CHM676 Final Project

1 Overview

The objective of the final project is for you to *learn about* and *present on* an experimental spectroscopic method that interests you. To complete the project, you will pick a research article that uses this technique and report on it in four forms:

- A one-page (single-space) executive summary of the paper.
- A Jupyter Notebook that uses a numerical simulation to reproduce one or more key figures from the paper. (The figure should be publication-quality and match the figure in the paper as nearly as possible in both form and content.)
- A one- to three-page (single-space) document describing your simulation of the results (including any figures, equations, or code snippets necessary to explain the calculation).
- A 12-minute presentation, given in class **between Nov. 25 and Dec. 6**, that describes the research article and your simulation/analysis of it.

1.1 Executive Summary

In one single-spaced page, the executive summary should explain

- **Background:** The scientific motivation for the study:
  - **Problem:** What is the problem that motivates the study? (This should be a "big-picture" problem that an educated lay person would likely recognize, e.g., global warming, breast cancer, or antibiotic resistance.)
  - **Progress:** At the time of writing, what had already been done to address this problem? (Here you should briefly summarize relevant literature. E.g., renewable energy sources that have been developed to limit CO_2 emissions.)
  - **Gap:** What is the gap that remains that this paper tries to fill? (This should be the "small-picture" problem, which may be recognized only by specialists; e.g., the limited efficiency of a particular class of solar cells.)
- **Proposal:** The (spectroscopic) strategy proposed to (at least in part) fill this gap.
- **Approach:** The specific steps taken to implement this strategy. (A bullet-point list of 2 - 4 items would be appropriate.)
- **Results:** The article's findings.
- **Significance:** How these findings have advanced *scientific knowledge in the relevant discipline* (i.e., Intellectual Merit) and what impact this will have on society more broadly (Broader Impact).

Your in-class presentation should summarize your work clearly and concisely. You should be prepared to answer any (reasonable) questions about the method posed by myself or the class.

1.2 Simulation and Write-up

Your numerical simulation should reproduce one or more key figures from the paper, illustrating **at least one** of the following

- How the measured signal is produced *at a molecular level.* (E.g., the MD simulations we used in class to illustrate pump-probe response.)
- How the raw signal *measured by the detector* is processed into an easily interpreted spectrum, time-trace, etc. (E.g., the Fourier transforms and scaled differences we used to extract the pump-probe spectrum from the raw polarization trace.)
- How the spectroscopic data can be analyzed (e.g., using curve-fitting, singular-value decomposition, or principle-component analysis) *to extract key physical parameters* about the system or process of interest.

Your write-up should concisely explain how your simulation works, including a summary of any necessary theory, equations, or data-analysis methods. The write-up should include a side-by-side comparison of the original figure from the paper and your simulated version. Include also any figures necessary to explain critical intermediate steps in your simulation/analysis.

1.3 Presentation

Your in-class presentation should *briefly* summarize the paper (following the same bullet-point progression outlined above for the Executive Summary) and describe your efforts to reproduce the selected key figure (as described in your write-up). You will have 12 minutes for the talk plus 4 minutes for questions from the class. (Note that you will be cut off promptly at 12 minutes and will not receive credit for any additional material not presented.)

2 Grading

Credit for the project will be assigned based on

- Your executive summary (25%)
- Your simulation code and write-up (25%)
- Your in-class presentation (25%)
- Your contribution to *in-class discussion* of other presentations (25%).

Each presentation will be followed by a 4-minute question/answer period. It is expected that all members of the class will participate in this discussion. For full credit, each student should ask **at least two** relevant, scientific questions during the course of the presentation series. (Hint: As you listen to each presentation, make a list of questions to ask at the end!)

3 Notes

- Your key objective in submitted materials (including the presentation) should be to **demonstrate your ability to understand, apply, interpret, and present the technique**. Beyond that guideline, the project is intended to be flexible enough to let you pursue whatever spectroscopic methods are most interesting to you.

- Choose the project based on what is interesting to you, **not** based on what is "easy". For grading purposes, expectations for the project will be calibrated against the simplicity of the technique. More detail will be expected in projects that focus on simpler methods; less detail will be expected for more complicated methods.

- Although all four learning objects – physical basis, instrumentation, analysis/interpretation, publication – must be adequately addressed, you may choose to emphasize some learning objectives more strongly than others. For example, a particularly detailed discussion of the physical basis of the technique can compensate for a less-detailed description of the instrumentation.

- If you are currently a member of a research group, you **may not** present on a technique that you are currently using in your research. You **may**, however, present on a technique that you intend to develop in the future but is not yet implemented.