

CSCI 596: SCIENTIFIC COMPUTING AND VISUALIZATION
Fall 2024 (section: 30280D—lecture & 30146R—discussion; session: 048)

Instructor: Aiichiro Nakano; office: VHE 610; email: anakano@usc.edu

TA: Taufeq Razakh (razakh@usc.edu)

Classes: Lecture: 3:30-4:50pm M W, SOS B2
Hands-on: 3:30-4:20 pm F, ZHS 159

Office Hour: 4:30-5:20pm F, VHE 610

Course Page: <https://aiichironakano.github.io/cs596.html>

Prerequisites: Basic knowledge of programming, data structures, linear algebra, and calculus.

Textbooks: W. D. Gropp, E. Lusk, and A. Skjellum, *Using MPI, 2nd Ed.* (MIT Press, 1999)—recommended
M. Woo *et al.*, *OpenGL Programming Guide, Version 4.5, 9th Ed.* (Addison-Wesley, 2016)—recommended
A. Grama, A. Gupta, G. Karypis, and V. Kumar, *Introduction to Parallel Computing, 2nd Ed.* (Addison-Wesley, 2003)—recommended

Course Description

Particle and continuum simulations are used as a vehicle to learn basic elements of scientific computing and visualization. Students will obtain hands-on experience in: 1) formulating a mathematical model to describe a physical phenomenon; 2) discretizing the model, which often consists of continuous differential or integral equations, into algebraic forms in order to allow numerical solution on computers; 3) designing/analyzing numerical algorithms to solve the algebraic equations efficiently on parallel computers; 4) translating the algorithms into a program; 5) performing a computer experiment by executing the program; 6) visualizing simulation data in an immersive and interactive virtual environment; and 7) managing/mining large datasets.

Syllabus

1. Basic molecular dynamics (MD) algorithms
 - Integration of ordinary differential equations; periodic boundary condition; linked-list cells
2. Parallel MD
 - Spatial decomposition (interprocessor caching and migration); load balancing; scalability analysis; asynchronous MD
 - Message passing interface (MPI) vs. shared memory (OpenMP) programming
 - Hybrid MPI+OpenMP programming
 - Data-parallel accelerator programming (*e.g.*, GPU—CUDA, OpenMP offload, SYCL)
3. Grid/cloud scientific computing
 - Computation steering on the Grid/cloud (*e.g.*, Globus, Grid RPC, MapReduce)
 - Grid/cloud enabling parallel applications
4. Scientific visualization
 - OpenGL programming
 - Scientific visualization software—OVITO, VMD, VisIt, ParaView
 - Virtual-reality programming—CAVE Library, ImmersaDesk, tiled display, head-mounted display
5. Scientific big data and machine learning
 - Data compression for scalable I/O
 - Graph-based knowledge discovery
 - *In situ* data analysis and machine learning
6. Scientific programming systems
 - Parallel software tools for irregular data structures; object-oriented MD; scripting wrappers
7. Other simulation methods
 - Stochastic simulations: Monte Carlo method
 - Continuum simulations: Schrödinger equation in quantum mechanics

Grading Scheme (assignment submission and grade posting on Blackboard; <http://blackboard.usc.edu>)

Assignments (6-8 programming projects), 85%; final project, 15%

A (100-90%); A- (90-85%); B+ (85-80%); B (80-75%); B- (75-70%); C (70-60%); D (60-50%)

Schedule

Final project report due (Dec. 13)