Courses on High Performance Computing and Simulations (HPCS)

Aiichiro Nakano

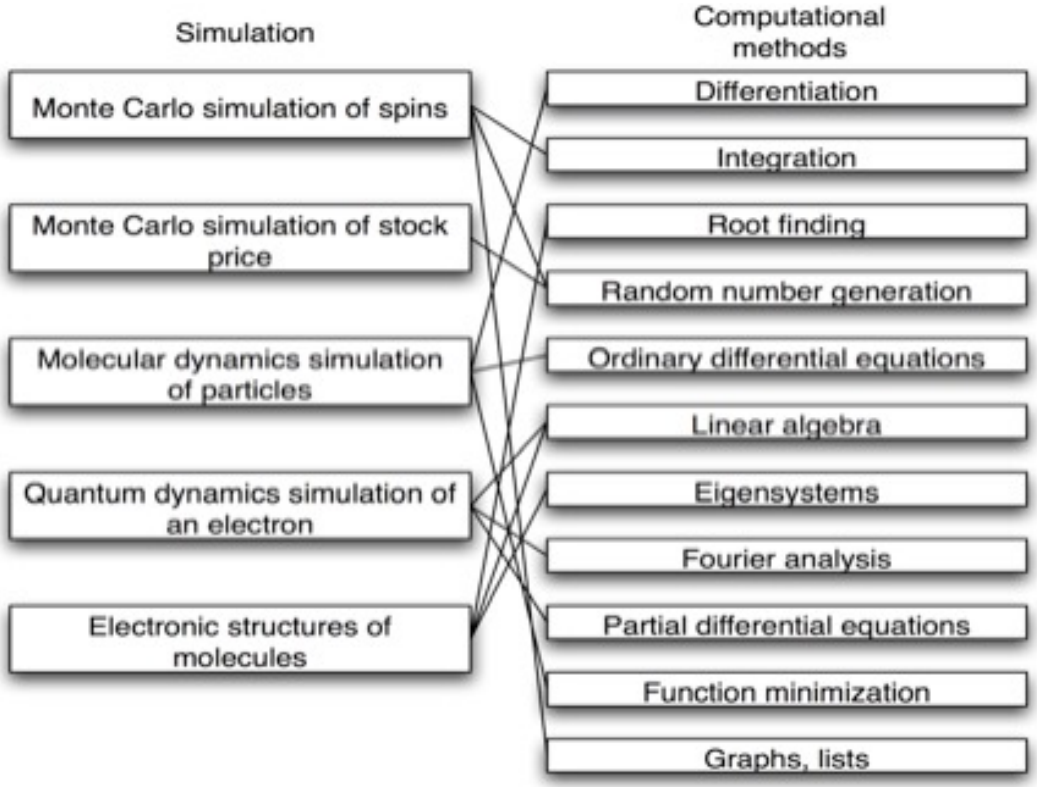
Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Quantitative & Computational Biology
University of Southern California

Email: anakano@usc.edu

https://sites.usc.edu/cacs/teaching

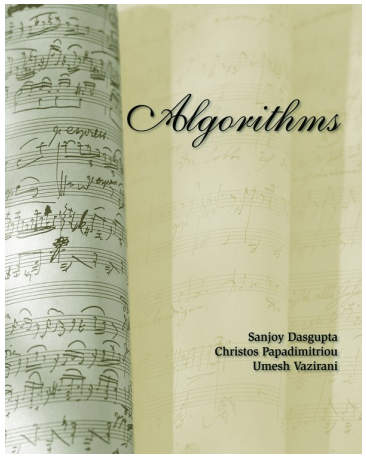
CACS HPCS Courses: Simulation!

