

Final Report
Summer 2007
LITRE 2005-2007
Computational Chemistry Laboratories I & II
Department of Chemistry
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Summary

Both Computational Chemistry Laboratory I (CCI) and II (CCII) lab manual have now been published and both courses have been taught one time in the Fall of 2006 and Spring of 2007. Each of these courses is 1-credit hour and taught in a weekly 3-hour lab period.

The main content of CCI is an exploration of the forces that hold molecules together, and its purpose is to provide a physical framework of how energy relates to the geometrical arrangement of atoms in space and how this guides chemical reasoning. There are several software packages that accomplish these objectives, and they each use different computational methods. Students are able to use those packages to solve problems in an inquiry-guided format. The final portion of CCI applies the skills they have learned to generate potential energy surfaces for common organic chemistry reactions (where organic chemistry is a pre- or co-requisite).

The second course in this two-semester sequence focuses on quantum mechanical calculations. The course proceeds from calculations involving only a single atom, and the electronic properties thereof, to trends in those properties across the periodic table. The middle portion of the course moves from atomic to molecular orbitals in simple molecules. Finally, the course applies that information to the structure and bonding of inorganic, metal-containing molecules. As such, the examples in this course draw from inorganic chemistry much like the examples in CCI drew from organic chemistry.

The enrollment in the fall was 17 students, and the spring 15. Many CCI students continued with CCII. This course is a required course, but the degree audits still do not reflect any of the changes the chemistry department has adopted. It has been challenging to get this last step approved, even though both courses have been approved for more than a year. The department now requires all BS chemistry students to take CCI and CCII. In the Spring 2007 CCII class, 4 chemical engineering students were enrolled, and the course is quite amenable to many engineering majors and physics majors.

Since the objectives of the courses, their scope, and the technological aspects of delivering them have been summarized in earlier reports, this report will focus on recent accomplishments, outstanding problems, and most importantly, course assessment. The students in both courses filled out a WebAssign survey which was not anonymous, and a survey at the website of Student Assessment of Learning Gains (SALG), which focuses on students' perceptions of what gains they perceive they have made in various content areas, rather than an evaluation of the effectiveness of the instructor.

I. Accomplishments and Activities

Computational Chemistry Laboratory II (LITRE 2005-07)

The CCII laboratory manual was written and published as an electronic manual via WebAssign. The format of the lab manual is identical to the first lab manual. It has 10 lab chapters in html format, and the design of the layout was done by Mr. Tim Mowrer, who was the software programmer who developed CCI. Students who enrolled in CCII were able to purchase lab manual access and homework access in a bundled price, and thus WebAssign became the web portal for this course, as all assignments were also handled through this software.

II. Course Delivery and Outstanding Issues

The laptops which were purchased in the Summer of 2006 by the chemistry department were almost exclusively used for this course. They are housed in a cabinet and must be rolled into and out of the classroom for each class period. The laptops have 7-hour batteries, which were needed because the classroom is not wired. The delivery of the course also depended on the campus wireless network, and of course the WebAssign server. Not once did any of these components fail. All software and hardware was robust, and course delivery was smooth.

The possibility of moving toward a laptop requirement is also underway in our department. The department is currently providing the laptops and software, but it must pay 5 times what it would cost the student for the same software. Since the software can be used in later courses, it would be more cost-effective and pedagogically superior to move to the point where the students come to class with their own laptops with the software installed. In addition to being able to ask them different types of questions outside of class in pre- and post-labs, this option would also alleviate course scheduling hassles, as there is only one classroom where this can currently be taught.

The only outstanding work to be done is for the 2nd edition of both laboratory manuals. Other than basic editing, explanations of certain concepts need to be expanded upon, and a few “quick-start” guides and reference pages need to be developed. As the surveys show, the lab manual was moderately to quite helpful in learning course content.

From a curriculum point of view, the only outstanding issue is the inclusion of this course on the Registration and Records web pages for BS chemistry majors. Even though long ago submitted, these pages do not reflect changes which were made 1-2 years ago.

Finally, from the standpoint of human resources, there needs to be more training of TAs and faculty for this course. Several faculty are interested in it, but have not had the time to devote to working through the lab manual on their own. As for teaching assistants, few have any background in this subject as we are one of the few departments which offer

such a course, so the course requires some extra time in the way of training TAs on the software and even on the theoretical ideas behind many assignments.

III. Course Assessment

For each course, a brief summary will be provided, followed by a more detailed appendix which includes data from student responses.

A. CH230 Computational Chemistry I

CH230 is a 3-hour lab, with reading assignments, pre-lab and post-lab assignments. There was a short lecture given at the beginning of each lab. Students worked semi-independently or sometimes in groups where group reporting was expected.

Overall, the feedback from students is positive. They were quite satisfied with the way the course was structured, the text, and the grading system.

There seems to be some bit of computational-phobia or technology backlash for some students. No one indicated that they would take this course in a distance education format when asked, which was surprising since it is most suitable for such an option.

The biggest complaints were the heavy workload and the material being too out-of-context for the student, or that the course was just too hard. This probably is the first course where they are integrating over many concepts and having to do that using software that is new to them presents too much of a challenge for some.

Appendix for CCI

End of Course Survey
not anonymous
delivered via WebAssign

1. This course was ...
 - far more advanced (19%)
 - more advanced (50%)
 - about the same (25%)
 - less advanced (6%)...than other Sophomore level chemistry courses.

