CSCI 596 & Master of Science in Computer Science with Specialization in High Performance Computing and Simulations (MSCS-HPCS)

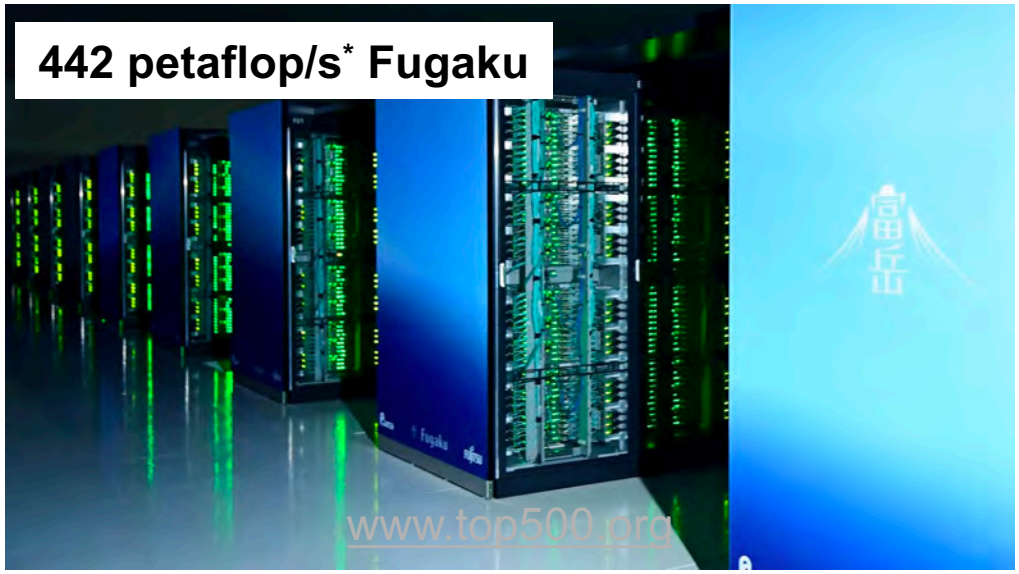
https://www.cs.usc.edu/academic-programs/masters/high-performance-computing-simulations

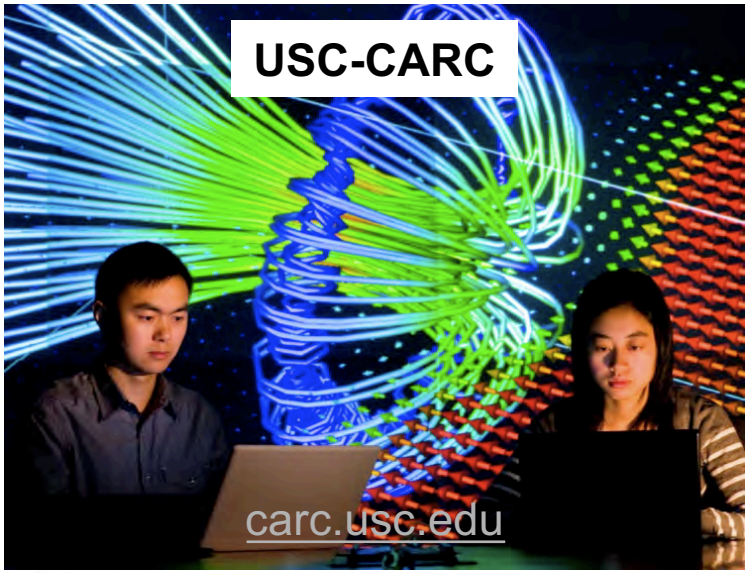
Computational Sciences at USC

Aiichiro Nakano

Email: anakano@usc.edu

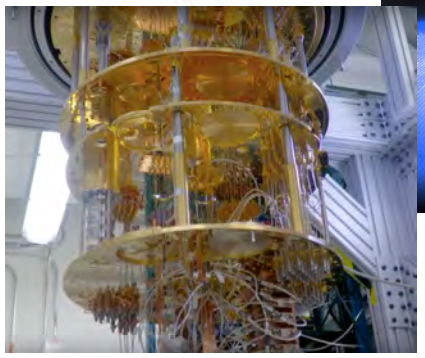
High Performance Computing





- *USC CARC (Center for Advanced Research Computing)*: **13,440 CPU-core GPU-accelerated 0.62 petaflop/s cluster**
- *USC ISI (Information Sciences Institute)*: **1,098-qubit D-Wave quantum computer**

