Transforming Math Education for Chemists with “MoCChA”

dB-SERC Course Transformation (Mid-Transformation)

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dB-SERC Lunch Discussion
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Mathematics on Computers for Chemistry Applications (MoCChA)

Mathematics for Chemistry (CHEM 1000)

Calculus 1
Calculus 2
Calculus 3

Physical Chemistry 1
(quantum mechanics)

Physical Chemistry 2
(thermodynamics - classical & statistical)
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.
Overview

• Practical Considerations & Implementing MoCChA
• Sample MoCChA Activity
• Challenges
• Attitudinal & Formative Assessment
• Summative Assessment
• Reflections
Implementing MoCChA: Jupyter Notebooks
Jupyterhub -> Jupyter -> Python -> Sympy, Numpy, ...

http://hub-dev.crc.pitt.edu

Dr. Barry Moore, CRC
Sharing/Developing Notebooks:
https://github.com/kaw112/jupyterNotebooks

Currently a private repository, email lambrecht@pitt.edu to request access.
Welcome to MoCChA - Mathematics on Computers for Chemistry Applications!

This notebook calculates the change $\Delta F$, given a differential $df = fx \times dx + fy \times dy$.
We approximate $\Delta F$ by taking finite steps in $x$ and $y$ and summing up the changes $df$.

This cell defines the differential $df$ and the curve along which we're calculating the change.
Feel free to experiment. You can change any line marked with "<---" below to change one of the parameters.

For example, you can choose a different differential to calculate or a different path along which to sum up $df$.
Or, you can change the numerical accuracy by varying the step size that determines the finite steps with which we approximate $dx$ and $dy$.

Hit Shift-Enter to execute each cell.

You can ignore the following four lines. They are necessary to load some libraries and set up the calculation.

```python
import sympy
```
What is the geometric interpretation the derivative of a parametric equation? The definition is similar to the derivative for a one variable function.
Top Hat Response System
Top Hat Clicker/Online Grading System

- Largest enrollment yet (41 students). Requires change in approach to handle in-class assessment & grading

- Using Top Hat for clicker questions and homework assignments

- Converted ~75% of homework into Top Hat questions (multiple choice, numerical & text answers, image selection)

- Used Top Hat to collect student answers in class; still asking one or more students to share their solutions

- Benefits: instantaneous student feedback & quantitative assessment, ability to offer & handle large number of homework & in-class problems
Top Hat Enables Timely Intervention
The concentration of H+ ions for a weak acid dissolved in water is given by the equation below.

Given the following definitions and constants, which term could be safely neglected to facilitate analytical solving of the equation? Click on the most suitable term in the image below. You can change your answer and resubmit.

\[ x = \frac{[H^+]}{c_0} \text{ is the H}^+ \text{ concentration. } c_0 = 1 \text{ mol is a constant to make } x \text{ unitless.} \]

\[ K_a = 1.40 \cdot 10^{-3} \text{ is the dissociation constant of the acid.} \]

\[ K_w = 10^{-14} \text{ is the autodissociation constant for water.} \]

\[ c = 0.010 \text{ mol is the initial concentration of the undissociated acid.} \]

Heat map of student responses:

\[ x^3 + K_a x^2 - \left( \frac{c K_a}{c_0} + K_w \right) x - K_a K_w = 0. \]
intervention
Sample MoCChA Activities
MoCChA Tutorial

- step-by-step instructions on how to use MoCChA notebooks
- in-class demonstration

MoCChA FAQ

1. **What is MoCChA and what’s its purpose?**
   “MoCChA” stands for “Mathematics on Computers for Chemistry Applications.” It’s a collection of web-based notebooks created by Daniel Lambrecht and Keith Werling from the University of Pittsburgh to allow users to solve and visualize math problems encountered in chemistry.

2. **How do I access the MoCChA notebooks?**
   MoCChA runs through a webserver hosted by Pitt’s Center for Research Computing. Follow the steps below to connect.
   
   *Note: Right now it is easiest to connect from within the campus network. See below if you need to connect from off-campus.*

   1. Go to [https://hub-dev.crc.pitt.edu/hub/home](https://hub-dev.crc.pitt.edu/hub/home)
   2. You should be directed to Pitt’s single-sign-on page to enter your credentials.
Your server is starting up.
You will be redirected automatically when it's ready for you.

5. You will see a directory listing once the server is ready. Select “Chem1000” to see a list of available MoCChA notebooks.

6. You can now open the MoCChA notebook by clicking on the file name (notebook files end in “.ipynb” (“interactive Python notebook”)).
Differentials and Changes along Different Paths

1. Let us recap some of the properties of differentials. Fill in the missing pieces below:

The general form for a differential in two variables is: \( df = f_x \, dx + f_y \, dy \)

- \( df \) describes the change of quantity \( f \) as we take an infinitesimal step (___) along the x-direction plus an infinitesimal step (___) along the y-direction.

- \( f_x \) and \( f_y \) are the _________________ of \( f \) along the x- and y-direction.

