Computational Physics Final Project Descriptions Spring 2015

T. J. Atherton

Below are a set of possible projects that you can attempt either together or individually. All projects below are potentially publishable: this will involve a fair amount of extra work—but great for your CV!

Semiclassical nonlinear optics

The following is a crude model of an electron confined to a delocalized π molecular orbital in a long conjugated molecule: Suppose an electron in the ground state of a potential well $V(x)$ is perturbed by an appied electric field $V'(x) = \epsilon x$ where ϵ is a small parameter. The position expectation value, representing the average location of the electron $\langle x \rangle$ will obviously shift in response. The linear response,

$$\alpha = \frac{\partial \langle x \rangle}{\partial \epsilon}$$

is called the *polarizability*. The *nonlinear* response is, however, of great interest for applications (google "nonlinear optics" to see why!). This is given by a set of parameters

$$\beta, \gamma ... = \frac{\partial^n \langle x \rangle}{\partial \epsilon^n}$$

where $n > 1$ called the first hyperpolarizability, second hyperpolarizability. Remarkably, there exists a fundamental limit on the magnitude of these quantities. The question then arises: how does one optimize the shape of the potential $V(x)$—which is supposed to capture broad features of the molecular design—so as to maximize β, γ, etc? The problem has been studied by your instructors in a sequence of papers, so some advice exists. To do so, one writes a program that solves the TISE for a particular potential, appropriately parametrized, calculates the hyperpolarizability, then adjusts the parameters to reach a maximum. Easy—and it works! The difficulty, however, is that the optimized potentials are difficult to interpret, and the reasons behind the fundamental limit remain only partly clear.

The problem can, however, be reformulated without recourse to the Schrödinger equation using semiclassical quantization. *[You may have seen this in Physics 13 as the Born-Sommerfeld quantization]*. In this approach, one solves the equivalent classical mechanics problem for $V(x)$ to find the classical trajectory $x(t)$ and momentum $p(t)$; one then imposes the Bohr quantization by requiring the *action* $\int p dx$ *[the area enclosed by the trajectory in phase space]* is quantized in units of $\hbar$, solving for the energy levels E_n. From the trajectory and the known energy levels, the hyperpolarizabilities can be calculated. The objective of this project would be to set up the optimization problem to find the potential that optimizes the hyperpolarizability within this framework.

Multi-electron nonlinear optics

This project is centered around the same fundamental problem—optimizing hyperpolarizability with respect to potential wells—as the previous one. The key difference is that here, we'll be trying to solve the *multi-electron* problem. This is important, because real molecules contain multiple electrons in π states, and the repulsive electron-electron interactions will tend to oppose redistribution of the charge under the application of an electric field. Hence, the nonlinear response could be attenuated by the presence of additional electrons.

A number of possible approaches could be taken to this project:—

1. *Density Functional Theory*. Rather than solving for the wavefunction ψ, it's possible to solve for the multi-electron charge density *[the powerful X theorem guarantees that the one can always be reconstructed from the other]*.
2. *Auf-bau*. A rather crude approach is to solve the one-electron problem, then to fill the states with multiple electrons using the *auf-bau* principle. *[A previous undergraduate student of mine made headway on this; it would be good to get further!]*

Having done either of these, the hyperpolarizability can be calculated from this and the potential then optimized.

Liquid Crystal Elastomer Strings

Liquid Crystal Elastomers (LCEs) are rubbery polymeric materials with cross-linked liquid crystal mesogenic groups. These included groups give the material a very strong response to an electric field. Therefore, when electric fields are applied, they deform (you can think of it as an artificial muscle); equally, when squeezed they produce an internal electric field of their own. Working with collaborators, the instructor has constructed a fundamental theory of such materials. By patterning the elastomer, one can make a material that self-folds into desired shapes. One fascinating problem that arises is: given a desired final shape, how should one pattern the material? This is a deep problem indeed—too complex for this class!—but there's a lot we could do to make progress.

A simpler subproblem is to look at the physics of 1D LCE "strings". Imagine, for instance, a rope that could stand up if you put it in an electric field, or that might buckle if you soak it in water to make it swell. The objective would be to write a program to predict the shape of the rope given an initial pattern and applied field or swelling protocol. From this, a sensitivity analysis of the final state to the initial conditions, within some appropriate norm, could be conducted as a precursor to the inverse problem. It is conceivable that analytical solutions may exist for restricted subproblems providing the opportunity for rich validation.

Shape changes with GPU computing

Another focus of the instructors' work has been to look at shape minimization problems, where a surface (represented by a triangulated mesh) is relaxed under forces like surface tension to identify the ground state (usually a sphere). Indeed, the instructor has written a large computer package—Morpho—to do so.

It seems likely that the problem could be formulated using a GPU computing language like CUDA, potentially with huge speedup. As well as the interest in fundamental physics, this could have wide applications in graphics, movie making, etc. as the physics of soft materials (think toothpaste, soap bubbles, etc.) are difficult to capture with generic algorithms. An important part of this project will be benchmarking the performance of the new algorithm against a non-GPU implementation that already exists.

[I think this might suit a comp sci student, or someone with a lot of programming experience; particularly if you've taken a computer graphics class]

Packing Spheres on Curved Surfaces

A significant focus of the softmattertheory group's work involves packing problems: how do we put spherical particles on a curved (and possibly time-evolving) surface so as to cover the highest fraction of the surface possible? On a plane, the problem is trivial: the particles pack into a hexagonal lattice. On a curved surface, the curvature necessitates the introduction of gaps in the packing called defects. How these defects are distributed on the surface, particularly where the curvature is non-uniform, is of great interest.

Because this is so closely related to the instructor's current research, many possible projects could be formulated within this space:

1. **Effect of polydispersity.** Even the very simple problem of packing spheres of different sizes onto a sphere has not been investigated! We should do so!
2. **Shapes beyond spheres, ellipsoids and cylinders.** Pick your favorite (interesting) surface—and pack!
3. **Continuum limit.** The placement of defects can also be described by a continuum elastic theory, so we could minimize this elastic energy to find the placement of the defects directly.

Computational Physics in the High School Classroom

Computation is a fundamental tool of physics: simulations are used to gain important insights into complex systems; it is used for fitting models to data; visualization is key to understanding physical processes. Additionally, it is a powerful classroom tool, allowing students to identify relationships between parameters and processes as well as

visualize the results. While it has grown ever-more important that practicing physicists are prepared to use these tools in their work, it is not a standard part of the undergraduate or high school curricula. However, the Next Generation Science Standards contains a lot of language about model-building, interpreting data, etc., that computation could provide a powerful approach to address *[anecdotally, these seem the hardest parts of the standards to implement too!]*. The objective of this project, therefore, is to **prototype** what computational physics in the high school classroom might look like and provide guidance for further work on this. Some possible activities within this project:—

1. Consultation with High School teachers on what the specification should look like, e.g. a quick and informal survey. Are there particular experiments students do that could be improved by computation? What challenges do they face? How much time should the activity reasonably take? *[It also needs to be really cheap! I'm thinking that aiming at a Raspberry Pi would be a great idea, for example.]* It would be great to leverage the extensive education research expertise available at Tufts to help with the design.

2. Implementing a sample activity as well as an associated teaching guide. What will the students do? Are there things the students could modify? Does it relate to something physic

3. If possible, a trial run! Or even feedback from high school teachers/education researchers on how to improve it.

Formulate your own project

Students already working in a physics research group may, in consultation with their adviser, construct a computational physics final project that is pertinent to their research. *It is essential for this to work that both student and advisor consult with the instructor for this course so that the grading criteria are clear to all.*
