Sabbatical Report, Fall 2025
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Introduction:

ChemCompute (chemcompute.org) is a Science Gateway (website) for students to perform computational chemistry for free. Commercial software packages for these types of calculations typically cost $1000 and up per license for a department to purchase or $60 per student per class if students purchase them. ChemCompute provides free access to research quality computational chemistry software to students around the world, with over 39,000 students using the site last year. ChemCompute also provides computational resources for students to use Jupyter Notebooks for Chemistry or other scientific areas.

ChemCompute also serves as a platform for me to research student attitudes towards using computers in science. It is shocking to find the number of students who are adept at digital devices, but not at using computers to solve chemical problems.

Sabbatical Report:

My sabbatical request was for time to work on required aspects of my ChemCompute NSF grant. One of the requests was to travel in the Fall semester to put on workshops and present. I ended up travelling during Summer 2025 quite a bit, putting on several workshops. This freed up my fall sabbatical to work on other portions of the NSF grant.

1. Revise course-based research class based on Spring 2025 feedback

a. One of the main requests from students was a way to collaborate on their projects. Projects in this class involved running python in Jupyter notebooks, and the ChemCompute site lacked a method to allow multiple students to simultaneously edit the same notebook. I have added that capability, so that students can collaborate and work together. My hope is that this will alleviate some of the anxiety that students felt last year.

b. I trialed an AI assignment last year which didn't go over well with the students: they didn't see the ultimate point of the assignment and had difficulty completing it. I have rewritten the assignment to focus on AI in chemistry (alphafold) instead of LLM usage in chemistry. I hope that this appeals more to the students.

2. Plan workshops for Summer 2026: I collaborated with the POGIL-PCL group and applied for a workshop at the Biennial Conference in Chemistry Education (BCCE), but was declined due to high demand. I am instead working on holding a conference at Sonoma State in Summer 2026.

3. Improve the accessibility of the ChemCompute site: Over the summer, several faculty contacted me and asked about the accessibility of the site. Most universities are starting to require WCAG compliance on sites used in their courses. Accessibility is a requirement of my grant, and so I decided to use Fall 2025 to update my site to WCAG compliance. This ended up being a much larger challenge than I anticipated. WCAG requirements are numerous and it was extremely difficult to meet them simultaneously.

      a. Screen reader compatibility: the site was reworked to make it compatible with screen readers. These changes aren't visible to sighted users, but involve behind the scenes changes to the way the site is rendered.

      b. 400% zoom compatibility: the flow of the site was changed to accommodate users who view pages at 400% zoom. For example, WCAG specifies that the site must only scroll vertically at this zoom level.

      c. Contrast: some elements did not have high enough color contrast and were fixed.

      d. Keyboard navigation: the site and many interactive elements on the site were adapted to allow usage by users who only use the keyboard.

      e. Accessible plots: all plots on the site were unified and now use an accessible plot library to assist screen readers and keyboard users and display alternate data tables.

4. Analyze past survey data: our external evaluator analyzed survey data that I have been collecting on the website for years. The site uses a pre-post anonymized survey scheme, which makes it difficult to draw pre vs post conclusions. Our next goal is to incorporate their feedback and rewrite the surveys to use a retrospective pre-post format instead.