CSCI596 (Scientific Computing and Visualization) Final Project  
Anything Related to What You Have Learned in the Class  
Due: December 11 (Fri), 2015

Submit a project report by Friday, December 11. In addition, a brief (~1.5 minutes) PowerPoint presentation on your project is required in class on November 30 (Mon), December 2 (Wed), or December 4 (Fri). The presentation is just an outline of the project—what is the problem, what methods were used, and what are the major results—and should not contain more than 5 slides. Please email me your PowerPoint file before the day of your presentation. Also, please see me to discuss and agree on your project by Friday, November 13.

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 metacomputing-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., Hadoop, OpenCL) 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?