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

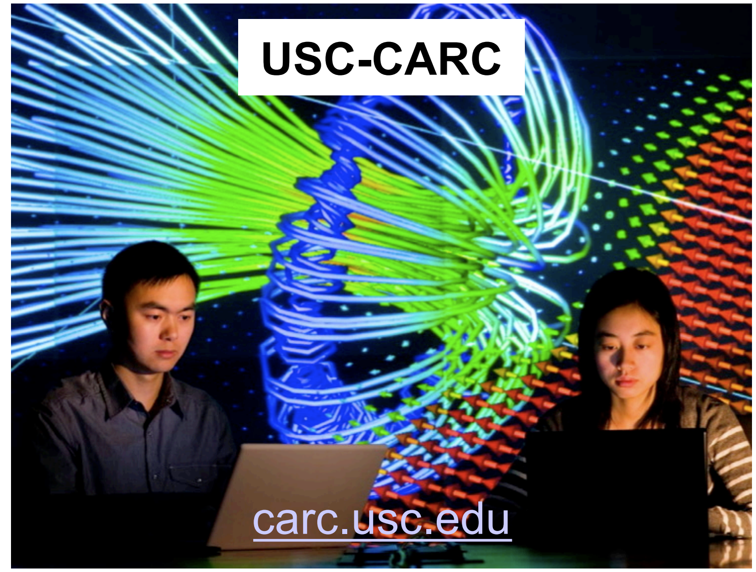
https://www.cs.usc.edu/academic-programs/masters/high-performance-computing-simulations

Computational Sciences at USC

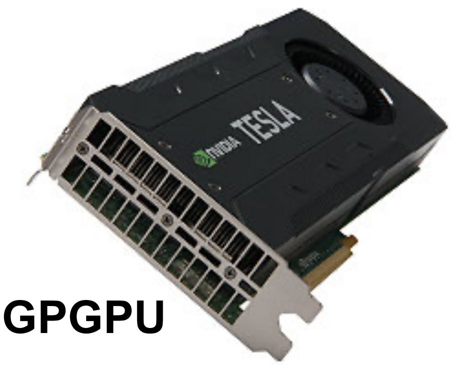
Aiichiro Nakano

Email: anakano@usc.edu

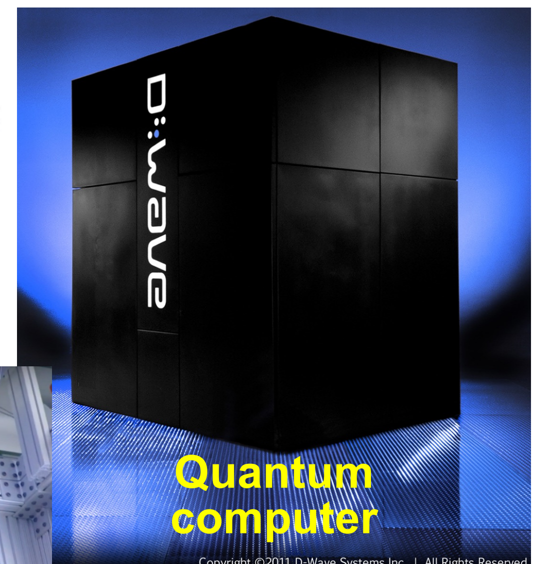
High Performance Computing

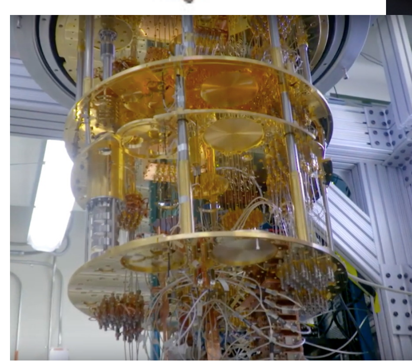


- *USC CARC (Center for Advanced Research Computing)*: **21,000 CPU-cores & 200+ GPUs**
- *USC ISI (Information Sciences Institute)*: **1,098-qubit D-Wave quantum computer**



