Transforming Math Education for Chemists with "MoCChA"

dB-SERC Course Transformation (Pre-Transformation Discussion)

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dB-SERC Lunch Discussion

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Mathematics **o**n **C**omputers for **Ch**emistry **A**pplications (MoCChA)

Overview

- “Mathematics for Chemists” (CHEM 1000) - objectives and need for transformation
- Goals for the proposed course transformation
- Implementation plan
- Example activities
- Assessment plan
- Discussion - your suggestions for topics, examples, activities, assessment, resources …

Chemistry majors

Physical Chemistry 1
(quantum mechanics)

Physical Chemistry 2
(thermodynamics - classical & statistical)

Mathematical Methods

→

graduate school/electives

Quantum Chemistry
Computational Chemistry
Statistical Mechanics
Biophysical Chemistry
Analytical Chemistry
Spectroscopy

"**Hard as hell** class."

"one of the **most difficult** chemistry classes at a lot of schools"

"Every other pre-med I know (and doctors with whom the subject has arisen) expressed an **explicit hatred** for pchem."

"P chem was a **life ruiner** for a couple people I knew, no joke."

"I think the problem most people have with pchem isn't the material itself, but the fact that the material **involves math**. People hate math."

1 in 3 Chemistry majors need more proficiency in mathematical methods to be 'conversant' in physical chemistry.

https://forums.studentdoctor.net/threads/physical-chemistry.863749/

Number of Mathematical Concepts Distracts from Teaching Physical Chemistry

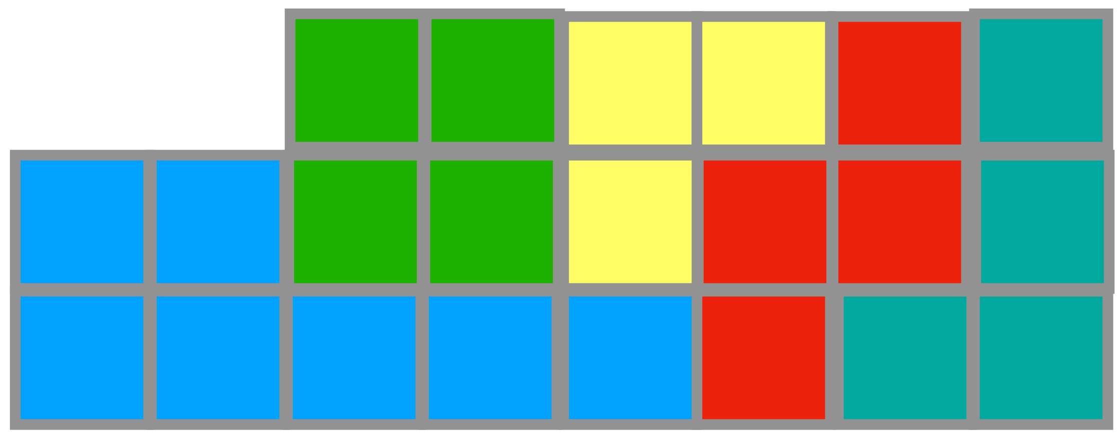
- Complex numbers (basic arithmetics, roots, equation solving)
- Linear algebra (vectors, matrices, equation solving, determinants, eigenvalue equations, symmetry)
- Multi-variable calculus (partial derivatives, differentials, line integrals, multiple integrals)
- Series expansions & basis sets (Taylor, Fourier, …)
- Differential equations (initial values, boundary conditions, eigenvalues, quantization, separation of variables)
- Probability & stochastics

Mathematics for Chemistry (CHEM 1000)

Calculus 1

Calculus 2

Calculus 3



Physical Chemistry 1
(quantum mechanics)

Physical Chemistry 2
(thermodynamics - classical & statistical)

Introduces math concepts in the context of specific Chemistry examples.

