CSCI 596: SCIENTIFIC COMPUTING AND VISUALIZATION

Fall 2021 (section: 30280D—lecture & 30146R—discussion; session: 048)

Instructor: Aiichiro Nakano; office: VHE 610; phone: (213) 821-2657; email: anakano@usc.edu

TA: Kuang Liu; email: liukuang@usc.edu

Classes: Lecture: 3:30-4:50pm M W, LVL 17 and online
Hands-on: 3:30-4:20 pm F, SOS B2 and online

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, DPC++)
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 (5-7 programming projects), 80%; final project, 20%
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. 15)