

## **CSCI653 (High Performance Computing and Simulations) Final Project: Completing Your GitHub Repository**

**Due: December 18 (Wed), 2019**

*Submit a final project report by the end of Wednesday, December 18. In addition, a brief (1-2 minutes) presentation on your project is required in class on December 4 (Wed) or 6 (Fri). The presentation is an executive summary about the big picture but not excessive details. Also, please see me to discuss and agree on the scope of your project by Friday, November 22.*

**Project:** Complete the GitHub repository initiated in your assignment 1. The repository should describe an application of high performance computing and simulations (HPCS) to a challenging scientific or engineering problem and seek an innovative solution to the problem of your choice. Your project can be one of the following two types: actual programming (if implementable within the semester) or research proposal. (The subject can be anything related to simulations such as molecular dynamics (MD), quantum dynamics (QD), parallel computing, or scientific data visualization and machine learning.)

- 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; analyze which curve performs better.
    - > Implement low-overhead load balancing based on movable partition boundaries and hypergraphs.
    - > 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, message renormalization, and computation-communication overlap.
  - Optimize the performance of the hybrid MPI+OpenMP+CUDA QD program by introducing CPU-GPU computational overlap and communication minimization.
  - Combine the OpenGL visualization program, atomv.c, and the MPI simulation program, pmd.c, so that you can animate a parallel MD simulation at run time; do it in virtual reality.
  - Integrate machine learning into parallel MD or QD program.
- 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 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. What will be the contribution?
  2. Specific objectives: Step-by-step path to the goal.
  3. Current state of the knowledge/previous work. What have been done, and more importantly, what have not been done that you are addressing?
  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?