Remaining challenges:

- Amount of material (could always use more examples & hands-on exercises)
- “Paper-and-pencil” heavy
- Scheduling

Goals of the Proposed “MoCChA” Transformation

- Empower chemistry majors with general problem solving skills to tackle problems in physical chemistry.
  - break down realistic chemistry problems into manageable sub-problems,
  - select appropriate mathematical models,
  - solve these models by the help of computer-based algebra systems,
  - evaluate the validity and limits of these models, and
  - interpret the results and their applications in chemistry.

Approach

- Create POGIL activity worksheets centered around a Chemistry problem plus a math concept required for its solution
- Interactive math solving & visualization via mobile computing (jupyter, Wolfram Cloud)
- Activities will be grouped into thematic modules
- Modularity will allow flexible uses as a supplement to existing math courses and as math refresher modules

Approach

- POGIL-style worksheets that pose a chemical problem or question
    - “What is the concentration of ozone in the atmosphere?”
- guide the students through the process of breaking the problem down into sub-problems and mathematical models
    - “What are the processes that lead to formation and depletion of ozone?”, “Which differential equations describe the breakdown/formation of ozone?”
- solve the math model using computer-based algebra or numerical simulation (http://jupyter.org, a web-based platform for Python worksheets featuring symbolic and numerical math solvers)
- worksheets link to jupyter using scannable barcodes to enable students to solve math and visualize solutions in real time from their cell phones, tablets, and laptops

Approach

- We will create several types of MoCChA activities:
  - In-class POGIL team worksheet
  - POGIL team-homework project
  - Math resource sheet for individual practice
- Aim: 1 of each activity per topic
- Low-stakes speaking assignments

Approach

- Transformation award will focus on MoCChA activities within Mathematics for Chemistry (CHEM 1000) and assessment within Physical Chemistry 1&2 (CHEM 1410 & 1420).

- Possibility of creating a “mini-course” centered around MoCChA that will allow students to supplement any general math course with chemistry-specific applications.

- MoCChA would allow students, e.g., to attend the general math class (Calculus 3) and to supplement with a MoCChA mini-course for chemistry-specific applications.

Expected Benefits

- More tailored math education for Chemistry majors will likely help students
  - succeed in their upper division coursework,
  - maintain competitive grades (as required, e.g., for graduate and medical school applications),
  - graduate more timely,
  - and learn techniques helpful for research and the workplace
- aligns with University goals of enabling students to think critically, work in teams, and communicate effectively & with Chemistry Department's "Computing across the Curriculum" initiative

Expected Benefits

- We expect that these new avenues will help engage and excite students at a broader and deeper level than possible within a traditional lecture, leading to improved learning outcomes and student attitudes.

- POGIL activities have been shown to improve learning outcomes for chemistry students (e.g., up to a 15.1 point improvement on a percentile scale in organic chemistry assessments).

  Hein, S. M. Positive Impacts Using POGIL in Organic Chemistry. *J. Chem. Educ.* 2012, **89** (7), 860–864.

Expected Benefits

- emphasizing “big picture” outcomes and chemical applications over tedious paper-and-pencil solutions
- training critical thinking skills within the context of chemistry, such as analyzing the applicability of a given model or switching between different models to solve a problem
- offering teaching and learning mechanisms other than “paper and pencil”, such as team exercises, team discussions, and oral communication

Expected Outcomes

- students will be able to switch and translate between different models in physical chemistry, such as different mathematical models or intuitive chemical pictures
- students will be able to apply computer-aided mathematical modeling and numerical simulations to solve canonical Chemistry problems
- team work & communication skills

Outline of a POGIL activity

- Worksheets with team exercises (2-3 students, each student will be assigned a specific role)
- Sample structure:
    1. Introduction and motivation based on a chemistry concept or application known to students from introductory courses such as General or Organic Chemistry.
    2. Critical thinking phase – students form hypotheses, e.g. around "which math models apply to the given situation?" or "which properties of a particular math model apply to the given chemistry problem?"
    3. Exploration phase – students run numerical simulations or symbolic solutions on their cell phones, tablets or laptops to explore the properties of the math model and its implications for the chemistry problem.
    4. Students report their findings to the class and the class discusses strengths and weaknesses of different solution strategies.
    5. Students confirm or revise their initial hypotheses based on class discussion.
    6. Students practice the newly discovered principle or technique by applying to additional problems and examples either in class or at home.
- Each topic module will come with a cover sheet for the instructor to define goals, prerequisites, expected outcomes, and expected problems together with suggestions