2. The average total time spent each week in CH230: 5 hours (3 were in class)

3. The amount of time necessary to earn a passing grade in this course was...

Very reasonable	7%
Reasonable	40%
No Opinion	13%
Unreasonable	40%
Very unreasonable	0

4. The course had 10 labs (lowest 1 was dropped) and one cumulative final exam. When asked if more exams are needed...

Stick to 1 final exam	44%
Use midterm + final	44%
No Opinion	12%

5. If there were a laptop requirement so that each student had their own computer and software, how would you prefer this class be taught?

Prefer to be in a classroom with other students and instructor	81%
Prefer distance ed option	0%
Don't Care either way	19%

CH230-001 Fall 2006 Grade Distribution

A 41%

B 59%

no other grades were assigned

End of Course Survey

anonymous

delivered via Student Assessment of Learning Gains (SALG)

The responses to this survey question is based on a 1-5 scale where

1 = no help

2 = little help

3 = moderate help

4 = much help

5 = very much help

1. Resources that helped your learning

a. The text 3.33

- b. Other reading material (generally articles) 2.38
- c. Use of software packages 3.53
- d. Use of WWW 2.73

The responses to this survey question is based on a 1-5 scale where

- 1 = not at all
- 2 = a little
- 3 = somewhat
- 4 = a lot
- 5 = a great deal

2. As a result of your work in this class, how well do you think that you now understand each of the following? [The following is a list of course objectives.]

The distinction between various forces that hold matter together.	3.07
How to graph potential functions.	3.07
How to build molecules and compute their properties such as energy.	3.87
The distinction between computational methods and their applications and limitations.	2.93
How to generate a potential energy surface.	2.73
How to search databases for chemical information.	3.2
How to verify results from computational studies with experimental data.	2.67

3. Using the same scale, how much has this class added to your skills in each of the following?

General problem-solving skills.	2.87
How to explore a chemical system via a computational method.	3.47
Finding trends in data	2.93
Critically reviewing articles	2.21

B. CH232 Computational Chemistry II

Like CH230, this lab is taught in a 3-hour lab/week format. There is a short introductory lecture followed by a lab portion where students used software to solve chemistry problems or to explore trends in bonding. They also had graded pre- and post-lab assignments.

The format worked very well and most students were satisfied with the grading structure of the course. Unlike the students in CH230 (and many to most were the same students), this time 23% would prefer a distance education option. However, by that one student just meant (as indicated in a free response question later) that students would have access to the software outside the lab setting.

In the free response section, many students commented on the fact that software was not available to them outside of class, and they felt pressured to complete the labs in the given time slot. A few students mentioned that they would gladly purchase software if that were an option.

Most students felt that very few changes, other than the planned editing and a few quick-start guides, are needed for the electronic manual.

Appendix for CCII

End of Course Survey
not anonymous
delivered via WebAssign

1. This course was more advanced (31%) or far more advanced (62%) than other Sophomore level chemistry courses. The rest thought it was the same difficulty level.
2. The only piece of software used was Spartan. When asked about the learning curve of this software,
8% no
31% small
23% moderate
38% significant

It could be that those who had not taken CH230 felt the learning curve was more significant.

3. The average total time spent each week in CH232: 4.5hours (3 were in class)

4. The amount of time necessary to earn a passing grade in this course was...

Very reasonable	23%
Reasonable	39%
No Opinion	15%
Unreasonable	23%
Very unreasonable	0

5. The course had 10 labs (lowest 1 was dropped) and one cumulative final exam. When asked if more exams are needed...

Stick to 1 final exam	69%
Use midterm + final	23%
No Opinion	8%

4. If there were a laptop requirement so that each student had their own computer and software, how would you prefer this class be taught?

Prefer to be in a classroom with other students and instructor	69%
Prefer distance ed option	23%
Don't Care either way	8%

CH232-001 Spring 2007 Grade Distribution

A 62%

B 31%

C 7%

End of Course Survey

anonymous

delivered via Student Assessment of Learning Gains (SALG)

The responses to this survey question is based on a 1-5 scale where

1 = no help

2 = little help

3 = moderate help

4 = much help

5 = very much help

1. Resources that helped your learning

a. The text 3.07

b. Other reading material (generally articles) 2.77

c. Use of software packages 3.13

d. Use of WWW 3.27

The responses to this survey question is based on a 1-5 scale where

1 = not at all

2 = a little

3 = somewhat

4 = a lot

5 = a great deal

2. As a result of your work in this class, how well do you think that you now understand each of the following? [The following is a list of course objectives.]

The process to compute electronic properties of atoms/molecules.	3.13
How to graph wavefunctions and determine nodal structures	2.67
How to apply molecular orbital theory to small molecules.	2.87
How to compute ionization energies, electron affinities, dipole moments.	3.47
How to graph IR spectra.	3.33
How to apply MO theory to metal-ligand complexes.	2.93
How to verify results from computational studies with experimental data.	2.93

3. Using the same scale, how much has this class added to your skills in each of the following?

General problem-solving skills.	2.67
How to explore a chemical system via a computational method.	3.0
Finding trends in data	2.8
Critically reviewing articles	2.4
Working effectively with others	4.13