PHSX 615/815, CHEM 914: Final Homework

Due at the latest by: Fri. May 13^{th}

You are very welcome to choose your own topic. The descriptions are sometimes over-specified (and sometimes not) and should not be followed literally but can be useful guidance.

Choose one computational topic that interests you

Possible Topics

1. Relaxation Methods for boundary value problems like Laplace's equation
2. Time dependent Schroedinger equation
3. Use of Metropolis algorithm / Bayesian inference
4. Stochastic modeling of infectious disease spread
5. Implement Genetic Algorithm or Simulated Annealing to a problem of your choice
6. Choose your own topic

As usual please write it up and submit your code. Topics 1,2,3, and 4 currently have written up descriptions / suggestions and notes that are distributed (likely on web page).

Guidance on Choosing Your Own Topic

Use techniques or ideas developed in the context of this class to explore some aspect of computational science. Four of the topics are reasonably well specified, and they may be a good choice if you don't have specific ideas on what you'd like to explore. It is important that personal project work that is done is original new work, is not too specialized to your particular research domain and is not rehashing/repackaging of existing work. As a guideline – it should be something that the other students in the class would grasp and understand.

As a general theme to guide your choice, one area that is particularly rich in its application is stochastic modeling using Monte Carlo techniques. Many systems in nature are rather complex, and do not lend themselves to exact solution. One very important technique, especially from my perspective as an experimental physicist, is the Monte Carlo technique, which can be used to simulate the behavior of many different systems. We already saw how the essence of Monte Carlo is integration by throwing random numbers. However the Monte

Carlo method is usually invoked, not just for its ability to solve N-dimensional integrals, but for its ability to simulate the results of an experiment. The experiment can be anything you can think of. Examples are: a simple toin coss, a game of poker, a ball game, a model of financial markets, models of infectious disease, results of a physics experiment. It can usually be used in a very natural way to simulate each step of converting the model parameters into the experimental observables.

An often essential aspect of the application of the technique, is the ability to simulate not just a possible result of one particular realization of the experiment, but to simulate an ensemble of results of the experiment. This can be particularly important when trying to assess the significance of the observed result from the actual experiment in the context of a particular model. The strength of the technique is that it deals explicitly with the stochastic nature of the processes and predicts not just average behavior, but the distribution of behavior. You are welcome to choose some system that you want to model using the Monte Carlo technique, and explore the behavior of. Some particularly apt examples might be from sport. For example, given particular statistics or educated guesses at them, and their distributions, sports like football, soccer, basketball, baseball, golf, cricket should be amenable to such an approach. You may also want to explore possibilities in other domains.

Bottom-line: pick something you are interested in, and try to make sure that it is reasonably self-contained and tractable. Building on techniques that you have already established is recommended. If you are uncertain that the project you are thinking of taking on is appropriate please feel free to discuss.