GPGPU





QPU

* exaflop/s = 10^{18} mathematical operations per second

Computational Sciences at USC

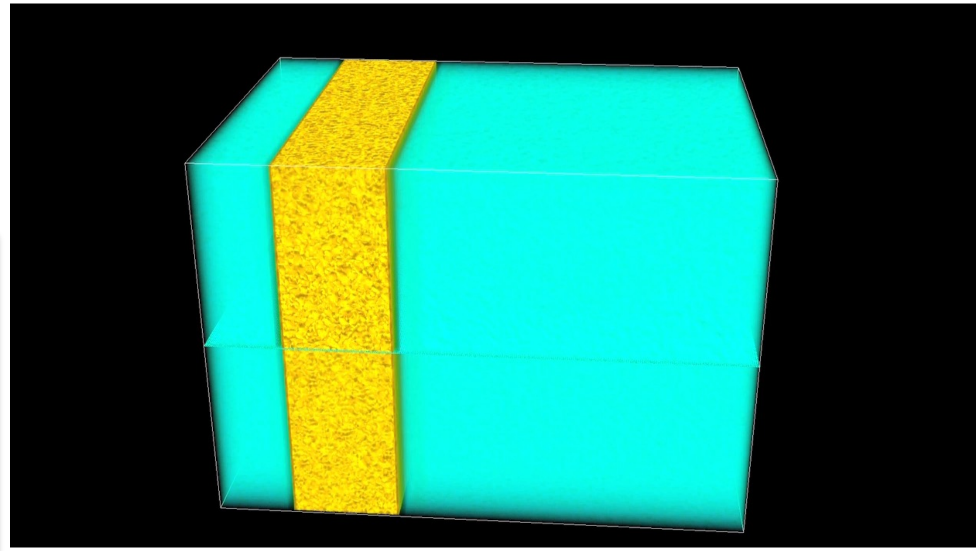
The Nobel Prize in Chemistry 2013

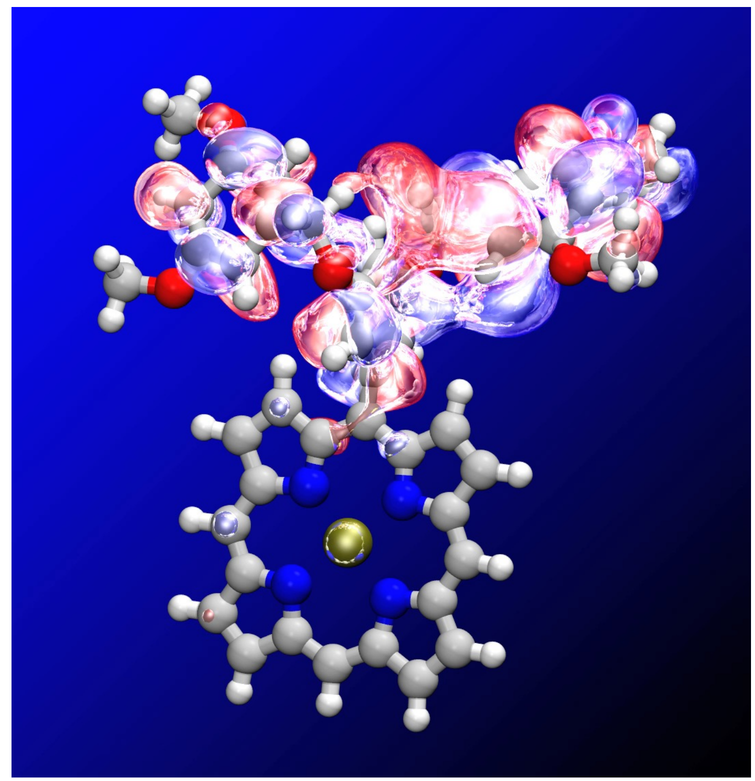
© Nobel Media AB
Martin Karplus

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 786,432 cores**

cacs.usc.edu

Current & Future Supercomputing

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

786,432-core IBM Blue Gene/Q
281,088-core Intel Xeon Phi
560-node (2,240-GPU) AMD/NVIDIA Polaris

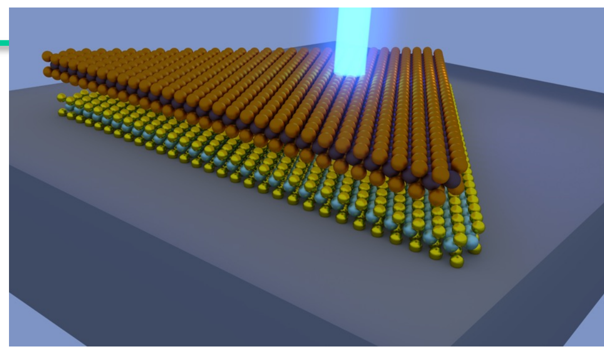
U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

- **Atomistic simulations on million cores (pre-exascale)**

Innovative & Novel Computational Impact on Theory & Experiment

Title: AI-Guided Exascale Simulations of Quantum Materials Manufacturing and Control
PI and Co-PIs: Aiichiro Nakano–PI, Rajiv K. Kalia, Ken-ichi Nomura, Priya Vasishta

