Modular Computational Chemistry and Biochemistry Curriculum

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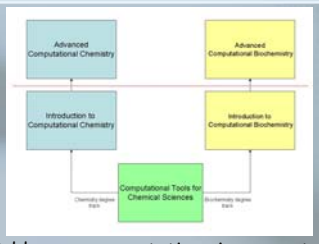
Overview

- Background and motivation
- Student learning outcomes
- Structure of courses and activities
- Assessments

Background and motivation

- Computer is essential tool to modern chemist/biochemist
- Introduction to Chemical Computation (1993)
  - National model; cited in the peer-reviewed literature
- AY 2002-3 re-examined content and delivery
  - Student opinion questionnaires; Dept. exit surveys; instructor frustrations
- Computer technology and software have advanced
- Advanced applications have become more specialized requiring separate coverage for chemistry and biochemistry majors

Background and motivation



- Addresses expectations in *computer fluency* for undergraduates as defined by
  - ACS Committee on Professional Training
  - National Research Council Guidelines for Undergraduate Education in Life Sciences

Student learning outcomes

- Chemistry 210: Computational Tools for the Chemical Sciences
  - Able to perform simple chemical computation and visualization of properties of molecular and macromolecular systems
  - Sufficiently familiar with elements of programming to carry out calculations and simulations
  - Adept at using computers to acquire and process data, carry out statistical characterization of data and perform statistical tests
  - Adept at using computers to graphically display data in a variety of representations
  - Skilled at using the Internet to carry out literature searches, access and mine major databases

Student learning outcomes

- Chemistry 410A: Introduction to Computational Biochemistry
  - Demonstrate ability to use computer algorithms, publicly available databases and server-based tools to search for and retrieve genomic information
  - Demonstrate ability to interrogate and critically analyze genomic data
  - Perform in silico mutagenesis and design of molecular biology experiments
  - Apply insights gained to intelligent design and formulation of hypotheses in own research

Student learning outcomes

- Chemistry 410B: Advanced Computational Biochemistry
  - Demonstrate ability to use computer algorithms, publicly available databases and server-based tools to search for and retrieve biomolecular information
  - Critically model, analyze and validate biomolecular data
  - Demonstrate ability to interrogate biological (protein/nucleic acid/complexes) structures
  - Perform in silico mutagenesis and screening of ligands
  - Apply insights gained to intelligent design and formulation of hypotheses in own research

Student learning outcomes

- Chemistry 410C: Introduction to Computational Chemistry
  - Perform basic computation and visualization of molecular geometry and properties
  - Run geometry optimization using semi-empirical molecular orbital theory and density functional theory methods for specific molecules
  - Calculate molecular energies, dipoles, and infrared frequencies
  - Determine thermodynamic properties such as enthalpies, entropies, and free energies of molecular systems
  - Properly interpret calculated results and make reasonable assessment of the accuracy and reliability in calculated properties
  - Solve practical problems in laboratory research using molecular modeling or calculation

Student learning outcomes

- Chemistry 410D: Advanced Computational Chemistry
  - Understand the basic theoretical concepts for advanced computational methods and techniques
  - Search for the transition state and determine the activation energy for a given reaction
  - Calculate the potential energy surface of a molecular system
  - Calculate the rate constants of a reaction at different temperatures
  - Properly interpret calculated results and make reasonable assessment of the accuracy and reliability in calculated properties
  - Solve practical problems in laboratory research using computational methods

Structure of courses and activities

- Chemistry 210
- Chemistry 410A
  - Final project topics (presented in technical report format)
    - Studies on the mutated pfcrt gene in Plasmodium falciparum: implications for drug development
    - Genetic and molecular characterization of human rhinovirus variants
- Chemistry 410B
  - Final project topics (presented in technical report format)
    - In silico analysis of human and E. coli thymidylate synthases: promising drug targets in the de novo dTMP biosynthesis pathway
- Chemistry 410C
  - Final project topics (presented in technical report format)
    - Stability of selected alkyl radicals in the atmosphere
    - Stability of fluoromethanes
- Chemistry 410D
  - Final project topics (presented in technical report format)
    - Characterization of intermediates in cholesterol biosynthesis using computational methods

Assessments

- Indirect formative and summative assessments
  - Pre- and post-course online surveys (www.zoomerang.com)
- Direct formative and summative assessments
  - Skills demonstrated in weekly assignments
  - In Chem 210, final exam demonstrates integrated skills
  - In 410ABCD, final projects demonstrate integration and extension of skills

Summary

- A modular restructuring of our computational curriculum that effectively addresses computer fluency and better meets training needs of majors
  - Formative and summative assessments
- Flexibility of modules
  - Upper division electives
  - Staffing
  - Graduate study plan
- Curriculum development
  - Repository of materials

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