NDSU Technology Action Plan Request

I. Action Plan Introduction and Authorizations

NDSU ORGANIZATION OR UNIT

Chemistry and Biochemistry Department

TITLE OF PROJECT

<table>
<thead>
<tr>
<th>Project Duration (3 years maximum)</th>
<th>From: 2/1/2010</th>
<th>To: 12/10/2011</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of Project (Check one)</td>
<td>New x</td>
<td>Previously Submitted</td>
</tr>
</tbody>
</table>

Total Technology Fee Request $16,000.00

Project Director
(Must be NDSU faculty or staff)

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Name (Type or Print) | Signature | Date
Project Director  
Svetlana Kilina  
Unit Head  
Gregory Cook  
IT Division Consultant  
Britt McAlister

Executive Summary (maximum of 175 words)

Atomic and molecular modeling via computer is an educational practice that's time has arrived. For educational purposes, a paradigm shift is towards making use of these tools to assist students in their studies in many disciplines (e.g. Chemistry, Microbiology, Nanotechnology, Engineering, etc) is clearly underway.

We propose the purchase of and installation of common atomic/molecular modeling packages on IT managed cluster machines to help NDSU students take part in this activity.

For primarily educational purposes (e.g. not research oriented), the primary cost is software based as most modern desktop computers (Mac, Windows or Linux) are performance-capable.

We also advocate the purchase (although not part of this proposal) and installation of other modeling software packages (e.g. structural engineering) on IT managed cluster machines.

We successful execution of this successful proposal will demonstrate the feasibility of discontinuing the practice of department owned and maintained computer labs.
II. Project Overview

1. How does this project meet student needs?

Modeling is an important vehicle for understanding atomic/molecular concepts. Commonly students have employed physical modeling kits which provide only a small fraction of what can be gleaned from visual computational modeling.

This is a move away from current department controlled instruction theaters/labs. Utilizing the existing classroom format, computer clusters with modern computational software packages makes the machines more available to the general student population and learning process is more enjoyable for students.

2. What audience does this project directly serve? What audience is indirectly served? How many students are affected?

Two categories of students are directly affected. (i) Students in certain classes would hold one or more classes in the shared IACC space as part of a course they're taking. This category is mainly consist, but not limited, of freshmen students taking General Chemistry classes (e.g. Chem 121 L, Chem 676, etc). (ii) The second category is any student in any class containing atomic/molecular content (e.g. Chemistry, Bio-systems Engineering, Coating and Materials, Electrical Engineering, Materials and NanoTech, Microbiology, Physics, etc.). This category is mainly oriented on graduate students at the above mentioned departments and undergraduate students majoring in different scientific disciplines.

The lab would be also available just as any regular cluster machine outside scheduled class time for all NDSU students who are interested in using the quantum chemistry software.

Indirectly, making use of the existing classroom format, computer clusters makes the machines more available to the general student population.

There are over 60 General/Introductory Chemistry labs for Fall 2010. At an average of 10 students per section that would be 1200 students/year. Adding indirect usage from departments listed above, usage could easily approach 2000 students/year.

3. For projects that target a subset of NDSU’s students, please describe the possibility for broader application in the future.

Many departments make use of atomic/molecular concepts (e.g. Chemistry, Bio-systems Engineering, Coating and Materials, Electrical Engineering, Materials and NanoTech, Microbiology, Physics, etc.). Also, if successful, there are many other areas of modeling (e.g. structural engineering) that could be targets for expanding the utilization of the lab with new software.

4. Describe both the immediate and long term impact of this project.

Currently (Fall 2010) only Chem 476/676 is using computational modeling as an integrated portion of the class. The computational lab is located at the Chemistry Department, and dated computers and computational chemistry software are used by students, which hinders the efficiency of the learning process.

Making use of shared IACC space, modern clusters, and updated software will significantly enhance learning process and adoption of complicated scientific concepts by students via practical exercises, visualization of result, and active learning technics with use of modern technology. In future, all of the departments (Chemistry, Biosystems, Electrical Engineering, Materials and NanoTech, Microbiology, Physics, etc) could make use of the modeling cluster/software.
5. Who will pay for ongoing expenses following the technology fee funded portion of this project (e.g., who will replace hardware or software after it has reached its end of life)?

