

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

Due: December 13 (Fri), 2024

Create a GitHub repository [1,2] containing your final project by **Friday, December 13** — **submit the URL of your GitHub repository to Brightspace** (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 **December 2 (Mon), 4 (Wed) or 6 (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 22**.

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 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 (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/>