AURORA | EARLY SCIENCE PROGRAM



Early Science Projects for Aurora Supercomputer Announced

Metascalable layered materials genome

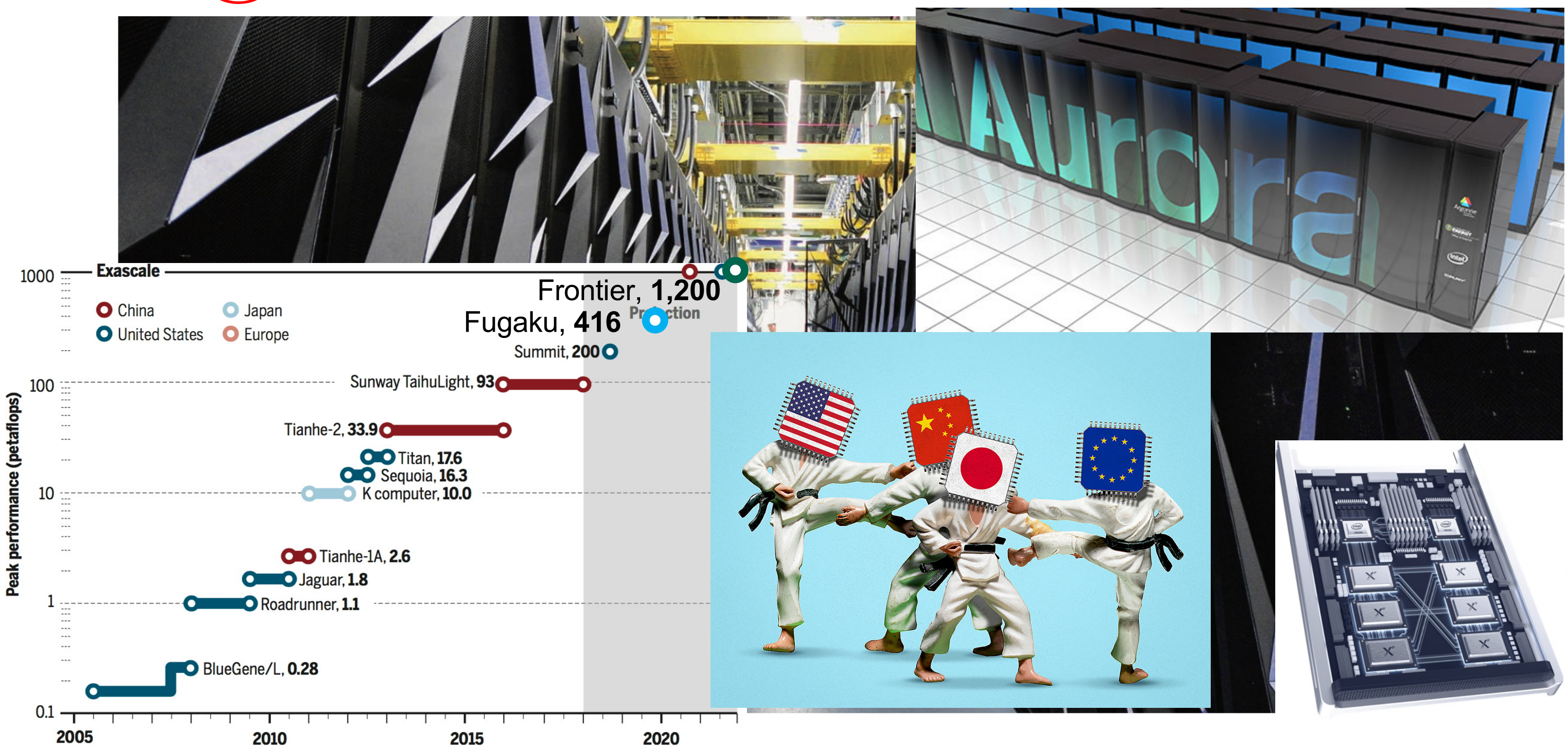
Investigator: Aiichiro Nakano, University of Southern California

2 exaflop/s
Intel Aurora (forthcoming)

exaflop/s = 10^{18} mathematical operations per second

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

CACS@Aurora in the Global Exascale Race



SUPERCOMPUTING

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

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

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.