GPGPU



QPU

* petaflop/s = 10^{15} mathematical operations per second

Computational Sciences at USC

The Nobel Prize in Chemistry 2013

© Nobel Media AB

Martin Karplus

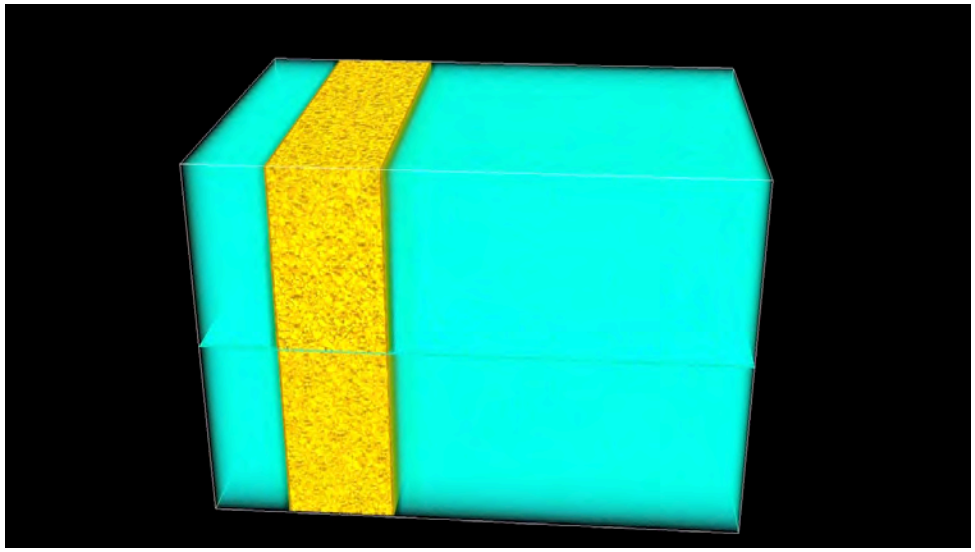
Photo: Keilana via Wikimedia Commons

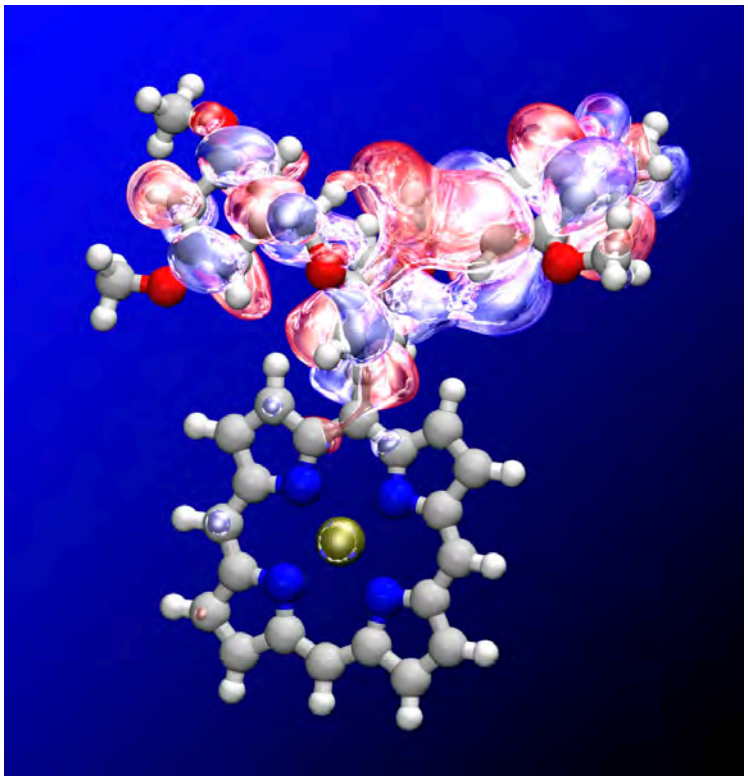
Michael Levitt

Photo: Wikimedia Commons

Arieh Warshel

The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*.





