CSCI596 (Scientific Computing and Visualization) Final Project
Anything Related to What You Have Learned in the Class

Due: December 12 (Wed), 2018

Submit a written project report by Wednesday, December 12. In addition, a brief (~1.5 minutes) informal presentation on your project is required in class on November 26 (Mon), 28 (Wed) or 30 (Fri). The presentation is just an outline of the project — what is the problem, what methods were used, and what are the major results — it should not contain more than 5 slides if you make a PowerPoint presentation, which is not necessary. Please email me your PowerPoint file (again only if you have decided to do so) before the day of your presentation. Also, please see me to discuss and agree on your project by Friday, November 16.

Project: Choose one of the following two options. (The subject can be anything related to simulations such as molecular dynamics (MD), parallel computing or scientific visualization.)

I PROGRAMMING: Write a program that is related to one of the subjects covered in the class. The following is a list of suggested topics (not exhaustive).

- Enhance the parallel MD program, pmd.c.
  - > Traverse the linked-list cells according to the Hilbert or Morton curve to enhance the data locality and cache performance.
  - > Implement simple load balancing based on movable but rigid partition boundaries.
  - > Send compressed messages to reduce communication.
  - > Modify the MD program such that it directly operates on compressed data to further avoid the compression/decompression overhead.
  - > Write a metacompting-enabled MD program based on processor grouping and message renormalization.
- Optimize the performance of the hybrid MPI + OpenMP MD program or write a hybrid MPI + OpenMP + CUDA program.
- Add new features to the OpenGL visualization program, atomv.c. For example, you can color-code the stress tensor of each atom and trace the trajectory of one of the atoms. Speed up the code by reducing the number of vertices to represent a sphere, for further atoms from the viewer.
- Write an OpenGL program to animate simulation in your own discipline.

II PROPOSAL: Write a short research proposal containing novel extensions of any of the techniques you have learned in the class. The proposal should contain: Goal, specific objectives, current state of the knowledge/previous work, techniques to be used, and expected results.

Guidelines for the Final Project

I. PROGRAMMING: Use your imagination; learn a new language (*e.g.*, TensorFlow, OpenCL, Hadoop) to make yourself marketable.

II. PROPOSAL

1. Goal: What's the "big" problem? Why important? Statement of the problem: If you can "clearly" state the problem, it often automatically suggests a solution.
2. Specific objectives: Step-by-step path to the goal.
3. Current state of the knowledge/previous work.
4. Techniques to be used: How to solve it? Big idea? Well-planned detail?
5. Expected results: Research full of surprises but needs hypothesis/test; broader impacts—so what?