Because the hardware is part of the already funded IACC cluster, that would be covered during standard refresh cycles. Although we're bringing a separate software ask to this cycle, it's expected that software would be rolled up into the refresh package/cycle that the IT division has in place.

Additionally, modeling software has a very long lifecycle. We're still running Gaussian 2003 at this point.

6. Describe how this project will follow NDSU's best practices in information technology. (Please make sure the NDSU IT Division staff you consulted signs in Part I of this form.)

(a) Make use of shared resources to drive utilization of fewer machines higher.
(b) Use IT division managed assets rather than dept controlled assets
(c) Make use of economies of scale (e.g. user support, desktop support, etc).

7. What service on campus is most similar to the one proposed here? How does this project differ?

The CHPC (CCAST) and current clusters are most similar.
The CHPC from the shared modeling perspective and the Clusters from the shared desktop and classroom usage perspectives. Both are currently managed or operated by the IT division.
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III. Project Description


**Computational chemistry not only for chemists.** Computational chemistry, also known as atomic-level modeling of molecules, can be considered as the “fourth leg” of modern research, joining observational, experimental, and theoretical science. The 1998 Nobel Prize in chemistry awarded to chemist John Pople and physicist Walter Kohn for their development of computational methods evidences the great importance of computational chemistry in modern science.

Being a highly interdisciplinary subject, computational chemistry is based on a mix of mathematics, physics, chemistry, materials science, and computer science. Using advances in theoretical algorithms and computer hardware, computational chemistry allows us to apply physical laws of quantum mechanics to model, understand, and predict—often ahead of experimental measurements—molecular structures, reaction energies, and spectroscopic properties of various novel composites. Such modeling can be done for materials of great technological importance, ranging from tiny nanomaterials for opto-electronics and photovoltaics to biomolecules for disease’s treatment and diagnostic in medicine. Today, computational chemistry has become an indispensible part of the modern researcher’s toolkit in chemistry, physics, materials science, bio-engineering, pharmacology, etc. Moreover, its use is no longer restricted to a small group of specialized theorists; rather, more and more scientists with various experimental backgrounds combine calculations and experiments in their work. Therefore, today, knowledge and skills in computational chemistry have become a common requirement for many research jobs in academia and industry.

**Applied computational chemistry course.** Given the increasing prominence of computational modeling in various professions, we propose to improve and extend the existing chemistry course CHEM-476/676 by a practical application of computation chemistry and computer-based molecular design. The course is oriented on both graduate and undergraduate students who are interested in science in general, or have a specific interest in chemistry, biochemistry, physics, materials science, polymeric materials, etc. The intent is to cross list this course in the Physics, Material Science, Polymeric Materials, and Computer Science departments. We expect that interdisciplinary nature of computational chemistry and its availability at different departments will appeal to diverse audience of NDSU students attracted to careers in science and will enhance the success of these students in their future professions.

The course will give an introduction to the methods of quantum chemistry with the goal of enabling students to perform their own computational studies. The best ways to learn the basic theories and algorithms behind computational methods is to simply practice using the software and try to analyze the physical meaning behind the computational results. For this purpose, (i) the lectures will be accompanied by practical exercises in which students solve computationally small problems providing insight into the various theoretical methods. (ii) Students will work in teams of two on the *final projects* performing calculations on topics of their research interests. At the final week, each team will present their work in 15-20 minute oral presentation following by questions from their peers and instructors. Incorporation of practice computational assignments requires to transfer 1-credit CHEM476/676 course (as it is now) to 4-credit course, which is typical for lab-based courses at NDSU.