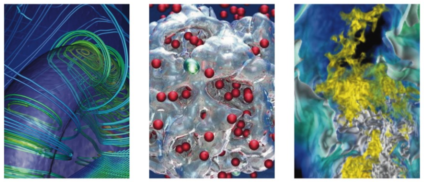
https://www.tomshardware.com/news/two-chinese-exascale-supercomputers

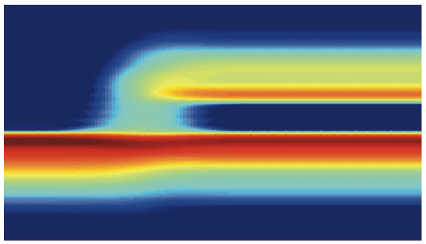
Exa-leadership

BES

BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW



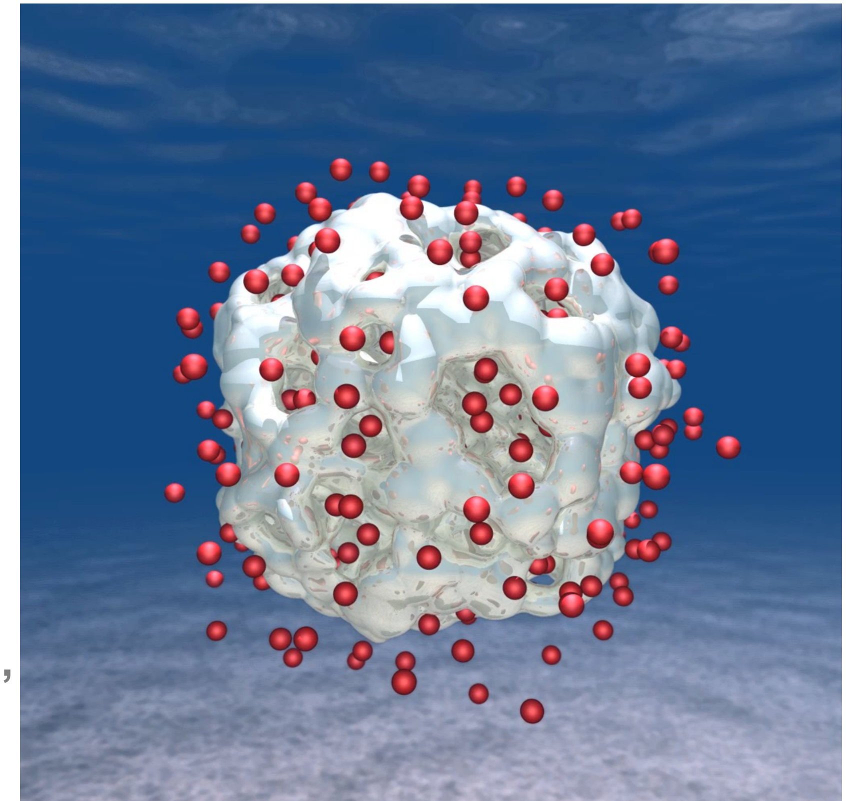


An Office of Science review sponsored jointly by
Advanced Scientific Computing Research and Basic Energy Sciences

NOVEMBER 3–5, 2015

ROCKVILLE, MARYLAND

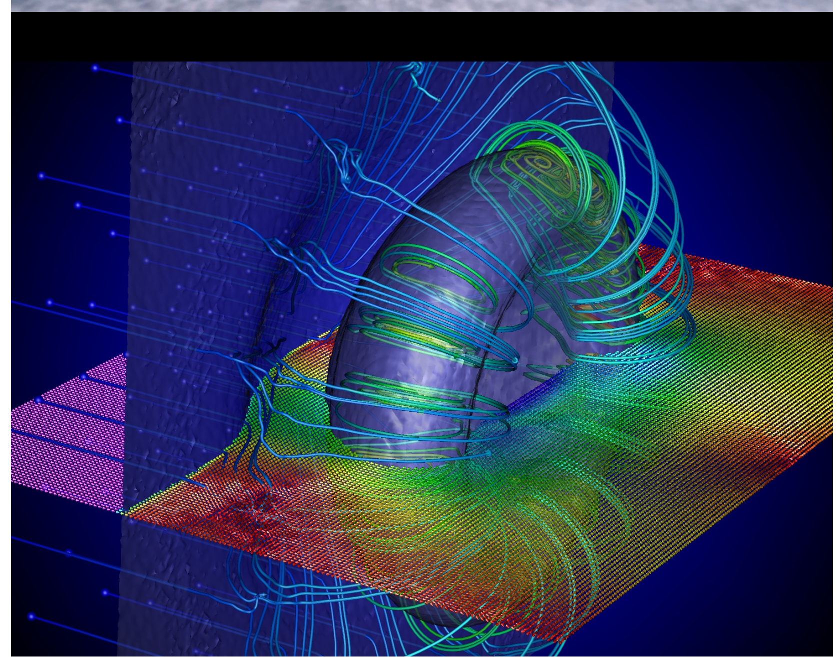
U.S. DEPARTMENT OF ENERGY



16,661-atom QMD

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

On-demand hydrogen production from water



10^9-atom RMD

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

Fluid dynamics atom-by-atom

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)

