

Intro to Computing in Chemistry

Kristi Closser

10-11-20

Teaching Computation Online with MATLAB

FRESNO STATE[®]

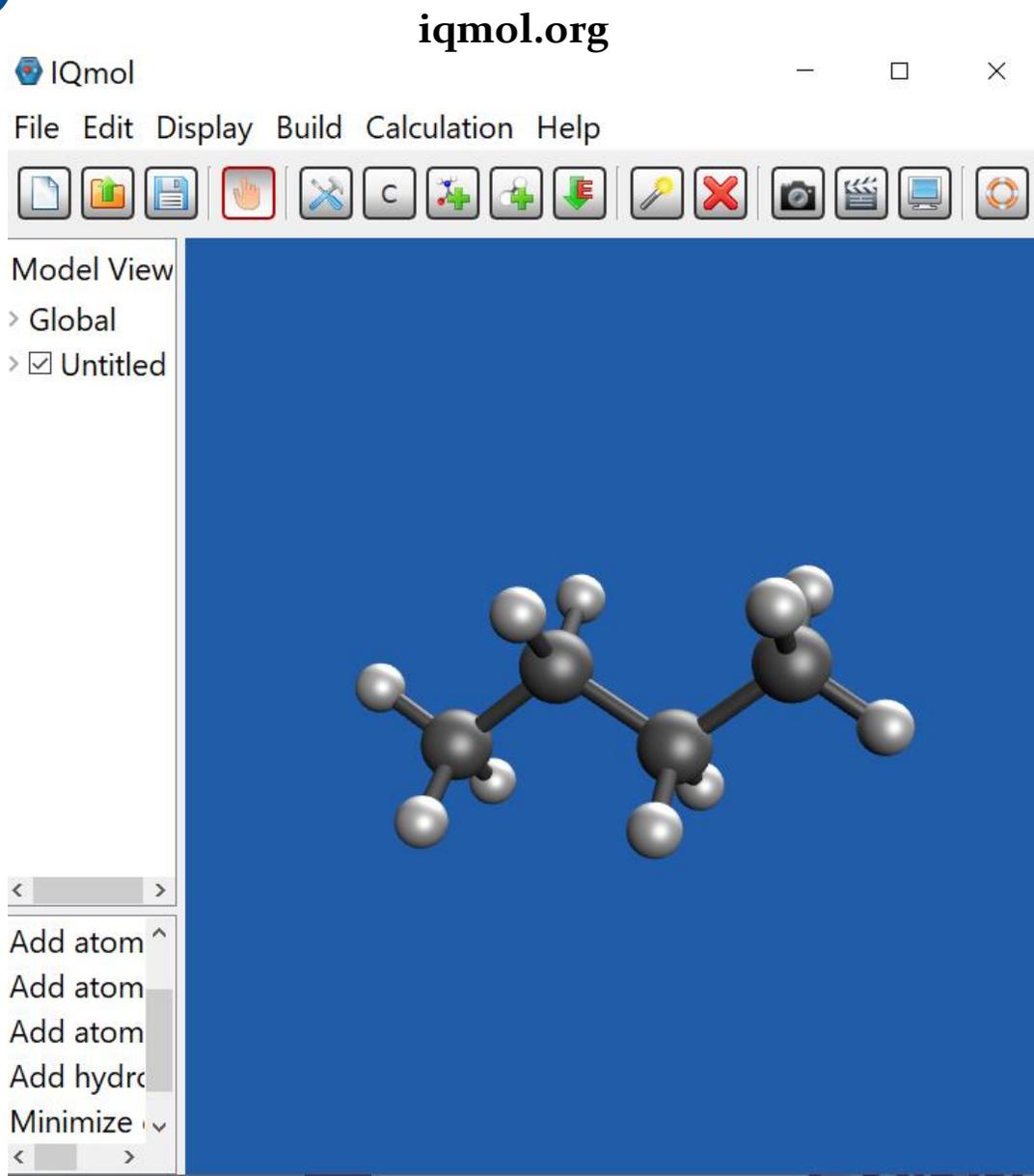
Chemistry and Biochemistry

Computation in Chemistry

Student understanding of computation is often undervalued in the discipline

“The ability to compute chemical properties and phenomena complements experimental work by enhancing understanding and providing predictive power. Students should have access to computing facilities and use computational chemistry software.”

American Chemical Society Committee on Professional Training, “ACS Guidelines and Evaluation Procedures for Bachelor’s Degree Programs” (2015)



Computation in Chemistry

Slowly gaining more acceptance in field

Introduce as part of other courses, where content is the focus

Fall 2019

Introduction to physical chemistry (upper division major class)

Spring 2020

Intro to computing in chemistry course (upper division elective)

Physical Chemistry—Content based course

Students use mostly pre-generated code to analyze data and model concepts

- ❑ Never require more than small code manipulations in live scripts (e.g. putting in a key equation, generating a plot)
- ❑ Focus on concepts, code is just there to support content
- ❑ Build in issues where students are forced to think about what is happening with data (e.g. divide by 0 due to missing data)

Computational Chemistry Specific Course

0 to programming in ~4 weeks

- ❑ Matrices and vectors
- ❑ Functions, loops and conditional statements
- ❑ Statistics and data processing (including plots)
- ❑ Using scripts

Week	Tu/Th dates	Topics
1	1/21	Intro, Complex Numbers, Matrices and Vectors
	1/23	Matrix Operations
2	1/28	Basic Math and matrix manipulation in MATLAB (McL 240)
	1/30	Mathematical Series, Intro to Computing
3	2/4	Functions, Loops and Conditional statements in MATLAB (McL 240)
	2/6	Descriptive Statistics and Data Processing
4	2/11	Graphing and data importing in MATLAB (McL 240)
	2/13	Good scripting and programming practices
5	2/18	Scripting in MATLAB (McL 240)
	2/20	Exam 1

Students and Programming

Students generally have minimal experience with any sort of computer based data analysis or coding

Sneak in programming as part of other courses. Focus on ways to make life easier (in the long run...often students find it very complex in the short term)!

In computing course, have students create code for very basic chemistry concepts

Heavy use of MATLAB online and Live Scripts for introduction of computational concepts

Decreasing Student Anxiety

- Low stakes assignments (course based on mastery grading, assignments, satisfactory/unsatisfactory assignments)
- In person computer lab (when possible...immediate assistance available to minimize frustration with syntax, etc.)
- MATLAB online: All students have same version, even off campus