Team work, in group questioning, and practical solving of problems that students posted to themselves based on their research interests will provide active learning experiences for students and encourage them to take responsibility for their own learning, meanwhile, making learning more enjoyable and interesting for students. Students who complete the course are expected to obtain a hands-on experience with widely used computational software, be able to ask questions that can be solved with modern computational methods, have some understanding of the capabilities, limitations, and reliability of various molecular modeling techniques, and be able to choose right computational tools to assist in their current or future research.
Privilege of understanding how the world works. The heart of computational chemistry is quantum mechanics. Since the beginning of the 20th century, quantum mechanics has forever changed the scientific picture of the world by introducing indeterminism, probabilities and nonlocality of electrons. Structure of any material and its physico-chemical properties completely relies on concepts of energy quanta and wave-nature of electrons. Fact is, however, that most of the NDSU students, who do not major in physics, never get a real chance to learn about the conceptual issues of quantum mechanics, which often seems strange and counterintuitive, and extremely challenging for students to be learned by them own. We think that not only physicists should possess the privilege to grasp this way of understanding how the world works. Educated citizens should at least have the possibility to become acquainted with the strangeness and beauty of quantum phenomena.

Applied Computational Course CHEM-476/676 cross listed at several NDSU departments will, indeed, provide such an opportunity for students majoring in deferent scientific disciplines, including chemistry, biochemistry, material science, engineering, computer science, and physics. This course will help students to learn and understand main concepts of quantum mechanics via application of these concepts to computational modeling of real systems and problems. Moreover, the benefits of applying computational chemistry for teaching extend beyond just this course.

Computational chemistry is beyond one advanced course. General Chemistry courses for freshmen provide another opportunity for the broad audience of beginning students to learn the main concepts of quantum mechanics dealing with atoms, atom bonding, and electrons. However, it is very challenging to understand something that we cannot see and touch. Computational chemistry aims to richly mimic, albeit in software, occurrences that is challenging – if not impossible – be observed. Some examples include things that happen too quickly, or too slowly (chemical reactions), or things that are too small (electrons, atoms, and molecules). Utilization of graphical programs for visualization typically used in computational chemistry provides a powerful teaching tool to help students "see" atoms and molecules in topics of General Chemistry, such as molecular bonding, polarity, the periodic table, etc. Each year, hundreds of freshmen who want to start their careers in chemistry, material science, technology, pharmacology, and medicine take General Chemistry courses challenging all these extremely complicated, but very important scientific concepts. Hard to be comprehended, course material on electronic structure of elements from the periodic table, different type of bonding in chemical compounds, chemical reactivity of different molecules and much more are hardly understood by students leading to lack of interest and disappointment in choosing careers. Through the use of simulations and visualization in frames of computational chemistry, students can gain an appreciation for all above concepts, while getting fun during their learning.

Redesign of Freshman Chemistry Laboratory. In this component, we propose to extend Freshman Chemistry Lab assignment with more applications of technology, computations, and active learning experiences. Two labs will be offered as a Virtual Lab on a regular basis of the General Chemistry courses. By taking advantages of computational chemistry programs (the same as we will use for Applied Computational Course CHEM-476/676), students will be able to perform a few simple simulations of several elements from the periodic table (e.g., hydrogen, carbon, oxen, etc.) and then visualize the s-,p-,d-, etc. atomic orbitals. Next, we will teach students to perform calculations and visualization of molecular orbitals (charge density distribution) of small base and acidic molecules, their vibrational motion and IR spectra. It should be noted that the students can see an animation of the vibrations, not just the static image shown in their textbooks. The students can also rotate the molecule, zoom in or out, and otherwise see the molecule and distribution of the electron density on different parts of the molecule from a variety of perspectives. They will learn how to compare computed results with that of experimental results by using resources such as the Computational Chemistry Comparison and Benchmark Database from the National Institute of Standards and Technology (NIST, http://srdata.nist.gov/cc-chdbv/). Discussions on who is “right”: experimentalists or computationalists will be encouraged.

Software for computational chemistry. In order to bring computational chemistry as a teaching tool into classrooms, special computational software allowing students to perform simulations and visualization of
molecules in a quick, simple and well organized form is required. The quantum chemistry software thus plays a central role in efficient learning of students in computational chemistry and, consequently, is a key element of our proposal that we ask for funding.