Module "Matrix Eigenvalue Equations"

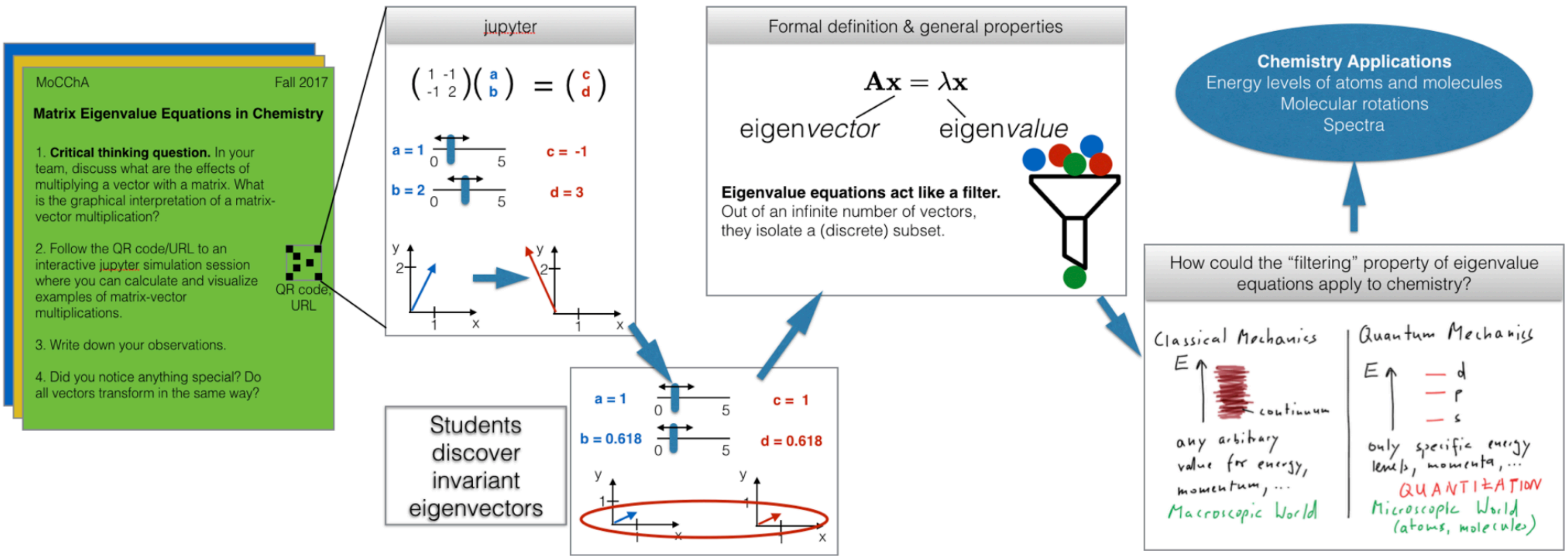
Goals: Students will discover that for a given matrix **A** there are special vectors **x** that stay invariant under application of that matrix. This insight will be used to formulate the concept of eigenvectors and –values. Students will discover that eigenvalue equations act as "filters" that identify specific vectors out of an infinite number of vectors in a given space. Students will identify applications in chemistry, such as orbital energy levels and spectroscopy.

Prerequisites: Coordinate representation of vectors and matrices; familiarity with matrix-vector multiplications.

Common pitfalls: (1) Students find the "trivial solution" with l=0. *Suggestion:* Challenge the students to explain what is the physical meaning of **x** = <0,0,...,0> by drawing a diagram of the solution vector: Void space (vacuum) is a mathematically correct solution, but chemists only care about particles. (2) ...