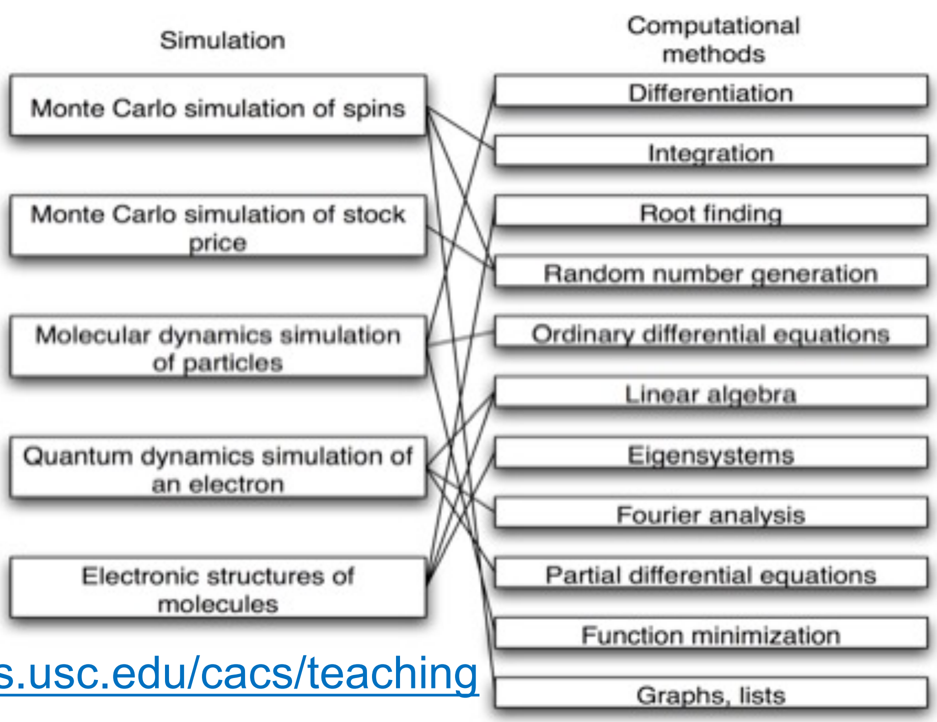
   (b) Computational Science/Engineering Application Track
   AME535 (comp fluid dynamics), CE529 (finite element), CHE502 (numerical transport),
   EE553 (comp optimization), EE653 (multithreaded arch), EE657 (parallel processing),
   EE659 (network), Math501 (numerical analysis), MAS575 (atomistic simulation),
   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**

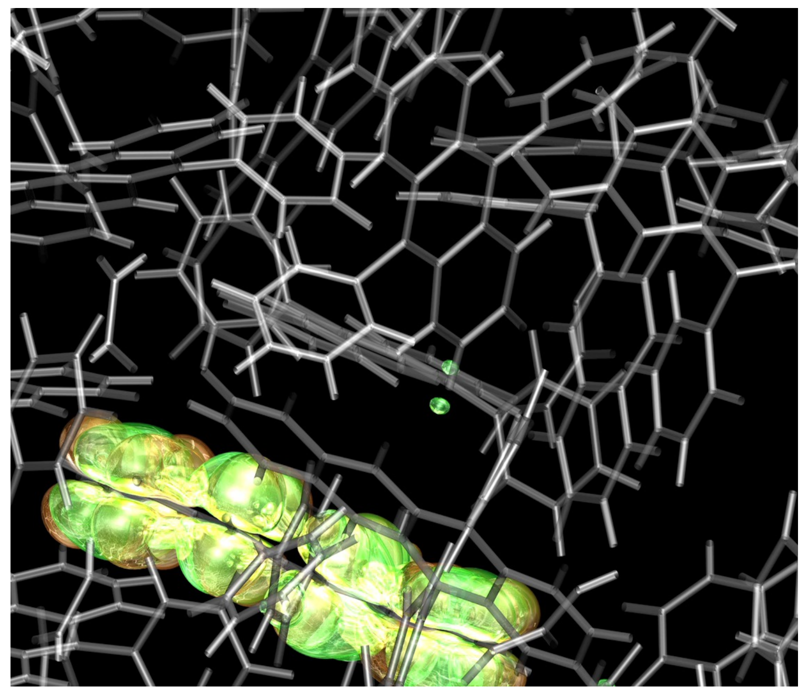
Q: Any addition to 3b?

