4 weeks to design and implement the first "notebook" lesson. After this each additional lesson should take much less time.

In basing my work off of the existing GUI we will follow the license guidelines for Tinker. Tinker is provided in a modular way that encourages user modification.

4. Technology

The heart of this project will be a redesign and front end for the Tinker program. Tinker itself is written in Fortran and C++, both of which I have 6 years of experience in programming in. The GUI will be written in Java, and requires the Microsoft developer program. The fortran compilers are available free, and the developer is available through the Rhodes IT department. Execution of the finished product will be on any 32 bit Windows platform.

5. Other Support

Rhodes college has provided PC and Linux programming platforms for development. The source code for both Tinker and the GUI are available freely from Jay Ponder at Washington University.

6. Learning Outcomes

The chemistry lesson "notebooks" which will be the end result of this project and which will be accessed through the GUI, will each provide an interactive, visual interpretation of chemistry lessons. Lessons I plan to design include: 1) a collision between molecules, 2) a phase change, 3) velocity distribution of molecules. These notebooks will allow the student to see for themselves how the motions of molecules lead to the reactions and equations they learn in the class. I believe by doping it themselves, it allows students to "own" the concepts, rather than memorize them.

7. Curriculum

General Chemistry at Rhodes is generally taught by 2 to 3 professors in sections of about 30 students. I plan to introduce the molecular dynamics examples in 1 section in Fall 2005, using the other 1 or 2 sections as controls. I believe that students will respond well to the lessons and I will be able to pass them along to other professors and other colleges the following year. Also, with students becoming comfortable with molecular dynamics in the freshman year, this will open up their ability to do more advanced modeling in organic and physical chemistry. It is the goal of our department to incorporate a strong computer/modeling component into our chemistry curriculum as a whole.

8. Assesment

As noted above, I plan to use these lessons in one section using the others as control. We will assess the popularity / success of the notebooks by quiz/exam grades and a questionnaire administered to the students. In the following year as we send the program out we will assess how other teachers like the lessons.

9. Collaboration and Dissemination

Strictly speaking, I can only disseminate the GUI and the notebook lessons I plan to develop. I hope to come to an agreement with Jay Ponder at Washington University to distribute Tinker along with the GUI. This can be made into a self-extracting downloadable file for use at other institutions. I plan to offer the package as a CD to freshmen chemistry students. With success, I plan to publish the results in the *Journal of Chemical Education* and /or present the results at a conference.

[1]http://dasher.wustl.edu/tinker/
[2] http://dasher.wustl.edu/ffe/