Although many various quantum chemistry software packages are available on the market, for practical assignments, we chose Gaussian-09 for simulations and Gausview graphical program for visualization. This is an integrated software system which offers pre- and post-processing capabilities (including a molecular editor and visualization of results), and which is linked to a variety of application programs offering a broad spectrum of computational methods applicable to many topics from different areas of physics, chemistry, and material science. This product provides an interface to some of the more powerful quantum chemistry simulators widely used by researchers all over the world, as well as a teaching tool commonly used at many US universities. With its user-friendly layout, Gausview allows students to build their molecules using a molecular editor with pull-down menus. More importantly, Gausview serves as a "front-end" not only for Gaussian, but also to several types of research-grade quantum chemistry software packages, such as GAMESS, SPARTEN, and MOPAC. All in, the interface and its corresponding quantum codes created a "portal" for students to easily select molecules and conduct calculations to illustrate molecular changes.

The use of such an environment helps to ensure efficiency and progress in the class (i.e., less time spent editing files, etc.). Another bonus, at least at an early stage of the class, is that most of these interfaces do not require a detailed understanding of all the options that the different application programs provide. The input generator provides reasonable defaults and the student is able to perform simple calculations quickly. However, the understanding is that the students shall not depend on the any one vendor or interface, but instead they will be able to execute any application program available to them.

The user-oriented and user-friendly interface and extended range of different computational functions incorporated to Gaussian-09/Gausview will help students to use this software not only in class under supervision of their instructors, but by themselves during their free time, if they want to practice their skills in computational chemistry. We also expect that other instructors from Physics, Material Science, or Engineering departments will use this software for their courses. In addition, graduate and undergraduate students involved in research in chemistry, biochemistry, physics, material science, and computer science will be able to utilize this software to perform simulations of their systems of interest to explain and interpret the experimental results they obtained in wet labs or to get some predictions to guide new experimental probe. Thus, we expect that the software will be utilized by a very broad audience of NDSU students for extending their skills and knowledge during learning process, as well as during their scientific research.

The move from department controlled computer labs. We believe the practice of department owned and maintained computer labs is flawed for several reasons and advocate a move away from this arrangement.

In order to realize maximum return on the investment of computer hardware and software, the most important metric to optimize is utilization. A tour through one of the shared computer labs (e.g. IACC 150) will show that the assets are utilized significantly less that 100%. For department controlled computer labs this situation is far worse. Decommissioning a department lab in favor of driving higher utilization on the IT managed cluster resources is just good stewardship of our financial assets. Additionally, department controlled computer labs are typically poorly supported (certainly the Help Desk is not a few steps away), poorly maintained to insure security and application stability and often has very limited hours of availability.

Finally, a move towards leveraging the assets purchased, supported and maintain through the IT division puts more mass between the common computer environments they select. The move in the future may well be to client or server based virtualization for cluster resources. Moving to a model where departments are already running on the selected configurations of the IT division will simplify the movement towards virtualization in the future.
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IV. Milestones

List the date for each project milestone. These milestones should represent the *significant* accomplishments that will be associated with the action plan. For each milestone, please indicate its expected outcome and the means for assessing that outcome. (The table may be extended as needed.)

<table>
<thead>
<tr>
<th>Date</th>
<th>Milestone</th>
<th>Expected Outcomes</th>
<th>Means of Assessment</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. First month</td>
<td>Contact Gaussian company, purchase license</td>
<td>Obtain Gaussian-09 and Gausview software license for MACs</td>
<td>Completed license agreement</td>
</tr>
<tr>
<td>2. 1 month after license signing</td>
<td>Installation of Gaussian-09 and Gausview software at the shared computer labs (e.g. IACC 150)</td>
<td>Completed installation; successful run of trial simulations</td>
<td>We will solicit user feedback</td>
</tr>
<tr>
<td>3. 1 month after software installed</td>
<td>Development and testing of practical exercises for computational chemistry course (CHEM-476/676)</td>
<td>All practical exercises are performed in reasonable time and with expected outcome</td>
<td>We will solicit feedback from grad students who took this class before</td>
</tr>
<tr>
<td>4. 1 month after development of practical assignments for CHEM-476/676</td>
<td>Development and testing of computational assignment for freshmen chemistry labs (virtual lab)</td>
<td>All simulations and visualizations are performed fast and with expected outcome</td>
<td>We will solicit feedback from grad students who TA these courses</td>
</tr>
</tbody>
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5.
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V. Supporting Documentation
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## VI. Budget

Edit the dollar amounts in the "clear fields." (click in area so that it appears "gray," then edit) The "darkly shaded fields" can perform arithmetic. Simple use Ctrl A to "Select All" and then press function key 9, F9.

