**Advanced Scientific Visual Communication – Syllabus**

ChE 3460 – Fall 2022

wilmerlab.com/sciviscomm.php

Mondays/Wednesdays, 3:00–4:15PM in room 309

**Instructor:** Prof. Christopher E. Wilmer
Office: Benedum 903 Email: wilmer@pitt.edu
Office Hours: Wednesdays 11am-noon, Fridays 2pm-3pm

**Teaching Assistant:** Ritesh Pawar Email: RIP36@pitt.edu

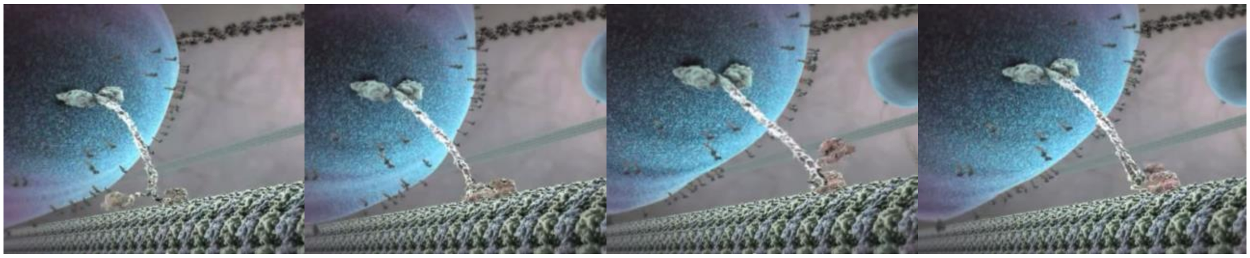

**Figure 1.** Images from an animation of a kinesin motor protein walking along a microtubule.

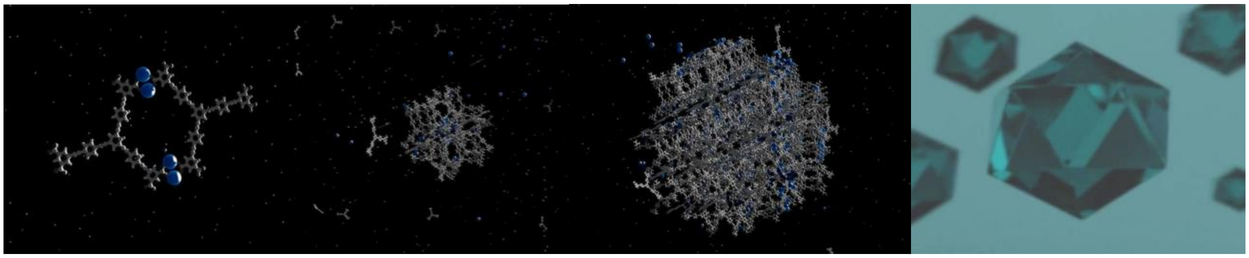

**Figure 2.** Images from an animation of the self-assembly of a metal-organic framework (MOF) crystal.

## Course Description

Scientific data, schematics, and even abstract concepts, are often most effectively communicated in visual form (see Figures 1 and 2, above). However, effectively depicting scientific ideas in a visual way often requires sophisticated visualization methods that have steep learning curves.

This course, primarily aimed at graduate students in engineering disciplines, will focus on teaching the advanced methods required to produce high quality scientific visual communication. Assignments take the form of producing publication quality figures, diagrams, posters, cover art, and short animations. We will also briefly explore emerging areas in scientific visualization such as 3d printing and interactive web graphics. The primary tools used will be Gimp, Inkscape, and Blender, all of which are open source, and the Python programming language for large dataset visualization. Powerpoint for presentations and limited figure production will also be used.

Each class focuses on depicting a particular scientific concept (e.g., microtubule self-assembly, nanoparticle growth, molten salt nuclear reactor) in a specific format (e.g., column figure, magazine cover, animation) and for a specific audience (e.g., lay public, non-specialist scientists, specialists). Each class will also develop skills and familiarities with different tools. Depicting a reactor may require precision drafting tools, while depicting an experimentally measured atomic-scale surface may require writing custom Python scripts to parse the data.

The final project of the class will involve creating a movie that meets the requirements of the annual NSF Visualization Challenge (for which the students would be encouraged to submit their work).

**Software & Hardware Required**

This will be a lecture-based course where students will follow the lecturer along on their laptops (and it is strongly advised that students also bring a mouse and keyboard). Students may also follow along using the classroom desktop computers instead. We will use the following software tools:

- Commercial: Microsoft PowerPoint (any version greater than 2007)
- [Free & open source] Gimp (www.gimp.org)
- [Free & open source] Inkscape (www.inkscape.org)
- [Free & open source] Blender (www.blender.org)

**Grading Structure**

| | | |
|---|---|---|
| • Individual assignments | | 40% |
| ○ Textbook figure | 10% | |
| ○ Journal figure | 15% | |
| ○ Cover art | 15% | |
| • Movie project (groups of 3-4) | | 30% |
| • Speed figures (~4 or 5 during semester) | | 20% |
| • Critical assessment | | 10% |

**Course Policies**

*Academic Integrity:* All homework and exams will be completed individually. Consultation with other students is permitted on homework, but not during exams. Violations of the University Academic Integrity Guidelines will result in penalties consistent with those guidelines, which may include receiving a failing grade in the course.

