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

Due: December 13 (Wed), 2023

Create a GitHub repository [1,2] containing your final project by ***Wednesday, December 13 — submit the URL of your GitHub repository to Blackboard*** (for a team project, every team member needs to submit the identical URL of the team repository individually for grading purpose). In addition, a brief (~one minute) ***informal presentation*** on your project is required in class on ***November 27 (Mon), November 29 (Wed) or December 1 (Fri)***. The presentation is just an outline of the project — what is the problem, what methods were used, and what are the expected results — you are only allowed to show your preliminary GitHub repository. Also, please discuss with me to ***agree on the topic*** of your project (during office hours) by ***Friday, November 17***.

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. If you are a Ph.D. student, try to enhance your own thesis research using techniques you have learned in this class. If you are a MS student, pick a compelling topic such that your GitHub repository becomes a good showcase in your job or Ph.D. application.

I PROGRAMMING: Write a program that is related to one of the subjects covered in the class. The following is a list of possible topics (just to give you an idea, please come up with your own topic).

- 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.
  - > 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 (or SYCL) 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

I. PROGRAMMING: Use your imagination; learn a new language (*e.g.*, SYCL, TensorFlow) 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?

References

1. https://github.com/
2. http://swcarpentry.github.io/git-novice/