- **PHYS516: Methods of Computational Physics (S)**
  ***Numerical methods (+ algebra & calculus)* in the context of simulations**
- **CSCI596: Scientific Computing & Visualization (23F, 24F)**
  Hands-on training on particle/continuum simulations, *parallel computing* & *scientific visualization*
- **CSCI653: High Performance Computing & Simulations (22F, 25F)**
  Deterministic/stochastic simulation *algorithms*, scalable parallel/distributed computing & scientific data visualization/analytics in virtual environment



	Particle model (ordinary differential equations)	Continuum model (partial differential equations)
Deterministic	molecular dynamics	computational fluid dynamics, continuum mechanics
Stochastic	Monte Carlo particle simulation	quantum Monte Carlo

Chapter 0: Prologue
Chapter 1: Algorithms with numbers
Chapter 2: Divide-and-conquer algorithms
Chapter 3: Decompositions of graphs
Chapter 4: Paths in graphs
Chapter 5: Greedy algorithms
Chapter 6: Dynamic programming
Chapter 7: Linear programming
Chapter 8: NP-complete problems
Chapter 9: Coping with NP-completeness
Chapter 10: Quantum algorithms



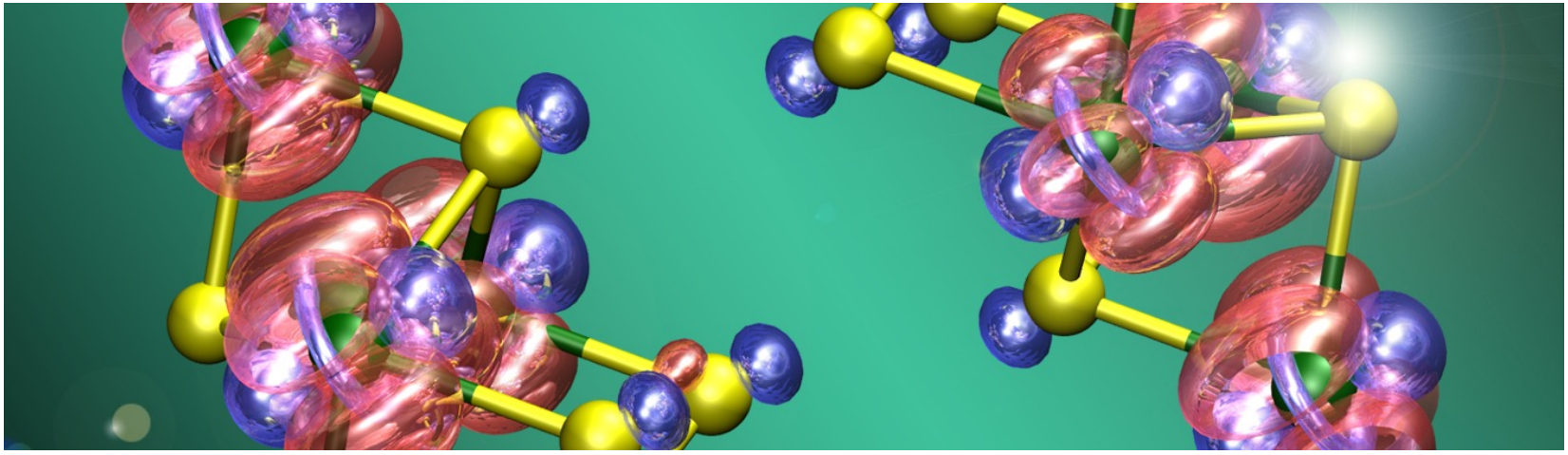
Additional HPCS Course

Detailed lecture notes are available at the course home page

CSCI 699: EXTREME-SCALE QUANTUM SIMULATIONS

Course Description

Computer simulation of quantum-mechanical dynamics has become an essential enabling technology for physical, chemical & biological sciences & engineering. Quantum-dynamics simulations on extreme-scale parallel supercomputers would provide unprecedented predictive power, but pose enormous challenges as well. This course surveys & projects algorithmic & computing technologies that will make quantum-dynamics simulations metascalable, *i.e.*, "design once, continue to scale on future computer architectures".