Collaboratory for Advanced Computing & Simulations

- **5.0 trillion-atom molecular dynamics**
- **39.8 trillion electronic degrees-of-freedom quantum molecular dynamics**
- **300+ million core-hrs/yr of computing on a 786,432-core Blue Gene/Q**

cacs.usc.edu

High-End Computing at CACS

- **Won two DOE supercomputing awards to develop & deploy metascalable ("design once, scale on future platforms") simulation algorithms (2017-2022)**

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

- **NAQMD & RMD simulations on full 800K cores**

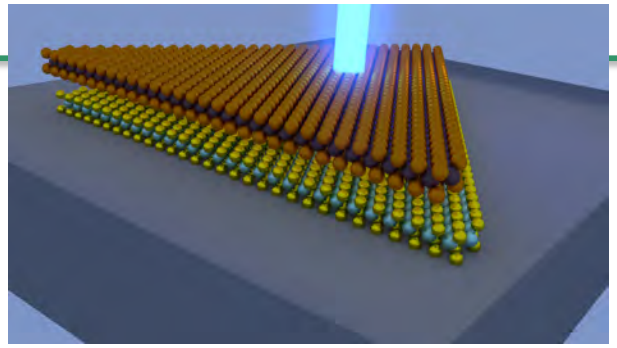
Innovative & Novel Computational Impact on Theory & Experiment

Title: "Petascale Simulations for Layered Materials Genome"

Principal Investigator: Aiichiro Nakano, University of Southern California
Co-Investigator: Priya Vashishta, University of Southern California

786,432-core IBM Blue Gene/Q

AURORA | EARLY SCIENCE PROGRAM



Early Science Projects for Aurora Supercomputer Announced

Metascalable layered materials genome

Investigator: Aiichiro Nakano, University of Southern California

Forthcoming exaflop/s computer, Intel Aurora

- **One of 10 initial simulation users of the next-generation DOE supercomputer**

Exaflop/s = 10^{18} floating-point operations per second

CACS@Aurora in the Global Exascale Race

R. F. Service, *Science* **359**, 617 ('18)

Design for U.S. exascale computer takes shape

Competition with China accelerates plans for next great leap in supercomputing power

By **Robert F. Service**

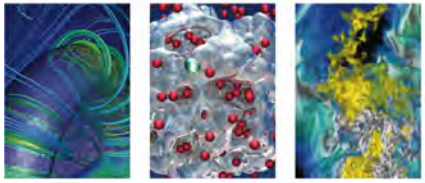
In 1957, the launch of the Sputnik satellite vaulted the Soviet Union to the lead in the space race and galvanized the United States. U.S. supercomputer researchers are today facing their own

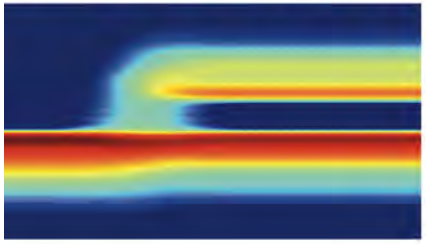
Lemont, Illinois. That's 2 years earlier than planned. "It's a pretty exciting time," says Aiichiro Nakano, a physicist at the University of Southern California in Los Angeles who uses supercomputers to model materials made by layering stacks of atomic sheets like graphene.

pace reflects a change of strategy by DOE officials last fall. Initially, the agency set up a "two lanes" approach to overcoming the challenges of an exascale machine, in particular a potentially ravenous appetite for electricity that could require the output of a small nuclear plant.