*Disability Concerns:* If you have a disability for which you are or may be requestion accommodation, you are encouraged to contact both the instructor and Disability Resources and Services (DRS) as early as possible in the semester. DRS is located at 216 William Pitt Union and can be contacted at (412) 648-7890 / (412) 383-7355 (TTY). DRS will verify your disability and determine reasonable accommodations for this course.

**Assignment Details**

Prior to doing any of the assignments, students must choose a scientific topic that they will visualize throughout the course. There are three topics to choose from, motivated by three different fictional grant proposals listed below:

**1. Metal-organic frameworks (MOFs) to capture $CO_2$ from the exhaust of coal power plants**

While in the best long term solutions to global warming are solar, wind, and possibly nuclear energy, in the short term, carbon capture technology retrofit onto coal power plants can significantly help reduce emissions. This research proposal describes the use of highly selective adsorbents called metal-organic frameworks (MOFs) to capture CO2 from the exhaust stream of coal power plants. Preliminary large-scale computational screening data, supported by early experimental adsorption data, support our hypothesis that a Zr-based MOF with a void fraction 80% is optimal for CO2 separation applications.

**Grant agency: Department of Energy, Requested amount: $5 million USD**

**2. Investigation of gold/palladium nanoparticle catalysts for water treatment applications**

Tricholroethylene (TCE) is a widely used industrial solvent that has been found in alarmingly high concentrations in ground water in major cities. Existing treatment technologies, such as activated carbon filters, are limited in their effectiveness for filtering out TCE. Recent research by Nutt et al. suggest that Pd/Au bimetallic nanoparticles may be effective catalysts for safely converting TCE to ethane, which can be easily separated from water. Here we propose to optimize the nanoparticle shape/size/composition and test their effectiveness on a pilot-scale filtration unit using an activated carbon support.

**Grant agency: Environmental Protection Agency, Requested amount: $4.5 million USD**

**3. Artificial nose for disease detection via large array of surface-acoustic wave sensors**

An increasing number of anecdotal reports exist of animals (and even an elderly woman) being able to detect diseases, such as Parkinson's disease, by smell. However, these reports are difficult to reproduce as it is unknown how the animals, typically dogs, can be trained to detect disease, and there are nonetheless unreliable diagnoses due to communication difficulties. An artificial nose, implemented via an array of thousands of microscale gas sensors, could potentially achieve the sensitivity and selectivity of a dog's nose while improving on reliability and analyzability. We propose to computationally design an optimal array of surface-acoustic wave (SAW) sensors and then build a small-scale prototype.

**Grant agency: National Science Foundation, Requested amount: $3.5 million**

If you feel strongly about pursuing a science topic that is not represented by the proposals above, please talk to the instructor to get approval on a topic of your own choosing. Keep in mind that this may substantially increase your workload, because the material covered in class may not help you as directly as it would if you picked one of the pre-selected topics.

**Assignment Details (continued)**

After choosing a grant proposal to work on, students will then do the following assignments throughout the course. The scientific concepts and data to visualize will depend on the grant proposal chosen.

*Textbook Figure*

A scientific concept will be described in words, which students must then illustrate in the form of a diagram. The diagram should be as accurate as possible, labelling all of the parts and adding text where necessary to explain vital parts. Besides overall dimensions, there are no constraints on how the diagram needs to be laid out.

*Journal Figure*

A scientific concept will be described in words, and also accompanied by raw data, which students must then illustrate in the form of a diagram and plot the associated data. Specific formatting guidelines are provided, in accordance with typical scientific journals. In addition to overall dimensions, the figure must be laid out in labelled panels and accompanied by a descriptive figure caption.

*Cover Art*

A scientific concept will be described in words, and students need to depict it in a striking and attractive way – in order to be suitable as a cover image for a top scientific journal. There is significant room for creativity in this assignment. Although it is always important to get preliminary feedback on draft images, it is particularly important for cover art, which must appeal to a wide audience.

*Movie Project (groups of 3-4)*

Students that have chosen the same proposal topic will form into groups of 3-4 and create a short descriptive movie (~3 minutes, ~5000 frames) depicting a scientific process. The movie should be made as if it was going to be submitted to the annual NSF Visualization Challenge.

*Speed Figures (individual, in class)*

An emphasis of the course will be on producing publication quality figures *quickly*. The "speed figures" will be analogous to quizzes in other courses. Students will be given a scientific concept that they need to depict and will then have a limited time (~an hour) to draft a figure using any tool they wish.

**Tentative Course Outline & Schedule**

A rough trajectory of the course:

Simple diagrams & data plots (Powerpoint, Inkscape)
↓
More complex diagrams, publication quality journal figures (Blender, Gimp)
↓
Advanced 3D rendering techniques, basic animations (Blender)
↓
Complex animations, python scripts, movies (Blender)
↓
(if there is time) Bonus: 3D printing, interactive web graphics