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



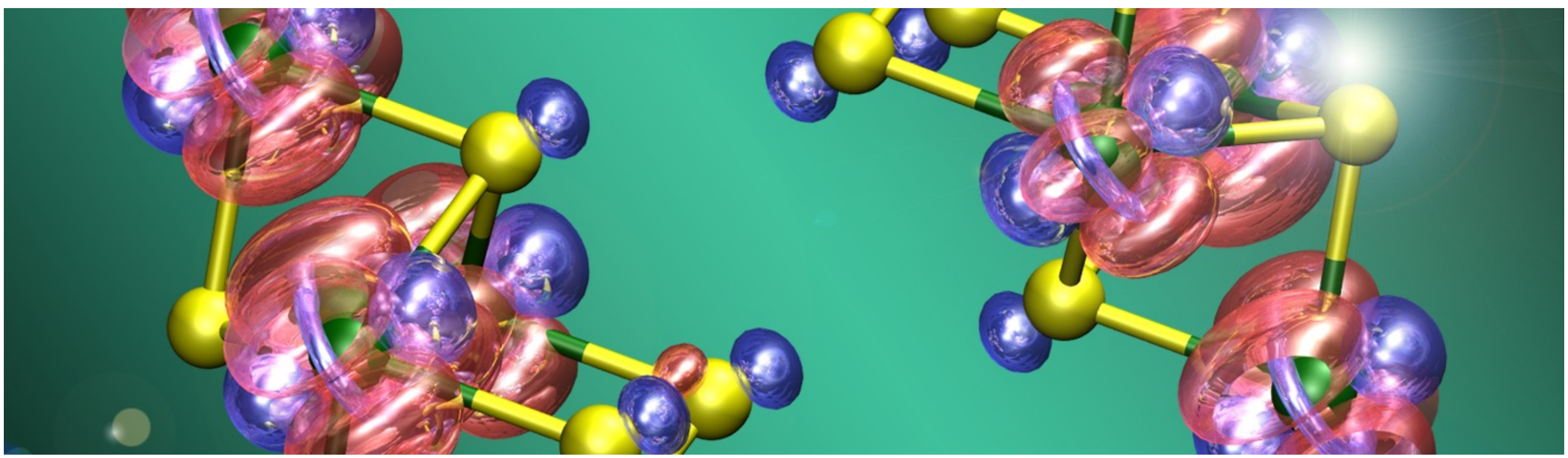
Additional HPCS Course

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 (EE 451): 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://www.carc.usc.edu/education-and-resources/workshops
https://www.carc.usc.edu/education-and-resources/office-hours