Exa(peta)flop/s = 10^{18} (10^{15}) floating-point operations per second

BES





NOVEMBER 3–5, 2015

ROCKVILLE, MARYLAND

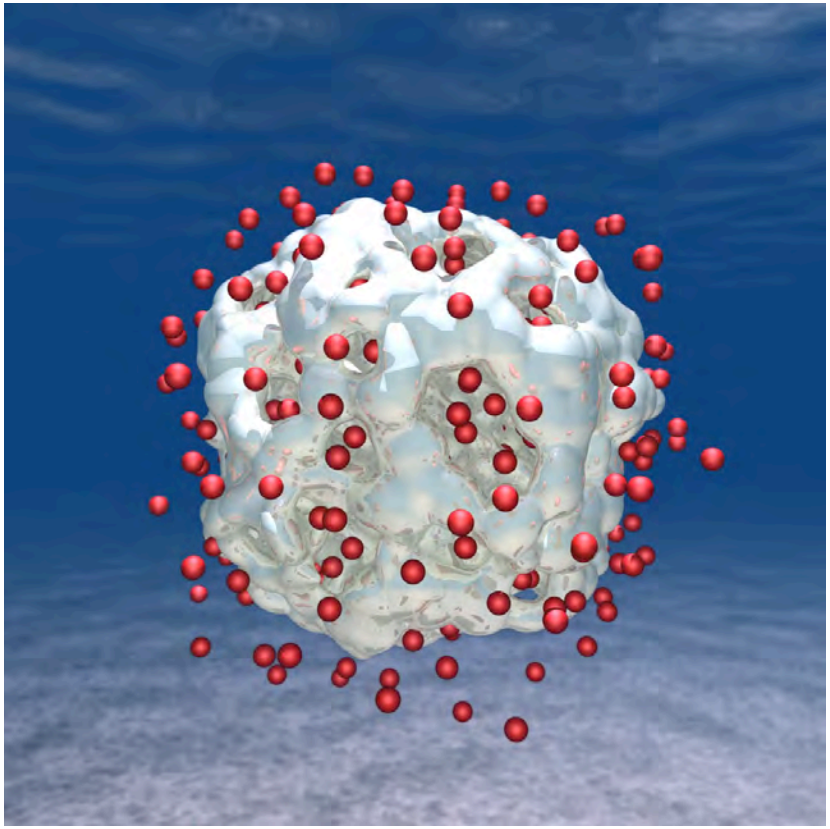
BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

An Office of Science review sponsored jointly by
Advanced Scientific Computing Research and Basic Energy Sciences

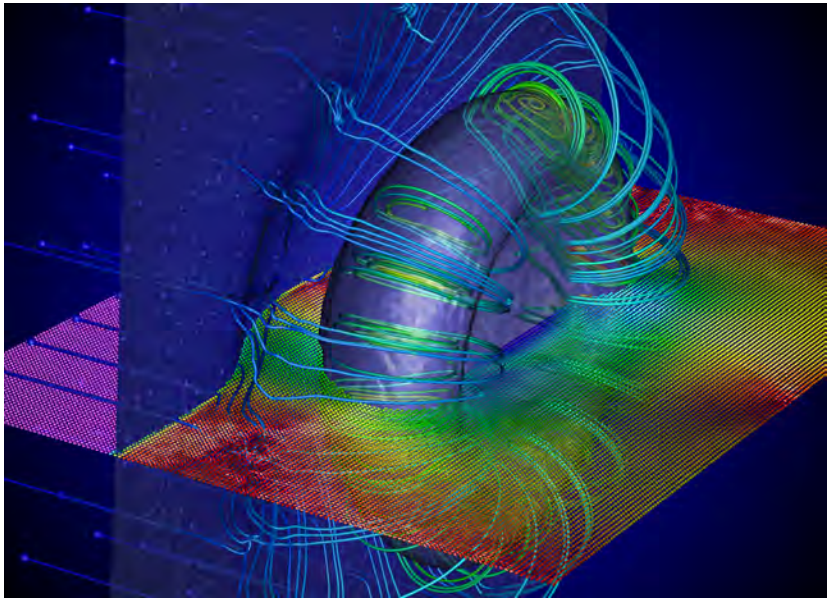
16,661-atom QMD

Shimamura *et al*.,
Nano Lett.
14, 4090 (’14)



10^9-atom RMD

Shekhar *et al*.,
Phys. Rev. Lett.
111, 184503 (’13)