https://aiichironakano.github.io/cs699.html

Related Course

- **EE599: Parallel Programming: Victor Prasanna**
  EE451: Parallel & Distributed Computation: Victor Prasanna

  Parallel and distributed computing using various programming models

- **EE599: Emerging Devices for AI/ML: Joshua Yang**

  Emerging materials, devices & how to use them to enable novel artificial intelligence & machine learning

CSCI 653 Prerequisites

1. CS596 (Scientific Computing & Visualization)

OR

2. Basic knowledge of
   - Numerical methods (CSCI 501, PHYS 516 or equivalent)
   - Parallel computing—MPI, OpenMP, CUDA programming experience (EE 451 or equivalent)
   - 3D graphics—OpenGL programming experience (CS580 or equivalent)

CSCI 653 will apply these knowledge & techniques to simulations (or scientific/engineering applications)

MSCS-HPCS Objectives

CSCI 653 is a core elective for MSCS-HPCS

- **Train a new generation of MS students in Computer Science to solve challenging scientific & engineering problems using high-end parallel computers, high-speed networks & advanced scientific visualization**
- **Support a unique dual-degree opportunity, in which students can obtain a Ph.D. in the physical sciences/engineering & an MS in Computer Science, to attract high-quality students**

https://www.cs.usc.edu/academic-programs/masters/

Simulation + Data + AI

Apart from the general Master of Science in Computer Science, the CS Department also offers the degree with the following specializations:

- Artificial Intelligence
- Data Science
- Game Development
- Computer Security
- Computer Networks
- Software Engineering
- Intelligent Robotics
- Multimedia and Creative Technologies
- High Performance Computing and Simulation

Actually, need ALL to do cutting-edge science (more in the next lecture)

MSCS-HPCS Requirement

A total of **32** units

1. Required Core Courses in Computer Science: 3 courses
   CSCI570 (analysis of algorithms)
2. Required Core Course for MSCS-HPCS
   CSCI596 (scientific computing & visualization)
3. Elective Courses for MSCS-HPCS: Total of 3 courses from both tracks (a) & (b)
   (a) Computer Science Track
   CSCI653 (high performance computing & simulations)*,
   CS520 (animation), CS551 (communication),
   CS558L (network), CS580 (graphics), CS583 (comp geometry),
   CS595 (advanced compiler)
   (b) Computational Science/Engineering Application Track
   AME535 (comp fluid dynamics), CE529 (finite element), CHE502 (numerical transport),
   EE553 (comp optimization), EE653 (multithreaded arch), EE657 (parallel processing),
   EE659 (network), Math501 (numerical analysis), MAS575 (atomistic simulation),
   Phys516 (computational physics), PTE582 (fluid flow), ...

Out of sequence

* **CSCI653 can substitute CSCI 596 for core requirement 2; however, once taken CSCI 653, CSCI 596 (its prerequisite) cannot be counted toward degree**

Q: Any addition to 3b?

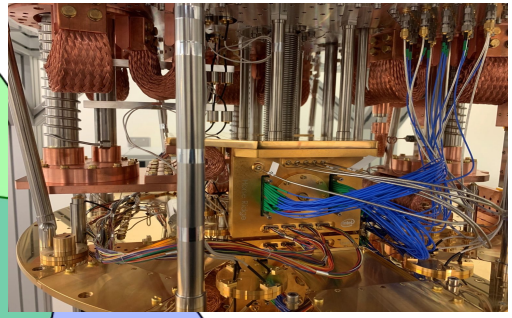
MS in Quantum Information Science

- New MS degree in Quantum Information Science (MSQIS) started in 2021
- Required foundational courses
  1. EE 520: Introduction to Quantum Information Processing
  2. EE 514: Quantum Error Correction
  3. Phys 513 (New): Applications of Quantum Computing
- Core—at least two courses from
  1. EE 589 (New): Quantum Information Theory
  2. Phys 550 (New): Open Quantum Systems
  3. Phys 559 (New): Quantum Devices
  4. Phys 660: Quantum Information Science & Many-Body Physics
- Phys 513: Application of Quantum Computing (will be co-taught with Prof. Rosa Di Felice)—quantum simulations on quantum circuits & adiabatic quantum annealer (syllabus)
- Phys 516, CSCI 596, CSCI 653: Core elective for MSQIS