- The differential \( df \) is called exact, if:

- If \( df \) is exact, then the change \( \Delta f \) obtained by summing up \( df \) ______________ depend on the path.
Hypothesis-Driven Virtual Experiments

Now we’re going to investigate several differentials for (in)exactness and we’ll calculate changes along different pathways. We’ll use the MoCChA online tool to calculate sums over differentials.

Differential #2:

\[ df = y \, dx + xy \, dy \]

1. Is this an exact or inexact differential?

2. Do you expect the sum of \( df \) to depend on the path? Explain your answer. hypothesis

3. Go to https://hub-dev.crc.pitt.edu -> run Chem1000/differentials.ipynb. This notebook calculates \( \Delta f \) by summing up \( df \) along a path.
   a. Calculate \( \Delta f_1 \), i.e. the sum over \( df \), along the path \( y_1(x) = x \) from \( x = 0 \) to \( x = 1 \). “experiment”
   c. Compare the results for both pathways. Are \( \Delta f_1 \) and \( \Delta f_2 \) equal? Explain your finding.

conclusion/refinement of hypothesis
Assessing Validity of Models

\[ df = \frac{1}{2} y^2 \, dx + xy \, dy \]

1. Is this an exact or inexact differential?

2. Do you expect the sum of \( df \) to depend on the path? Explain your answer.

3. Go to https://hub-dev.crc.pitt.edu -> run Chem1000/differentials.ipynb. This notebook calculates \( \Delta f \) by summing up \( df \) along a path.

   c. Compare the results for both pathways. Are \( \Delta f_1 \) and \( \Delta f_2 \) equal? Explain your finding.

4. How could you improve the numerical simulation to achieve agreement with the expected result?

assessing validity of the numerical approach
Identifying Appropriate Math Models

Based on our discussion of work differentials (\(dw\)), which of the following is an appropriate minimalistic model for describing the work required to walk up and down the Cathedral of Learning?

1. \(dw = mg \, dx\)
2. \(dw = mgh \, dx\)
3. \(dw = (mg + kv) \, dx\)
4. other: _______________

Explain your answer.

How would you describe the path on the right using your own words?
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Attitudinal Assessment
MoCChA Survey

Please help me understand how effective the MoCChA notebooks are and whether you have any suggestions for improvement. This survey is anonymous and has no impact on your grade in this or any other class. However, I would greatly appreciate your feedback!

I found the MoCChA notebook(s) helpful.

- [ ] Strongly Agree
- [ ] Agree
- [ ] Neutral
- [ ] Disagree
- [ ] Strongly Disagree
Conclusion

- Students are overwhelmingly positive about MoCChA (85% approval)

- Students feel that the notebooks help them solve math problems in chemistry & focus on big picture (85-95%)

- Students want to continue using MoCChA in this class (85%)

- Students expect to reuse MoCChA notebooks in future classes (75%)

- MoCChA stimulates teamwork, but can be improved (55%)
Summative Assessment
How Do Students Perform after MoCChA Activity Compared to Historic Performance?

- Used two exam questions from previous year & administered as unannounced in-lass assessment.
- Participation was voluntary, but earned 5 point bonus.
- Students were told outcome would not impact their grades.

Same questions
Same conditions (open notes)
Same time (10 minutes)

Unannounced
Wording slightly simplified
Ungraded
MoCChA Assessment

I would like to understand whether the MoCChA handout(s) have a measurable impact on students’ abilities to solve math problems. You can receive a 5 Point HW bonus for turning in this assessment. Don’t worry - your solutions will be anonymous. This is done by writing your name only on this top page, but not on the solution page.

1. Your name:  ____________________________________________

2. Solve the practice question on the next page. Do not put your name on the solution to remain anonymous.
Given the following differential:

\[ df = (1 + a \cdot y) \, dx + y \, dy, \quad \text{where} \quad a \quad \text{is a constant.} \]

a. Determine whether \( df \) is exact or inexact.  \( \text{ (5 Pts)} \)

b. Calculate the change \( \Delta f \) along a path from \((0, 1)\) to \((2, 5)\) with \( y(x) = 1 + x^2 \).  \( \text{ (10 Pts)} \)
MoCChA Prepares Students Remarkably Well

**Historical Data (2016)**
- No MoCChA
- Performance in an *announced* exam
- Preparation: two practice exams, homework, review sessions

**Course Transformation (2017)**
- Two MoCChA activities
- *Unannounced* assessment
- 10 days prior to exam
- No practice exam, no additional review session

With MoCChA, students achieved the same average score in an *unannounced* test as 2016 students did in an *announced* exam.
Potential for Improvement

• Off-campus access

• Mobile device support

• More teamwork

• Give option to hide/reveal code

• Provide general tutorial of Jupyter demonstrating & practicing commonly used, elementary tasks (e.g., algebraic operations, equation solving, integrating, differentiating, matrix-vector operations, …)
Reflection

• MoCChA notebooks working & stable, will make GitHub repository public when activities are mature

• Student attitudes improve with MoCChA

• Initial assessment of education outcome promising

• Top Hat online response system helpful for quantitative assessment & timely feedback

• Encouraging to develop more MoCChA activities!