U.S. DEPARTMENT OF ENERGY

MSCS-HPCS Objectives

- **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/

MSCS-HPCS Requirement

A total of **32** units

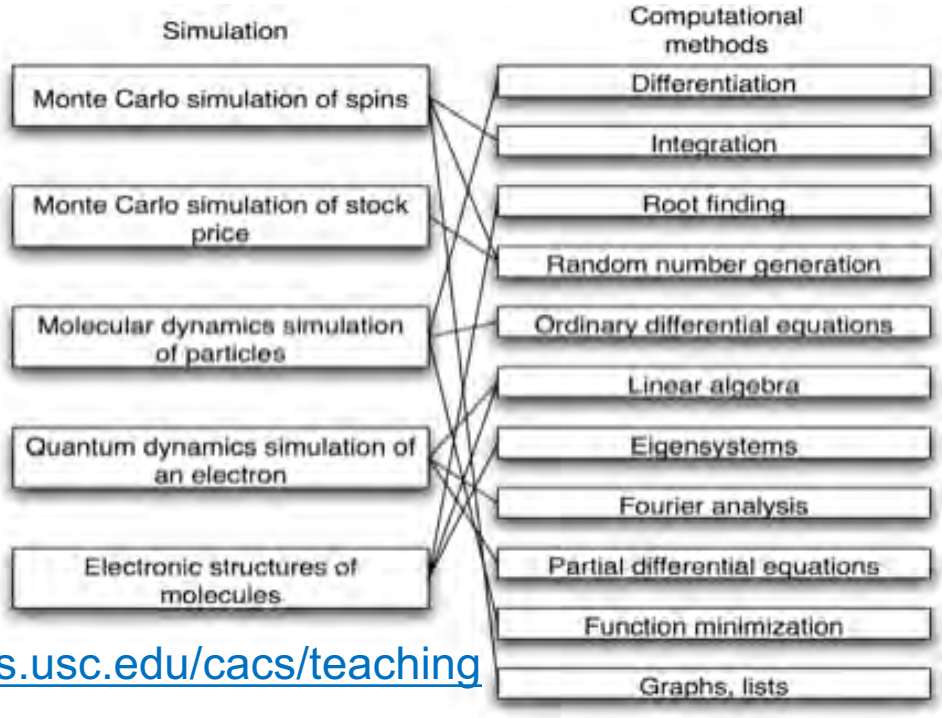
1. Required Core Courses in Computer Science: 3 courses
   CSCI570 (analysis of algorithms)
2. Required Core Course for MSCS-HPCS
   CSCI596 (scientific computing & visualization)
3. Elective Courses for MSCS-HPCS: Total of 3 courses from both tracks (a) & (b)
   (a) Computer Science Track
   CSCI653 (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), ...

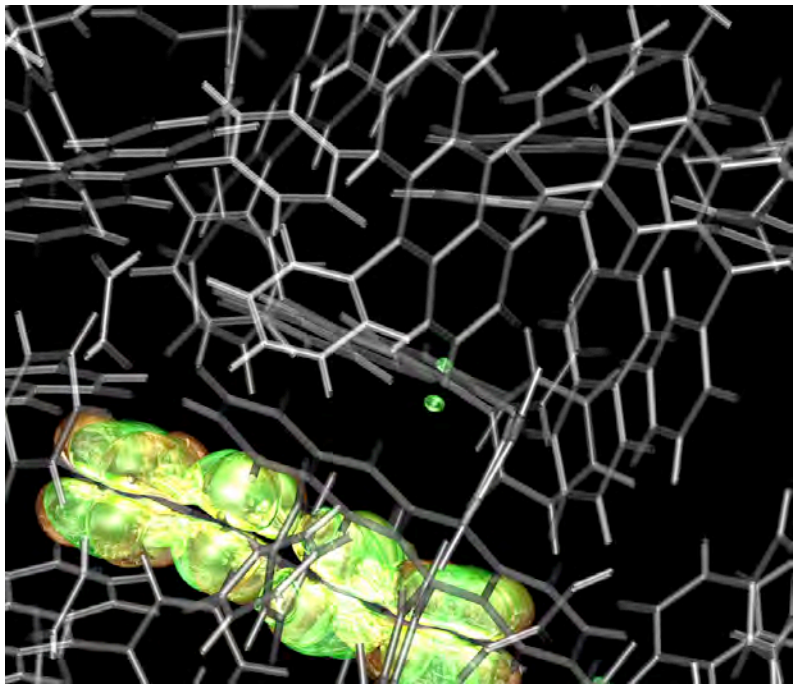
* **CSCI653 can substitute CSCI 596 for core requirement 2; however, once taken CSCI 653, CSCI 596 (its prerequisite) cannot be counted toward degree**

Q: Any addition to 3b?

CACS HPCS Courses

- **CS596: Scientific Computing & Visualization**
  Hands-on training on particle/field simulations, parallel computing, & scientific visualization (MPI, OpenMP, CUDA, OpenGL)
- **CS653: High Performance Computing & Simulations**
  Deterministic/stochastic simulations, scalable parallel/Grid computing, & scientific data visualization/mining in virtual environment
- **Phys516: Methods of Computational Physics**
  Numerical methods in the context of physics simulations





