FY04 Innovations in Teaching with Technology Awards: Development of a Graphical User Interface for Molecular Modeling in Chemical Education

Investigators: Jan H. Jensen
Department(s): Chemistry

What do you intend to do?
My objective is to develop a graphical user interface (GUI) to a molecular modeling program called GAMESS (General Atomic and Molecular Electronic Structure System) in order to make it more accessible to chemistry students. Specifically, the development will involve the modification of GChemical, a freely available program for building molecules.

Currently there is no molecular modeling/GUI software package that has all of the following important characteristics:

- Completely free
- Source code provided
- Works on Windows, Macs, and Linux machines

Thus the software package we propose to create, which has all these features, would be the first of its kind.

How will it improve student learning?
The software package will be used this semester by students enrolled in Introduction to Molecular Modeling (04:180). Currently 10 students are enrolled and I expect that at least three more students will enroll.

Impact in Other Departments
Introduction to Molecular Modeling has been taught four times so far, and has included students from the Departments of Biochemistry, Mechanical Engineering, Chemical Engineering, Physics and Astronomy, Pharmacy, as well as Chemistry. This project is thus inherently cross-disciplinary.

Additional Impact
Once operational, the software package will be used in other chemistry courses currently employing molecular modeling (4:011-012, 4:141, and 4:233).

Also, since GAMESS and GChemical are freely distributed the project will benefit chemical education world-wide.

What resources will you need? Itemized Budget

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graduate student salary for Spring 04 (Based on COGS minimum FY ’04 of $18,780 plus 12.5% fringe)</td>
<td>$7043</td>
</tr>
<tr>
<td>Dell Dimension 4600</td>
<td>$983</td>
</tr>
<tr>
<td>Total</td>
<td>$8026</td>
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</tbody>
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Budget Justification

The necessary modifications to Ghemical will be performed by a graduate student to be hired from the Computer Science Department. I anticipate that all necessary changes can be made during the Spring 04 semester and tested by the students enrolled in Introduction to Molecular Modeling.

It is important that Ghemical works on both Macintosh and PCs (running both Linux and Windows). The student will be housed in my laboratory where a Macintosh is available. However, to ensure that the code also runs on PCs, I would like to purchase one and house it in my lab. This machine will be made Windows/Linux dual-boot so that the code can be checked on both operating systems.

Cost Sharing

As mentioned above, I will supply a Macintosh computer for code development and testing.

Rough estimate of costs $8,000