### NDSU ORGANIZATION OR UNIT

### PROJECT DIRECTOR(S)

(Must be NDSU faculty or staff)

<table>
<thead>
<tr>
<th>A. Salaries and Wages (Number)</th>
<th>Number of Months</th>
<th>FUNDS REQUESTED</th>
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</thead>
<tbody>
<tr>
<td>1. Staff ()</td>
<td></td>
<td>$ 0.00</td>
</tr>
<tr>
<td>2. Graduate Students ()</td>
<td></td>
<td>$ 0.00</td>
</tr>
<tr>
<td>3. Undergraduate Students ()</td>
<td></td>
<td>$ 0.00</td>
</tr>
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</table>

| B. Total Salary and Wages (Sum A.1., A.2., and A.3.) |                  | $ 0.00         |

| C. Fringe Benefits |                  | $ 0.00         |

| D. Total Salaries (Sum B and C) |                  | $ 0.00         |

| E. Equipment (List each item; include installation and maintenance costs in your estimates) |                  | $16000.00         |
| 1. Gaussian-09 for Power PC-based Macs (site license for G09M, single CPU version) |                  | $5000         |
| 2. GausView 5 for Mac OS X (site license, unlimited computers) |                  | $8000         |
| 3. training of IT personal for installing and testing new software |                  | $3000         |

| F. Total Equipment (Sum items in E.) |                  | $ 16000.00         |

| G. Materials and Supplies (List each item) |                  | $ 0.00         |
| 1. |                  |
| 2. |                  |
| 3. |                  |
| 4. |                  |
| 5. |                  |

| H. Total Materials and Supplies (Sum items in G) |                  | $ 0.00         |

| I. Total Salaries; Equipment; Materials and Supplies (Sum: Line D + Line F + Line H) |                  | $ 0.00         |

| J. Total Technology Fee Request |                  | $16000.00         |

| K. Match (Describe in Match Section) |                  | $ 0.00         |

| L. Total Project Expenditure (Sum: Line J + Line K) |                  | $16000.00         |
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VII. Budget Justification

Although many various quantum chemistry software packages are available on the market, for our computational chemistry course, we chose Gaussian-09 for simulations and Gausview graphical program for visualization based on the following reasons.

1. This product provides an interface to some of the more powerful quantum chemistry simulators widely used by researchers all over the world. Therefore, students who complete the course will gain a hands-on experience with very useful and commonly used computational software. Such experience will help NDSU students attracted to careers in science to enhance their success in their future professions.

2) This software is commonly used as a teaching tool at many top US universities (University of Washington, University of Florida, MIT, University of California, Santa Barbara, etc.), which proves its efficiency in learning processes.

3) Among all quantum chemistry software, Gaussian-09/Gausview software has the most user-oriented and user-friendly interface and extended range of different computational functions.

4) This is an integrated software system which offers pre- and post-processing capabilities (including a molecular editor and visualization of results), and which is linked to a variety of application programs offering a broad spectrum of computational methods applicable to many topics from different areas of physics, chemistry, and material science. The uniqueness of this software is that it was specifically designed for broad type of applications, rather than focused on some specific simulations. Gaussian can perform simulations beyond of those typically performed by other quantum chemistry software, such as GAMES, MOPAC, CHYPERCHEM, SPARTEN, etc. In particular, in addition to geometry optimization and normal mode calculations, Gaussian can simulate absorption spectra and, more importantly, emission spectra. The last one is a challenge for most available software. In addition, it provides calculations and visualization of excited state orbitals, that is beyond of typical performance of other software.
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VIII. Budget Match