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

Changing Computing Landscape for Science

Post-exascale Computing for Science

Compute Cambrian explosion

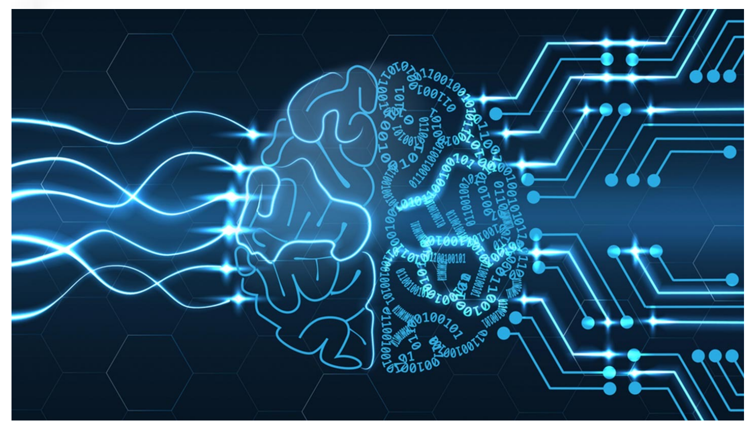
AI for Science

DOE readies multibillion-dollar AI push

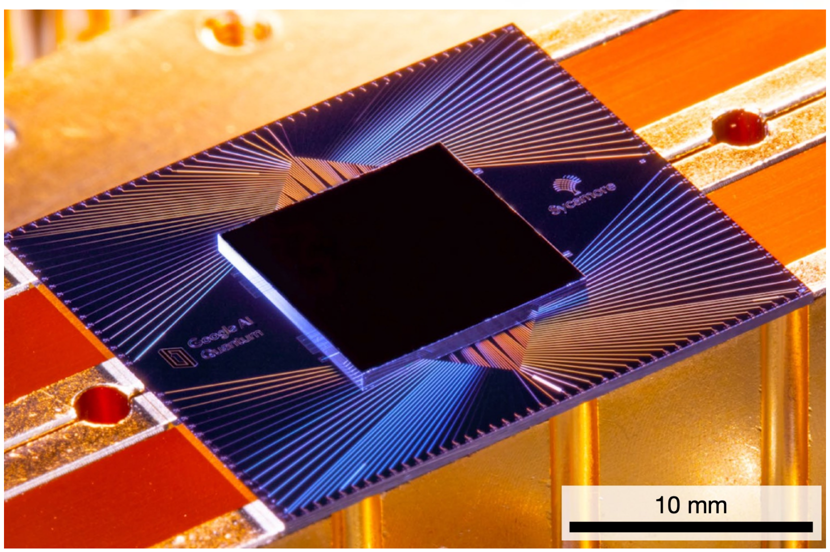
U.S. supercomputing leader is the latest big backer in a globally crowded field

By **Robert F. Service**, *in Washington, D.C.*

Science **366**, 559 (Nov. 1, '19)



Quantum Computing for Science

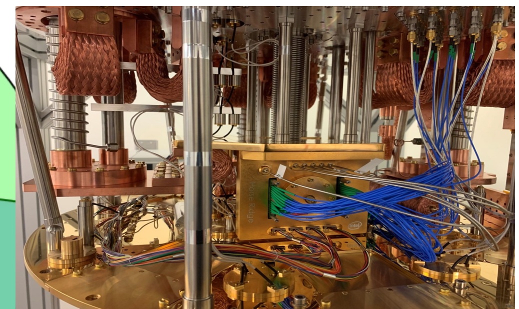


Use all to advance science!