Training Cyber Science Workforce

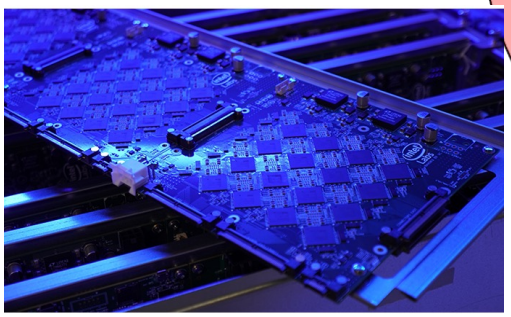
- New generation of computational scientists at the nexus of exascale computing, quantum computing & AI
- Unique dual-degree program: Ph.D. in science or engineering, along with MS in computer science specialized in high-performance computing & simulations, MS in quantum information science or MS in materials engineering with AI

Horse Ridge II
Quantum computer



Cybertraining on exa + quantum + AI platforms

Neuromorphic
Pohoiki Springs



Exascale
Aurora

NSF CyberTraining

CyberMAGICS - Cyber Training on Materials Genome Innovation for Computational Software (2021-25)

A. Nakano, K. Nomura, P. Vashishta (*University of Southern California*)
P. Dev, T. Wei (*Howard University*)

AIQ-XMaS: AI and Quantum-Computing Enabled Quantum Materials Simulator

QXMD

Nonadiabatic quantum molecular dynamics

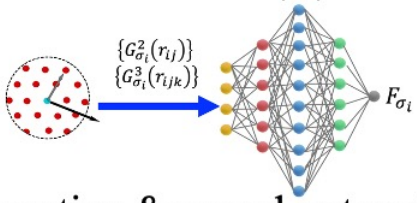
GEARS

Augmented-reality user interface

MISTIQS

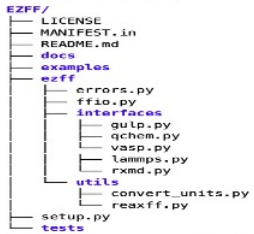
Quantum many-body dynamics on quantum computers

RXMD-NN



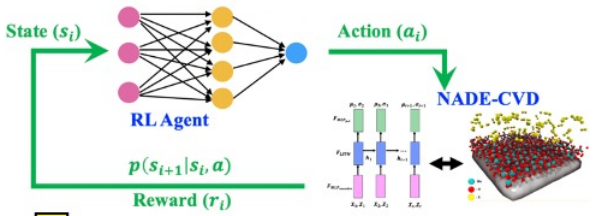
Reactive & neural-network molecular dynamics

EZFF



Easy force-field parameterization & uncertain quantification

MAITAI



AI tools for materials design

CARC Tutorials & Office Hours

Series of tutorials + office hours (T, 2:30-5 pm, LVL 3L) at the USC Center for Advanced Research Computing (CARC):

- **CUDA computing on GPU (Sep. 9): Register here**
- **HPC with Julia**
- **...**

https://www.carc.usc.edu/education-and-resources/workshops
https://carc.usc.edu

Students registered by the end of this week will get a CARC account

Master of Science in Computer Science with Specialization in High Performance Computing and Simulations (MSCS-HPCS)

https://www.cs.usc.edu/academic-programs/masters/high-performance-computing-simulations

Computational Sciences at USC

Aiichiro Nakano

Email: anakano@usc.edu