Part 1: Brief Bio

Bio

My name is Asmit Bhowmick. I am a fifth year Ph.D student in Chemical Engineering working in the field of protein engineering. I use computer simulations of biomolecules to rationally improve efficiency of enzymes.

Research Interests

Using computer simulations to gain predictive understanding of enzymes and different materials.

Personal Goals in the course

I hope to learn how to write good parallel codes that can help me in the future when I want to write customized simulation codes. I also have some interest in learning how to write GPU code but not sure how much that will be covered in this course.

Part 2: Application problem of interest

I took CS-294-73 with Prof. Phil Collela (Software engineering for scientific computing) where a couple of labmates and I wrote our own molecular dynamics code from scratch with emphasis on using particle mesh methods for electrostatic calculations. However, it’s a single core code with no parallelization. I was interested in parallelizing it either using MPI or OPENMP or maybe writing a GPU version of the code for this course.
The code we wrote is available at: https://github.com/asmit3/SoftwareEngg_Fall15