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

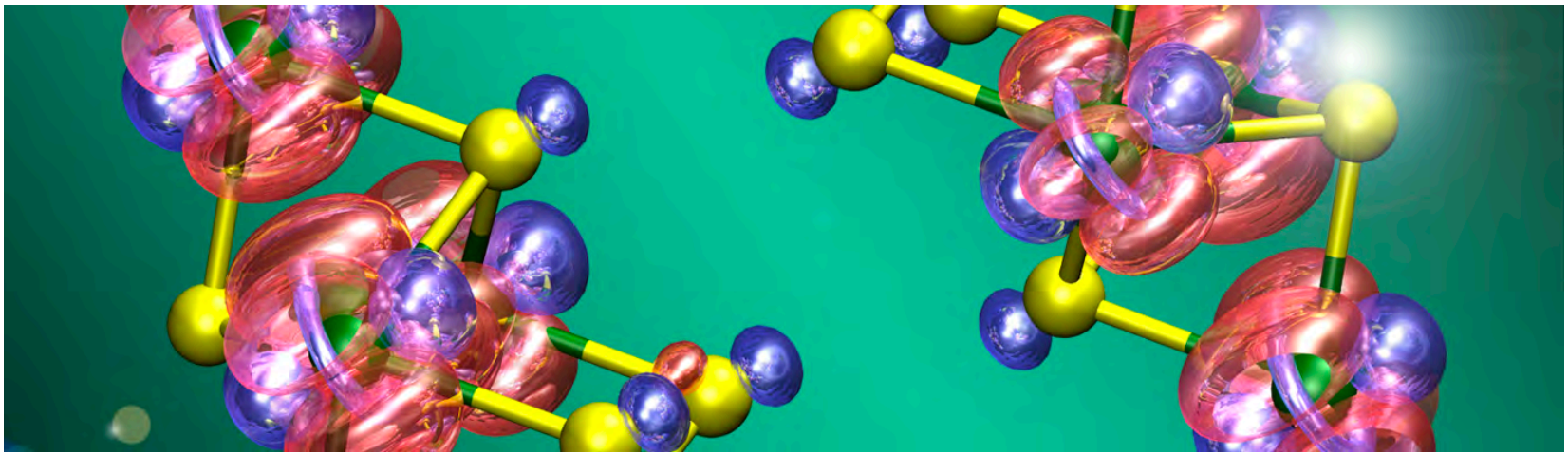
Additional HPCS Course

Detailed lecture notes are available at a USC 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
Prof. Viktor Prasanna

Topics: Parallel computation models, message passing & shared memory paradigms, data parallel programing, performance modeling & optimization, memory system optimization techniques, fine grained computation models & high level design tools for programming parallel platforms, communication primitives, stream programming models, emerging heterogeneous computing & programming models.

This course will study the abstractions for parallel programming as well as provide students with hands-on experience with state-of-the-art parallel computing platforms & tools including large scale clusters, edge devices & data center scale platforms.

- **Count toward MSCS**
- **To replace former CSCI 503 (Parallel Programming)**

CARC Tutorials & Office Hours

Series of tutorials + office hours (T, 2:30-5 pm) by USC Center for Advanced Research Computing (CARC):

- **Introduction to Python, R**
- **Parallel MATLAB**
- **...**

https://carc.usc.edu/education-and-outreach/seminars-and-workshops
https://carc.usc.edu/education-and-outreach/office-hours

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

MS in Quantum Information Science

- **New MS degree in Quantum Information Science (MSQIS) in 2021**
- **Required foundational courses**
  1. **EE 520: Introduction to Quantum Information Processing**
  2. **EE 514: Quantum Error Correction**
  3. **Phys 513: Applications of Quantum Computing**
- **Core—at least two courses from**
  1. **EE 589: Quantum Information Theory**
  2. **Phys 550: Theory of Open Quantum Systems**
  3. **Phys 559: 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**
- **CSCI 596, CSCI 653, Phys 516: Approved electives for MSQIS**

