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
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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

* petaflop/s = $10^{15}$ mathematical operations per second
The Nobel Prize in Chemistry 2013

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, 8.6 petaflop/s 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)
- NAQMD & RMD simulations on full 800K cores

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

786,432-core IBM Blue Gene/Q

Early Science Projects for Aurora
Supercomputer Announced
Metascalable layered materials genome
Investigator: Aiichiro Nakano, University of Southern California

- One of 10 initial simulation users of the next-generation DOE supercomputer
Exaflop/s = $10^{18}$ floating-point operations per second
CACS@A21 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 challenges.

Lemont, Illinois. That’s 2 years earlier than planned. “It’s a pretty exciting time,” says Alichiro 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
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)

10⁹-atom RMD
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? Please type in Chat
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

http://cacs.usc.edu/teaching.php
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".

http://cacs.usc.edu/education/cs699-lecture.html
CARC Tutorials & Office Hours

Series of tutorials + office hours (T, 2:30-5 pm, Zoom) 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
New MS degree in Quantum Information Science (MSQIS) coming to USC 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 XXX: Quantum Information Theory
2. Phys XXX: Open Quantum Systems
3. Phys 559: Quantum Devices

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
Dual-Degree Education at USC

MS in Quantum Information Science (MSQIS)

MS in Computer Science — Data Science & AI (MSCS-DS)

Ph.D. in Physics or Materials Science

MS in Computer Science — High-Performance Computing for Simulation & Machine Learning (MSCS-HPCS)

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