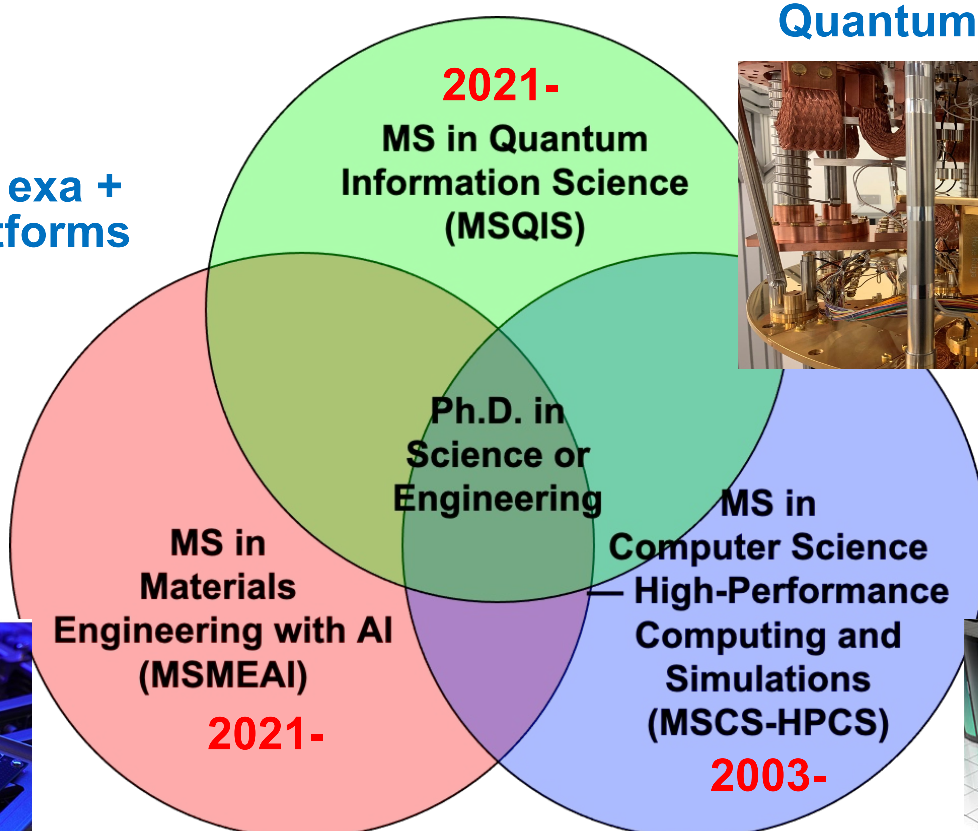
Training Cyber Science Workforce

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

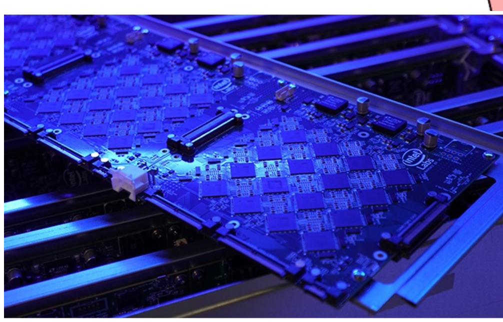
Horse Ridge II
Quantum computer



Cybertraining on exa + quantum + AI platforms



Neuromorphic
Pohoiki Springs



Exascale
Aurora

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: Applications of Quantum Computing

- Core—at least two courses from
  1. EE 589: Quantum Information Theory
  2. Phys 550: Open Quantum Systems
  3. Phys 559: Quantum Devices
  4. Phys 660: Quantum Information Science & Many-Body Physics

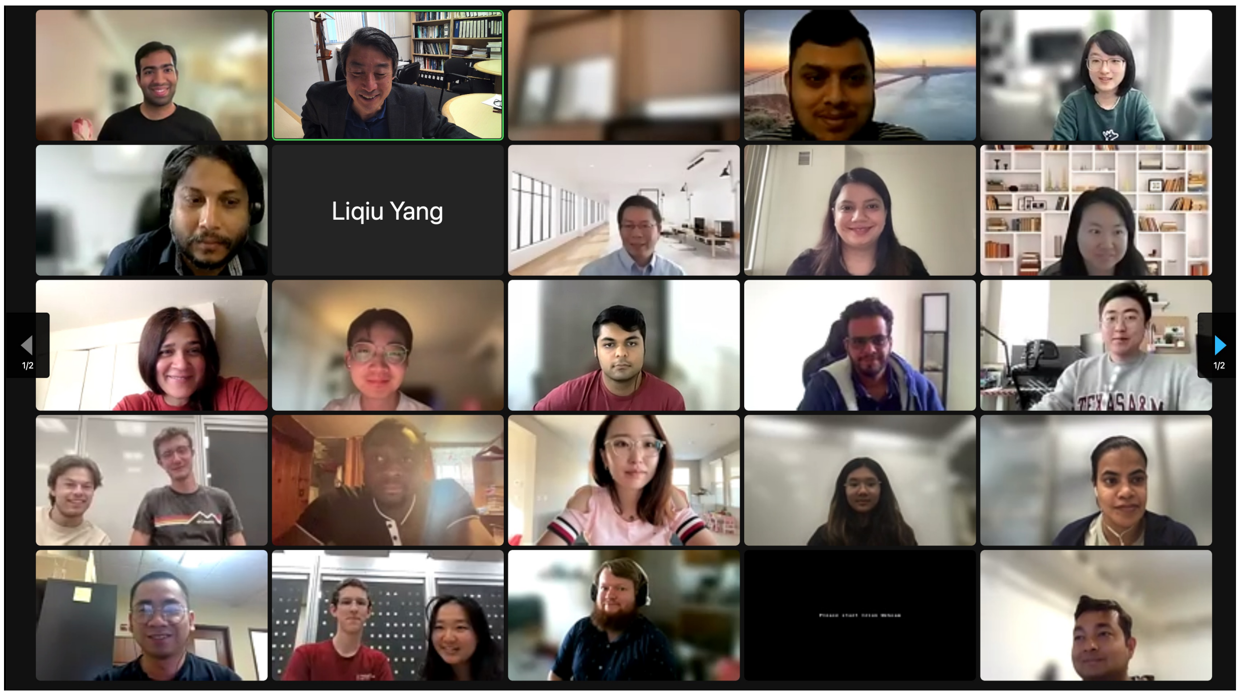
- Phys 513: Application of Quantum Computing (co-taught with Prof. Rosa Di Felice)—quantum simulations on quantum circuits & adiabatic quantum annealer (syllabus)

- CSCI 596 (this course): Elective for MSQIS

USC-Howard Cybertraining

CyberMAGICS: Cyber Training on Materials Genome Innovation for Computational Software

- Train a new generation of materials cyberworkforce, who will solve challenging materials genome problems through innovative use of advanced cyberinfrastructure at the exa-quantum-AI nexus



Second CyberMAGICS workshop
(June 29 – July 1, 2023)

$1M NSF CyberTraining (2021-25) project

Nakano, Nomura, Vashishta (USC); Dev, Wei (Howard)

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

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