https://catalogue.usc.edu/preview_program.php?catoid=14&poid=17742&returnto=5196

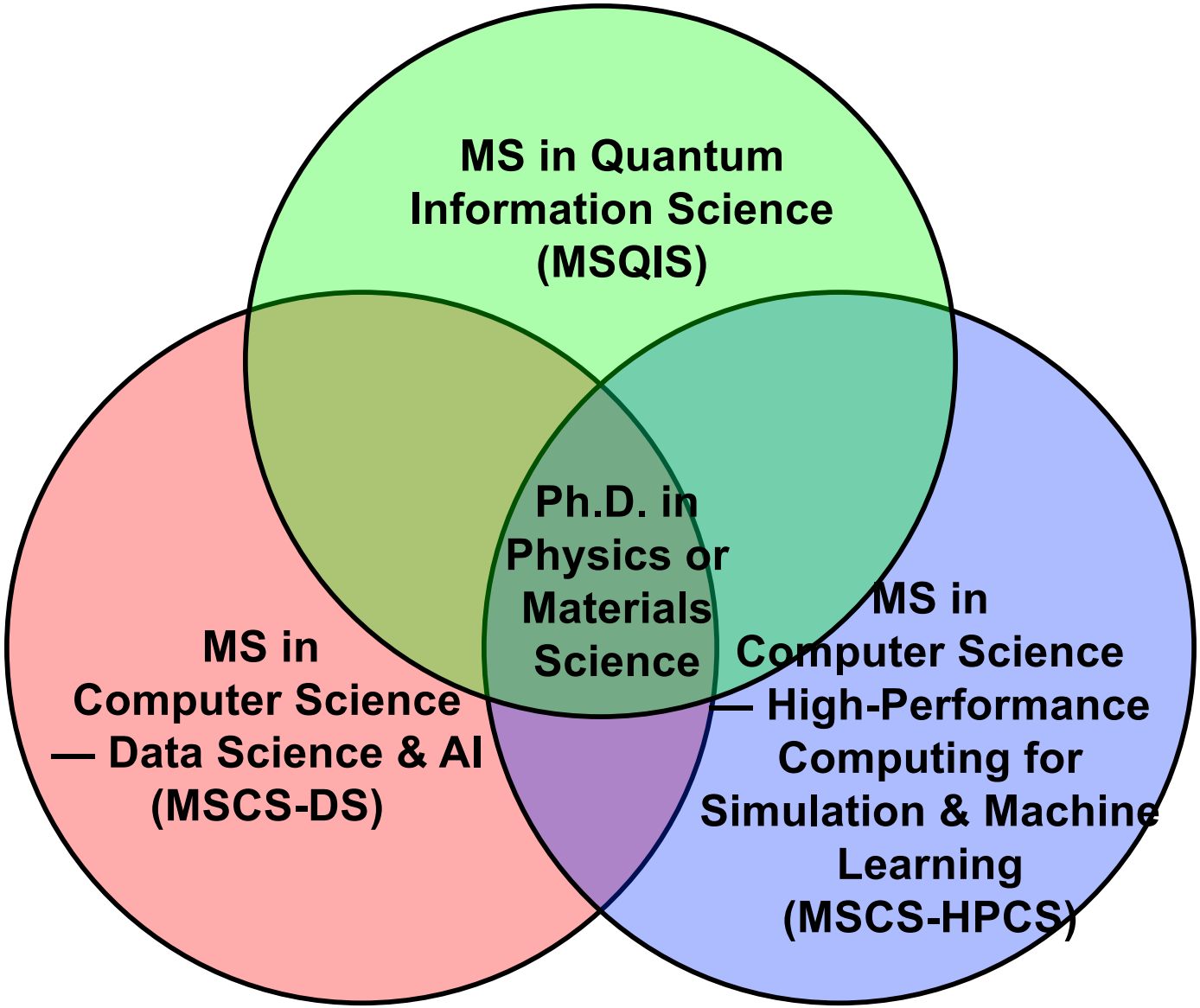
Phys 513: Application of Quantum Computing

Co-taught with Prof. Rosa Di Felice (Spring 2022)

- Training on available quantum computing hardware & respective functional principles, software and algorithms
- Students will have the opportunity to program quantum computers and run sample problems
- **Topics:** Gate-logic quantum computing, adiabatic quantum computing, applications to quantum chemistry & quantum dynamics

Hands-on quantum computing!

Dual-Degree Education at USC



Achieve what is impossible by one discipline alone—only at USC!

NSF Cyber Training Project

CyberMAGICS - Cyber Training on Materials Genome Innovation for Computational Software (2021-2025)

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

- Train a new generation of materials cyberworkforce to solve challenging materials genome problems (*i.e.*, computational design of new materials with desired functionalities) through innovative use of advanced cyberinfrastructure at the exa-quantum-AI nexus
- Develop training modules for a new generation of quantum materials simulator named **AIQ-XMaS (AI & quantum-computing enabled exascale materials simulator)**, which integrates exascalable quantum, reactive and neural-network molecular dynamics simulations with unique AI and quantum-computing capabilities to study a wide range of materials and devices of high societal impact such as optoelectronics and health (pandemic preparedness)

CSCI 596 & 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