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ConfChem Conference on Mathematics in Undergraduate Chemistry Instruction: Applied Mathematics for Chemistry Majors

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Supporting Information

ABSTRACT: To succeed in physical chemistry courses, students need competence with a significant amount of mathematics, including ordinary and partial differential equations and linear operators. This can present a barrier to student success because many of these topics are not taught in the traditional prerequisite calculus sequence. Through a collaboration of the Departments of Chemistry and Mathematics, Colorado State University has developed and implemented a two-semester sequence of courses, Applied Mathematics for Chemists, aimed specifically at providing students with the mathematical tools necessary for success in physical chemistry. This report summarizes one of the invited papers to the ConfChem online conference on Mathematics in Undergraduate Chemistry Instruction, held from October 23 to November 27, 2017, and hosted by the ACS DivCHED Committee on Computers in Chemical Education (CCCE).

KEYWORDS: *Physical Chemistry, Mathematics/Symbolic Mathematics, Curriculum, Upper-Division Undergraduate*

MOTIVATION

Instructors of physical chemistry, at Colorado State University and elsewhere, suggest that a significant barrier to student success in physical chemistry arises from discomfort and low proficiency with requisite math and the ability to connect mathematical concepts to the physical systems they describe.[1] Understanding physical chemistry requires student dexterity with topics such as differential equations and linear operators that are not covered in traditional prerequisite math sequences at most universities.

In response to missing mathematical skills and to improve student success in the two-semester upper-division undergraduate physical chemistry course, faculty members from the Departments of Chemistry and Mathematics collaborated to create Applied Mathematics for Chemists (MfC), a sequence of two 4-credit, semester-long math courses designed to address math literacy for chemists. Taught as an experimental course for two academic years, MfC was accepted into the curriculum of the Mathematics Department (course numbers MATH 271 and MATH 272), fulfilling the mathematics requirement for chemistry majors, and as a prerequisite for physical chemistry.

Conference discussion of the paper focused on the logistics and success of implementation rather than the need for such a course. A vital component to our success was the collaboration between Departments of Chemistry and Mathematics, as well as strong support from department chairs. Finding math instructors willing to learn some chemistry and teach the nonstandard material of MfC was also important. To continue offering MfC in the long term, there needs to be sufficient enrollment to warrant the resources necessary to offer the curriculum. Given the positive feedback from chemistry students who have taken the MfC course and urged their peers to do so also, we expect to attain sufficient enrollment. Students from other majors may also benefit from this applied math curriculum. Faculty from the Departments of Physics, Computer Science, and Chemical Engineering have expressed interest in allowing their majors to take the MfC sequence.

COURSE CONTENT

MfC aims to provide students with a working proficiency of the mathematics they will use in physical chemistry so that they can focus on learning and understanding the chemistry rather than struggle with math. The two texts used, Erich Steiner's *The Chemistry Maths Book*[2] and Donald McQuarrie's *Mathematics for Physical Chemistry*,[3] take a straightforward approach to mathematical topics relevant to chemists. The prerequisite for this course sequence, Calculus for Physical Scientists I, covers the basics of derivatives, integrals, and their essential relation given in the fundamental theorem of calculus. MfC begins with a fresh look at the fundamental theorem of calculus, developing foundational understanding of physical phenomena in terms of an initial condition and a rate of change. This sets up a new way of scientific thinking that leads naturally to the first topic of MfC, ordinary differential equations. Starting with this paradigm allows questions from chemistry to motivate the mathematics. Various types of differential equations and solution techniques are motivated by applications to chemical kinetics, the harmonic oscillator, and a first look at Schrödinger's equation for a particle in a box. The need to solve certain second-order differential equations motivates complex numbers. Taylor series are motivated as a

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tool to solve second-order differential equations with non-constant coefficients. The next section covers linear algebra, emphasizing the insights given by eigenvalues and eigenvectors of models of physical systems. Symmetry and group axioms are taught through linear transformations of planar molecules.

The second semester of the MfC sequence begins with vector spaces and linear operators, which provides students a concrete foundational understanding into topics that they often find very abstract, including infinite-dimensional inner product spaces and orthogonal polynomials. This set of topics is followed by multivariate calculus. Armed with partial derivatives, students are introduced to partial differential equations. Solving the wave equation using separation of variables, students review much of the material from the start of the first semester. The second semester ends with a group project, which guides students through the analytical solution to the Schrödinger equation for the hydrogen atom.

IMPACT

Instructors of physical chemistry have remarked on significant differences in students who have taken MfC compared to students who completed the traditional calculus sequence to fulfill mathematical requirements. Students who have taken MfC were much more engaged in the physical chemistry course. They also showed much more confidence in the mathematical manipulations used in physical chemistry classes, for example in the context of Maxwell relations in thermodynamics. Students could therefore focus on deepening their understanding of the chemistry. Student feedback, in particular from students who have taken MfC and then physical chemistry, has been positive as well.

CONCLUSION

This report summarizes one of the invited papers to the ConfChem online conference on Mathematics in Undergraduate Chemistry Instruction,[4] held October 23 to November 27, 2017, and hosted by the ACS DivCHED Committee on Computers in Chemical Education (CCCE). This paper was discussed November 15–23, 2017;[5] the paper itself and the related discussions are available in the Supporting Information.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.8b00107.

Full text of the original paper with associated discussions from the ConfChem Conference (PDF)

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Notes

The authors declare no competing financial interest.

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