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)
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 (5-6 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. 9)