HomeWork 0 , CS267 , SP14
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1. Brief bio:

**Background:** I am an AS&T PhD student with a kind of mixed background, as I have been to different fields. I began as a freshman in traditional mechanical engineering and got my bachelor followed by master. After that, I started working and researching in the field of nanothermodynamics for a couple of years. Finally I ended up with computational biology and biophysics. To clarify, by ‘computational biology’ I mean *Brownian and molecular dynamic simulations*, not bioinformatics or biostatistics.

**Current:** I have been using serial FORTRAN 90 *(no OOP)* to develop a computational model intracellular activities.

**Out of this class:** My hope from this class is to be able to deeply learn parallelization and its implementation as a hybrid of MPI and OpenMP platforms. Ideally, I like to combine these with GPU computing for the most computational-intensive parts.

**Programming:** I know FORTRAN pretty well, but not C. I am learning it though.

**Project for this course:** The project I have in mind for this course is:

*Modeling and simulation of polymer-derived nano-filters that selectively filter different kinds of particles, based on their sizes, charges, etc.* These have numerous biological (blood test, sample purification, selective drug delivery, ...) as well as industrial applications (air pollution, oil industry, water purification,...). The model itself is kind of challenging, but I can establish it fairly straightforward, as I have a long experience in these kinds of modeling.

2. Application of parallel computing

The application problem that I found for which they have used parallel computing, is a molecular dynamic study conducted in 2009 in the University of Illinois at Urbana-Champaign *(here is the paper)*. There, they made an array of 5X5 long polypeptides and studied the conformational changes of this system in an ionic solution in the presence of explicit water molecules *(see Fig.1)*. This system includes a total of one million atoms, including water molecules and ions.

Due to the high computational cost of this system and the fact that they needed to simulate it for long a simulation time in the order of microseconds, they used multiscale modeling. Thus, they have conducted two scales of simulations: all-atom and coarse-grained. In all-atom scale, as the name suggests, all atoms and their relevant interactions are taken into account. This scale was simulated about 100 ns. In the coarse-grained scale, they have lumped several atoms into a bead (=coarse atom) to reduce the total number of coarse atoms to about 300,000. Then, they simulated the coarse-grained system for about 4 µs
They have compared their results with similar published results and found a good agreement, which is kind of confirming the approach of molecular dynamics.

In their molecular dynamics package (NAMD), they benefit from both shared and distributed memory platforms. In the most recent version of this package, they also implement GPU computing as well to maximize the efficiency of this computational package. Indeed, the NAMD is a written in FORTRAN.

The application were run on two main national supercomputers: 1. Texas Advanced Computing Center, and 2. the Pittsburgh Supercomputer Center. As of November 2013, TACC was ranked 7 in top500, but Pittsburgh Supercomputer Center was not among the first 500 supercomputers. This application is scalable to massive processors, and I believe it reaches a very good performance compared to similar works.

Reference: