

# Big Picture: CSCI 596 & Cyber-science Nexus

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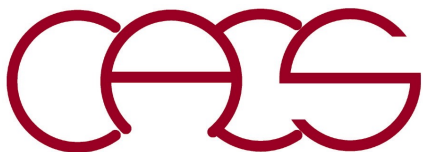
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**Aiichiro Nakano**

*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](mailto:anakano@usc.edu)**

**Science at the nexus of post-exaflop/s computing,  
quantum computing, and AI at USC**



# Changing Computing Landscape for Science

## Post-exascale Computing for Science



Compute Cambrian explosion



## AI for Science

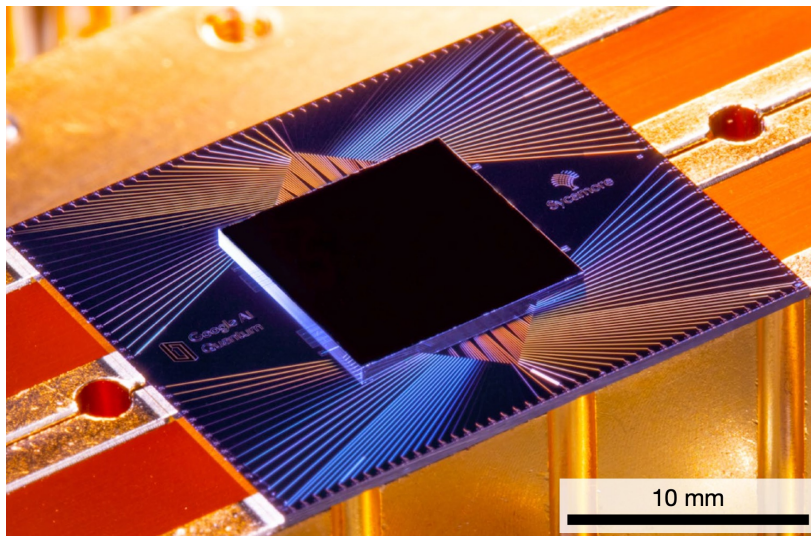
### DOE readies multibillion- dollar AI push

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!**



**Why cyber-science nexus at USC?**

# **USC Frontiers of Computing**

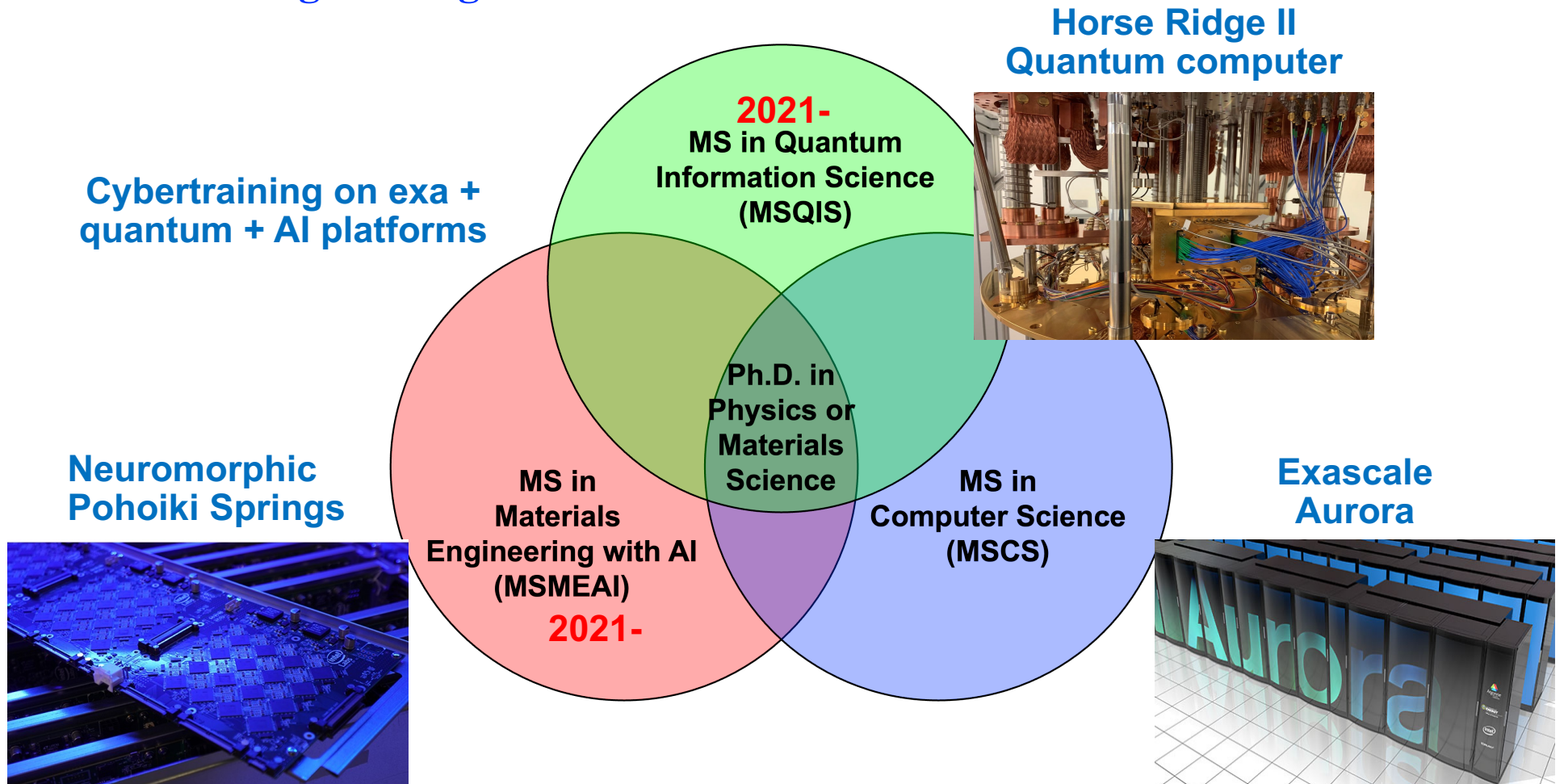
**USC launches computing into the next frontier**

<https://computing.usc.edu>

- **\$1 billion+, 10 years initiative**
- **New School of Advanced Computing:** <https://sac.usc.edu>
- **30 senior & 60 junior & mid-level hires**

# Training Cyber-Science Workforce

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

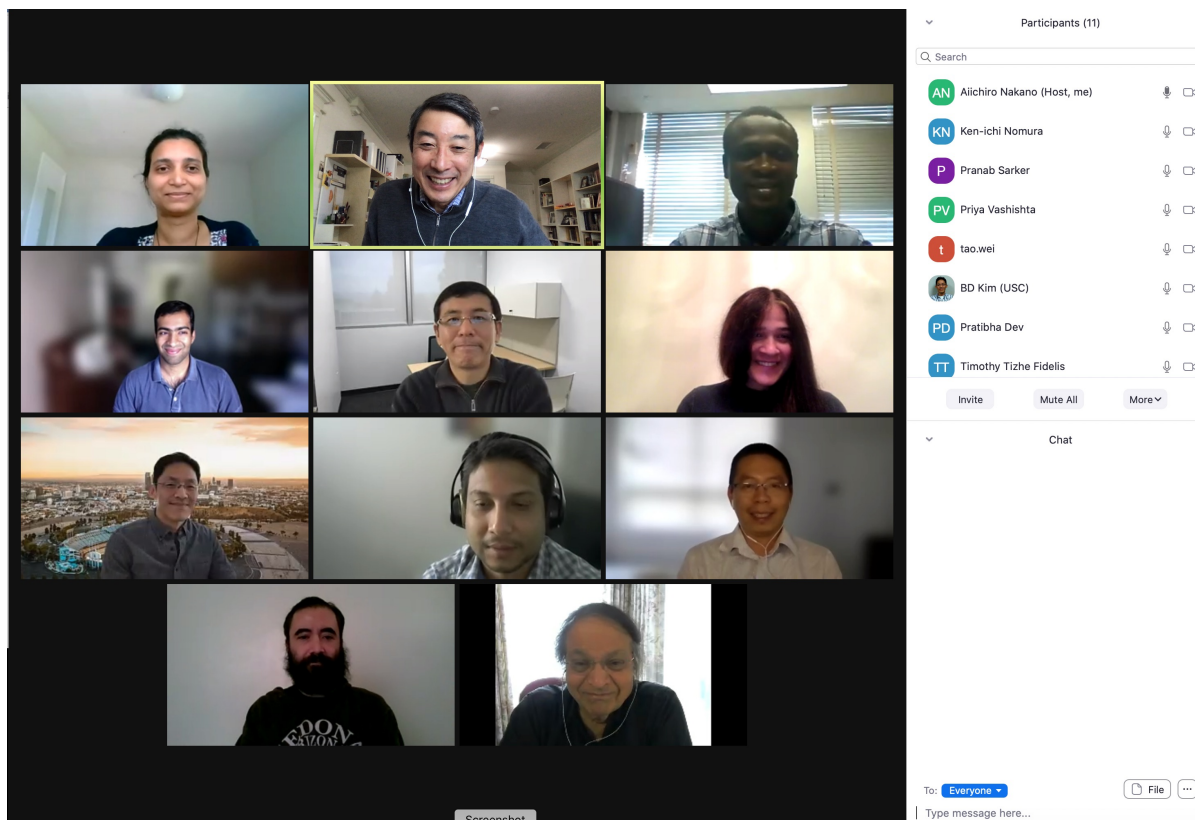




# USC-Howard Cybertraining

## CyberMAGICS: Cyber Training on Materials Genome Innovation for Computational Software

- This project trains 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*

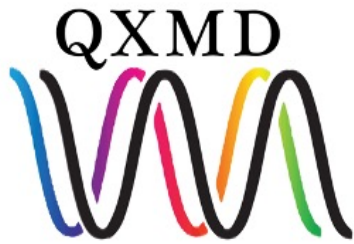


**\*Materials genome:  
Applying informatics to  
design new materials  
significantly faster than  
the conventional trial-and-  
error approach**

**NSF CyberTraining (2021-25) project**  
**Nakano, Nomura, Vashishta (USC); Dev, Wei (Howard)**

# AIQ-XMaS Software Suite

AI & Quantum-Computing Enabled Exa Quantum Materials Simulator



Nonadiabatic quantum molecular dynamics

GEARS



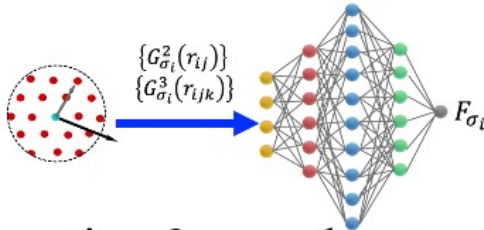
Augmented-reality user interface

MISTIQS



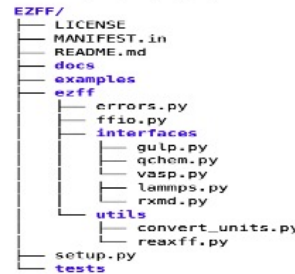
Quantum many-body dynamics on quantum computers

RXMD-NN



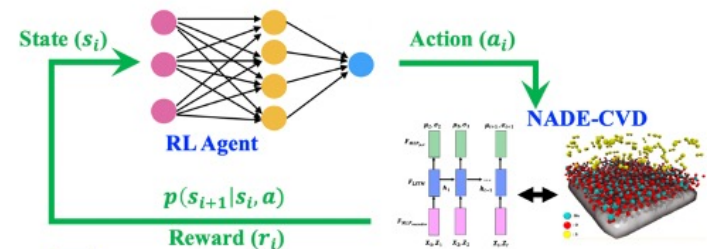
Reactive & neural-network molecular dynamics

EZFF



Easy force-field parameterization & uncertain quantification

MAITAI

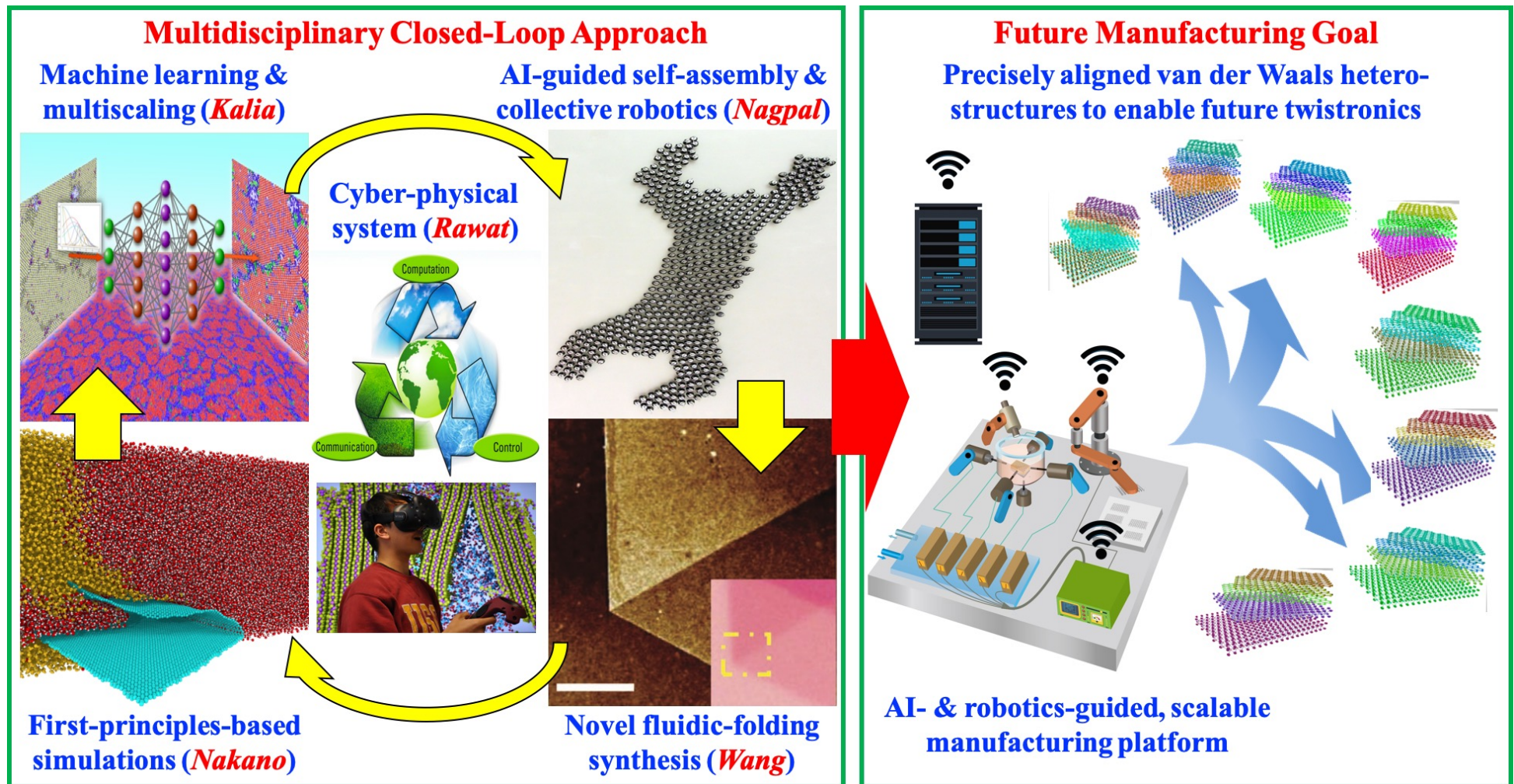


AI tools for materials design



# USC-Howard Future Manufacturing

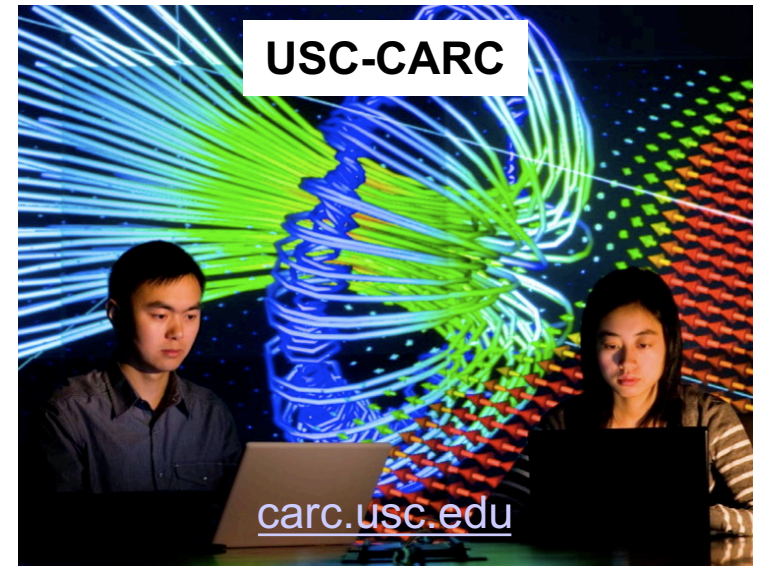
*FMRG: Artificial Intelligence Driven Cybermanufacturing of Quantum Material Architectures*  
\$3.75M NSF project (2020-2025)



Nagpal (Princeton); Kalia, Nakano, Wang, Yang (USC); Rawat (Howard)

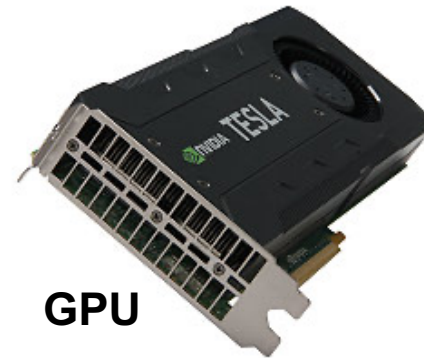


# High Performance Computing

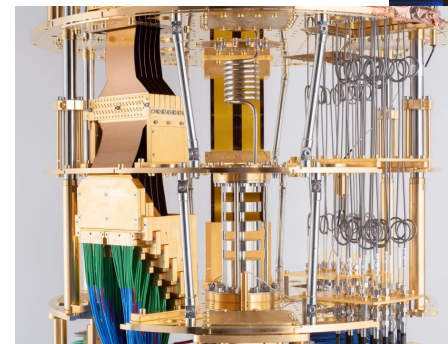


- **USC CARC (Center for Advanced Research Computing): 21,000 CPU-cores & 200+ GPUs**
- **USC ISI (Information Sciences Institute): 1,098-qubit D-Wave quantum computer**
- **USC-IBM Quantum Innovation Center: Cloud access to 100+ qubit IBM quantum computers (2024-)**

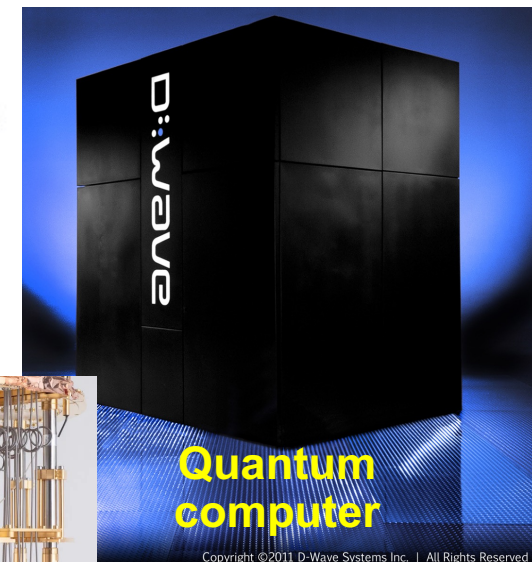
\* exaflop/s =  $10^{18}$  mathematical operations per second



GPU



QPU





# Computational Sciences at USC

## The Nobel Prize in Chemistry 2013



© Nobel Media AB  
Martin Karplus



Photo: Keilana via  
Wikimedia Commons  
Michael Levitt



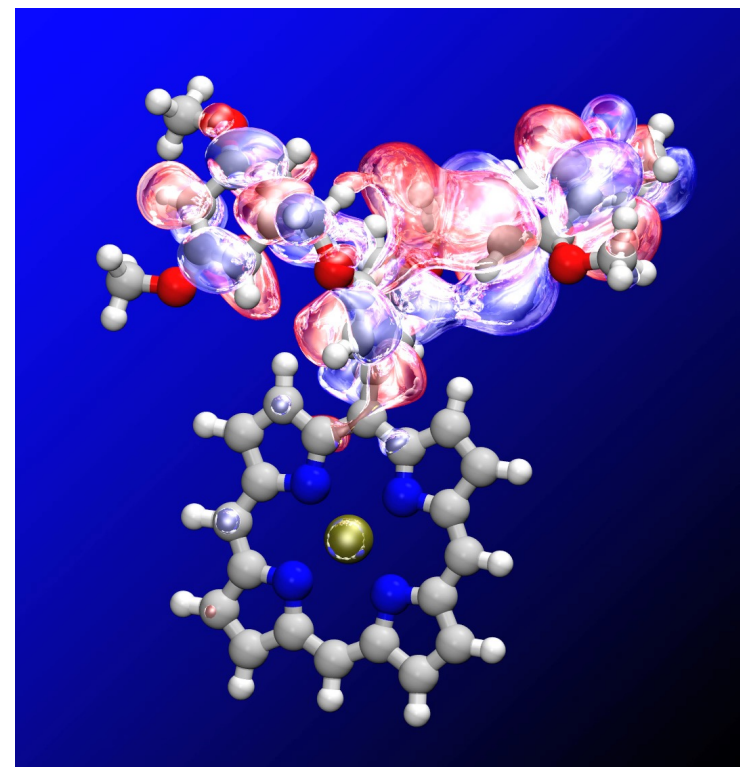
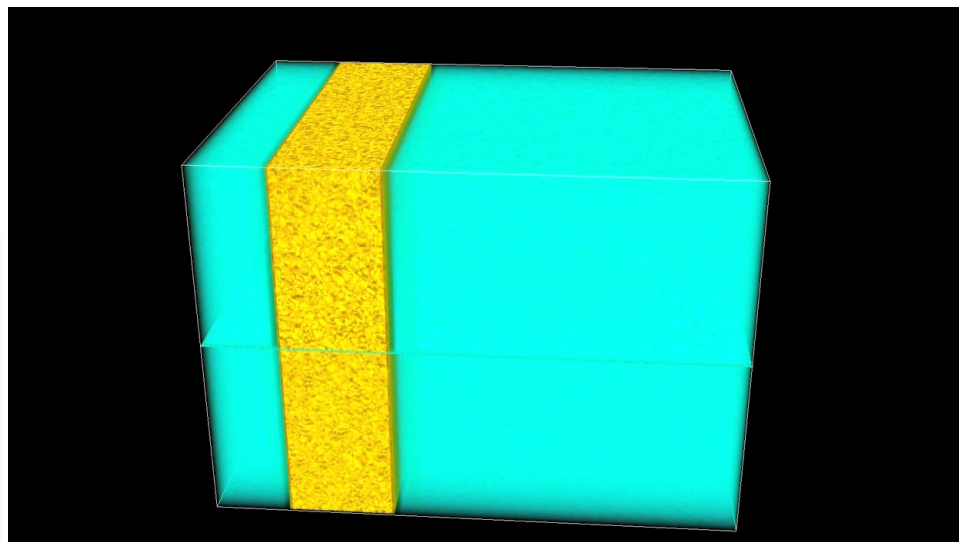
Photo: Wikimedia  
Commons  
Arieh Warshel

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
- 40 trillion electronic degrees-of-freedom quantum molecular dynamics
- 300+ million core-hrs/yr of computing on 786,432 cores

[cacs.usc.edu](http://cacs.usc.edu)



# Current & Future Supercomputing

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



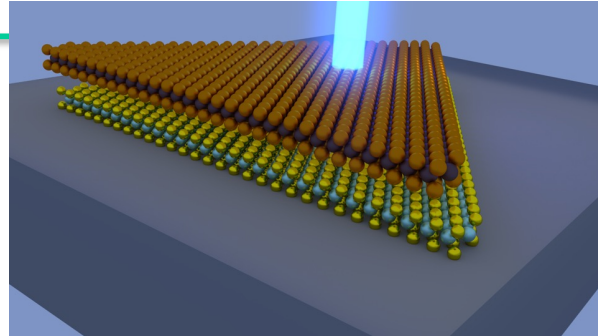
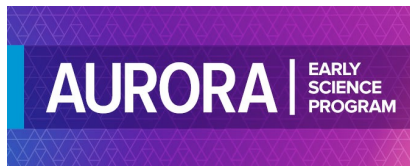
- Atomistic simulations on million cores (pre-exascale)

**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



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



Early Science Projects for Aurora  
Supercomputer Announced

**Metascalable layered materials genome**

*Investigator: Aiichiro Nakano, University of Southern California*



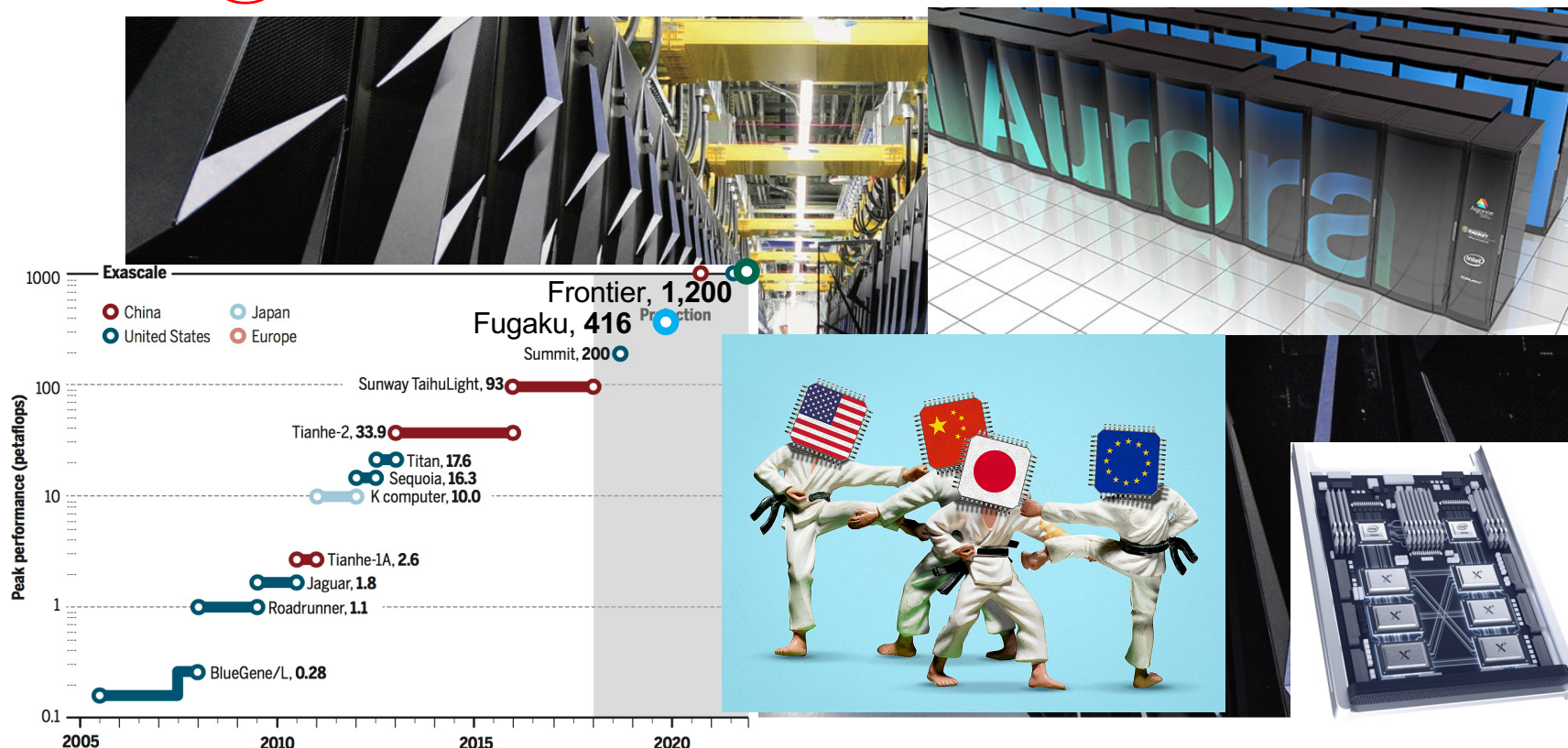
**1.01 exaflop/s**  
**Intel Aurora**

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>



# BES

# Exa-leadership

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)

*On-demand hydrogen  
production from water*

### 10<sup>9</sup>-atom RMD

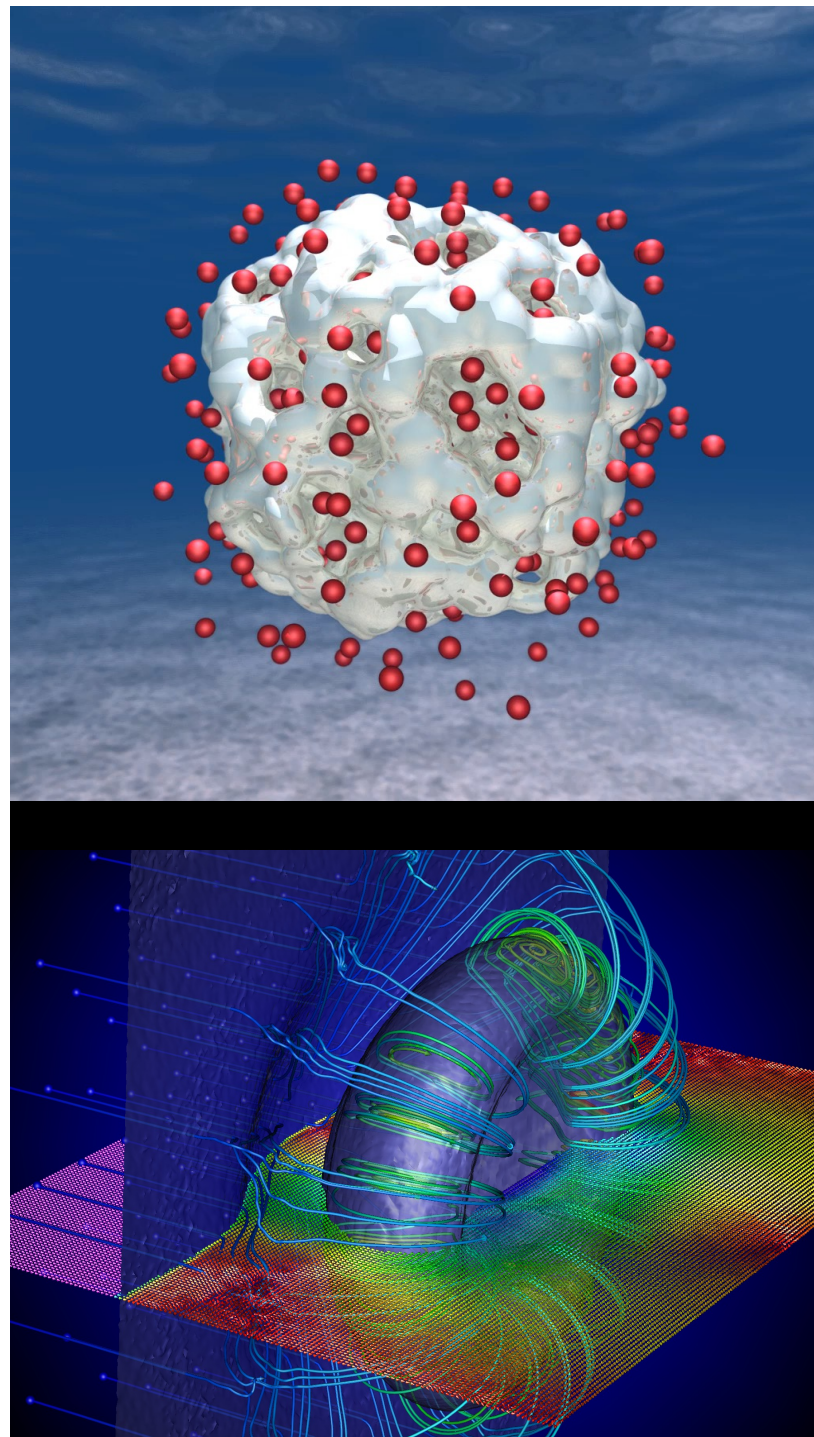
Shekhar *et al.*,  
*Phys. Rev. Lett.*

111, 184503 ('13)