Expected outcomes: After completing this module, students will be able to name applications of eigenvalue equations in quantum mechanics and solve simple eigenvalue equations using SymPy within the jupyter environment.

Example:
Matrix Eigenvalue Equations



Assessment

- We will administer pre- and post-assessments immediately before and after MoCChA modules.

- We will compare these results to historical results from the CHEM 1000 “Mathematics for Chemistry” course.

- Performance assessment for untransformed course: historical data for homework sets, exams, and group projects from the 4 semesters that I have taught the course previously.

- Compare performance outcomes for the POGIL worksheets for students who attend the transformed CHEM 1000 course (Fall 2017 & Spring 2018) and students who did not attend the transformed course but worked through the POGIL worksheets (CHEM 1410 & 1420, Fall 2017).

Assessment

- Will work with instructors in upper-division physical chemistry courses to assess the impact of the chemistry-specific math modules as compared to the more traditional "general" math classes.

- Will use Peoplesoft ID to match student performance outcomes and survey responses (as well as future course performance such as grades)

- How does the proposed transformation affect students' mastery of the content compared to the untransformed course? These tests will assess students' ability to reproduce, apply, analyze, and the material covered in the module.

- How does the course transformation affects students' general problem solving/ metacognitive skills?

  Cooper, M. M.; Sandi-Urena, S. Design and Validation of an Instrument To Assess Metacognitive Skillfulness in Chemistry Problem Solving. *J. Chem. Educ.* 2009, **86** (2), 240.

Assessment of In-Class Activities

1. level of participation (e.g., “did all students make useful contributions?”)

2. progress made in the discussion (e.g., “are the students making progress toward the desired result?”)

3. tone of the discussion (e.g., “did the group members help each other in approaching a solution?”)

4. relating the discussion/project to course content (e.g., “do the students apply/build on the concepts introduced in the MoCChA handouts?”)

5. Is the discussion focused?

If particular teams should not make progress as expected, then I will intervene e.g. by leading the discussion (e.g., by asking questions to ensure the discussion goes in a productive/deeper direction or by asking different groups to exchange their ideas) and by facilitating discussion (e.g., encouraging contributions from everyone).

Moreover, observing similar problems across multiple teams may indicate a systematic problem in the activity, course materials, or facilitation. I will record these observations and discuss them with the students to find a resolution (e.g., identify whether a component of the activity needs to be modified).

Assessment of In-Class Activities

- five minutes within every MoCChA activity reserved for studens self-evaluation and feedback about the activity and the facilitation.

- students create a table listing something they did well in the discussion (marked with "+") and an improvement they think they should make (marked with "Δ"). The group's "scribe" will record these suggestions and will review them at the start of the next activity to reinforce improvements. Teams will discuss what they found was strong about the activity and the facilitation and will suggest possible improvements; I will record these suggestions and use them to improve future activities and facilitation, if necessary.

"Guidebook for Student-Centered Classroom Discussions" by Jack Byrd, Jr., Publisher: Interactivity Foundation, Parkersburg, WV, 2008.

Assessment

- How does the course transformation impact students' attitude toward chemistry?

  Bauer, C. F. Attitude toward Chemistry: A Semantic Differential Instrument for Assessing Curriculum Impacts. *J. Chem. Educ.* 2008, **85** (10), 1440.

  Xu, X.; Lewis, J. E. Refinement of a Chemistry Attitude Measure for College Students. *J. Chem. Educ.* 2011, **88** (5), 561–568.

- How does the course transformation affect self-efficacy?

  http://userpage.fu-berlin.de/~health/engscal.htm

- Furthermore, we will use interactions with the students during team exercises, discussion and oral presentation as a chance to collect oral feedback.

“Dream” Outcomes

- CHEM 1000: Average scores in learning assessments of math skills improve by 10 percentile points. FDW rates decrease from 10% to 5%.
- P-Chem: More time to focus on Physical Chemistry, elimination of “double challenge” of learning math concepts and p-chem.
- Student attitudes toward math and p-chem improves.
- All Chemistry majors can have some MoCChA!