*Fluid dynamics  
atom-by-atom*

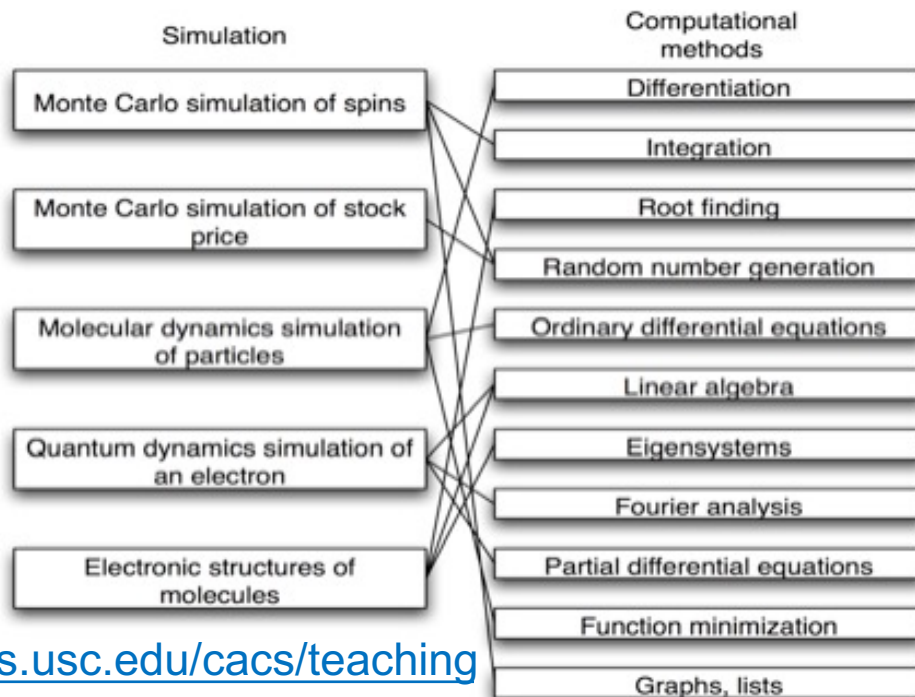
NOVEMBER 3-5, 2015

ROCKVILLE, MARYLAND

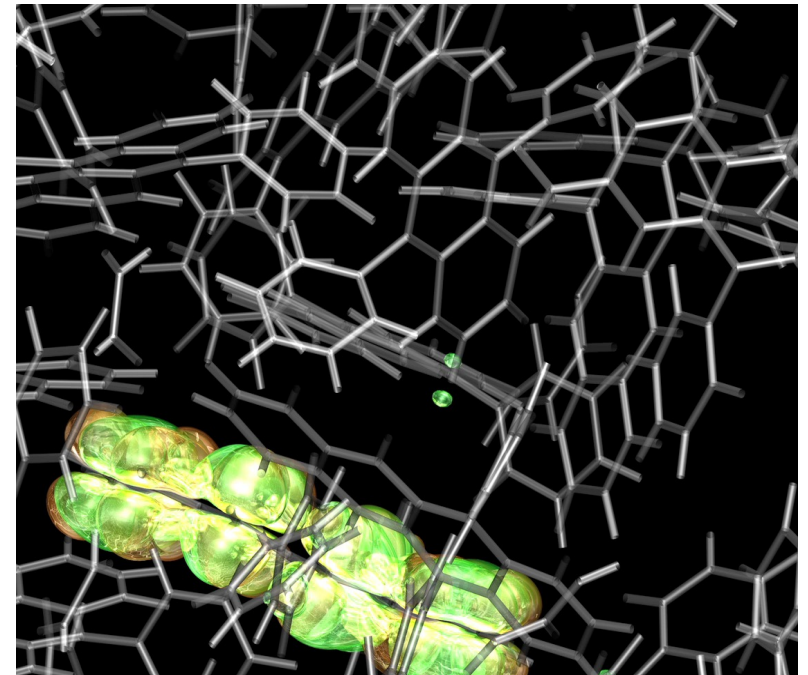


# CACS HPCS Courses

- **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

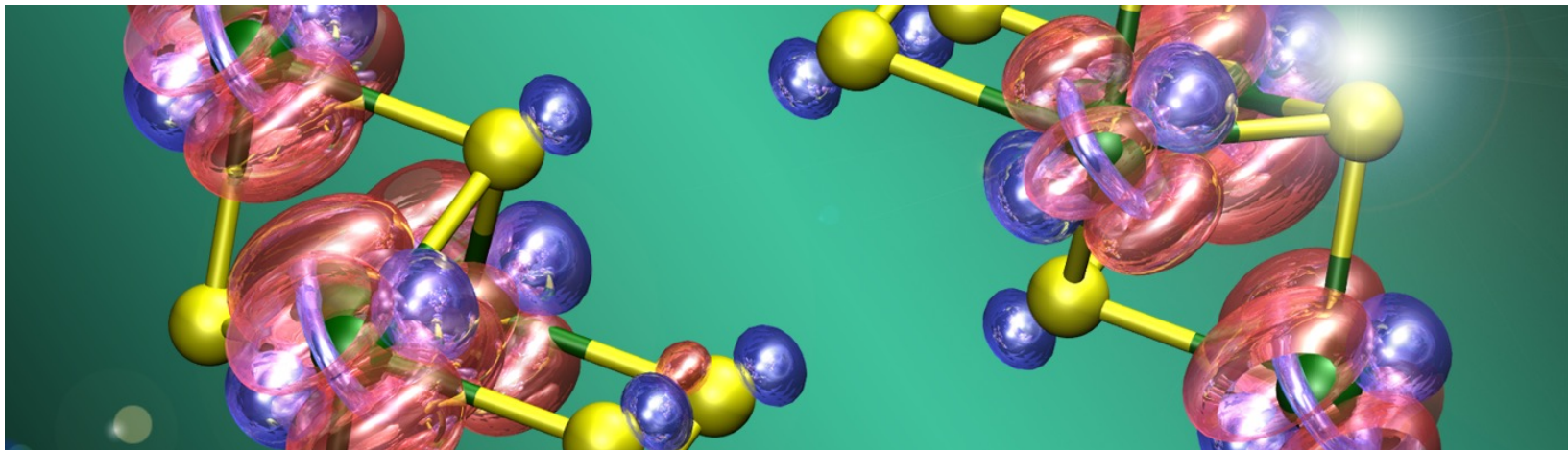
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Detailed lecture notes are available at a USC course home page

## PHYS 760: 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/phys760.html>

# Related Course

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## **EE 451: Parallel Programming** **Prof. Viktor Prasanna**

**Topics:** Parallel computation models, message passing & shared memory paradigms, data parallel programming, 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.

- **To replace former CSCI 503 (Parallel Programming)**



# CARC Tutorials & Office Hours

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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/services/education/workshops>

<https://www.carc.usc.edu/user-support/office-hours-and-consultations.html>

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

# MS in Quantum Information Science

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- 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**