Big Picture: CSCI 596 & Cyber-science Nexus

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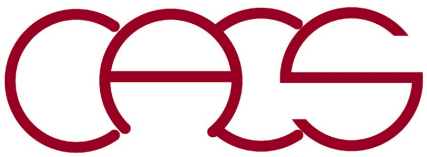
Science at the nexus of post-exaflop/s computing, quantum computing, and AI at USC



Changing Computing Landscape for Science

Post-exascale Computing for Science

Compute Cambrian explosion

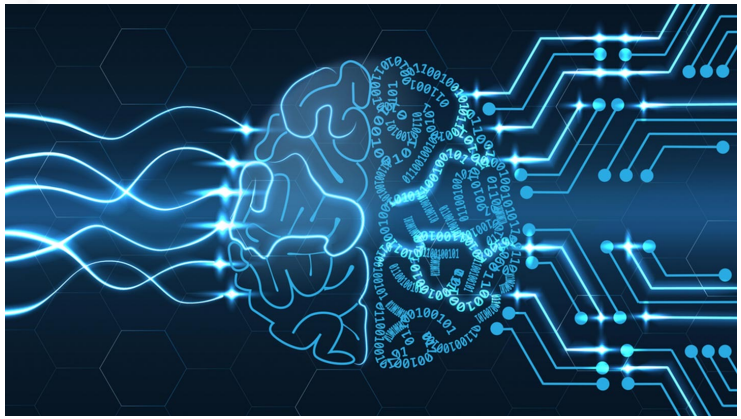
AI for Science

DOE readies multibillion-dollar AI push

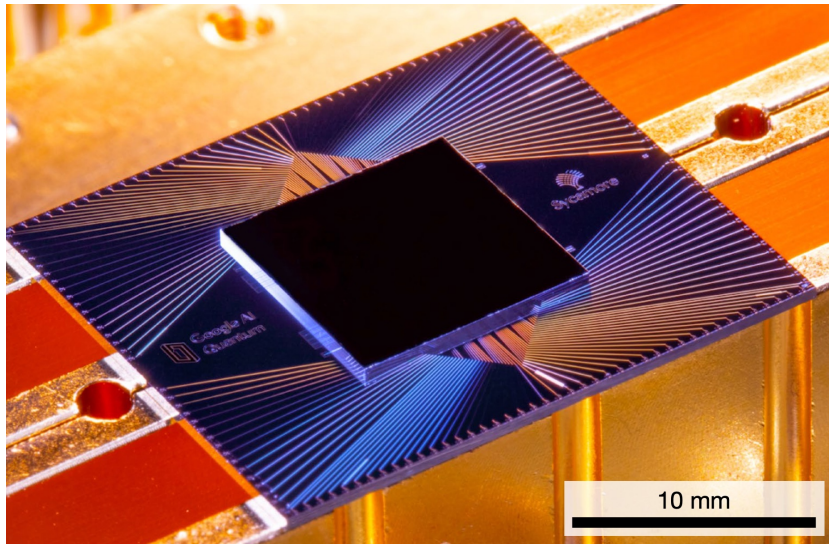
U.S. supercomputing leader is the latest big backer in a globally crowded field

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

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



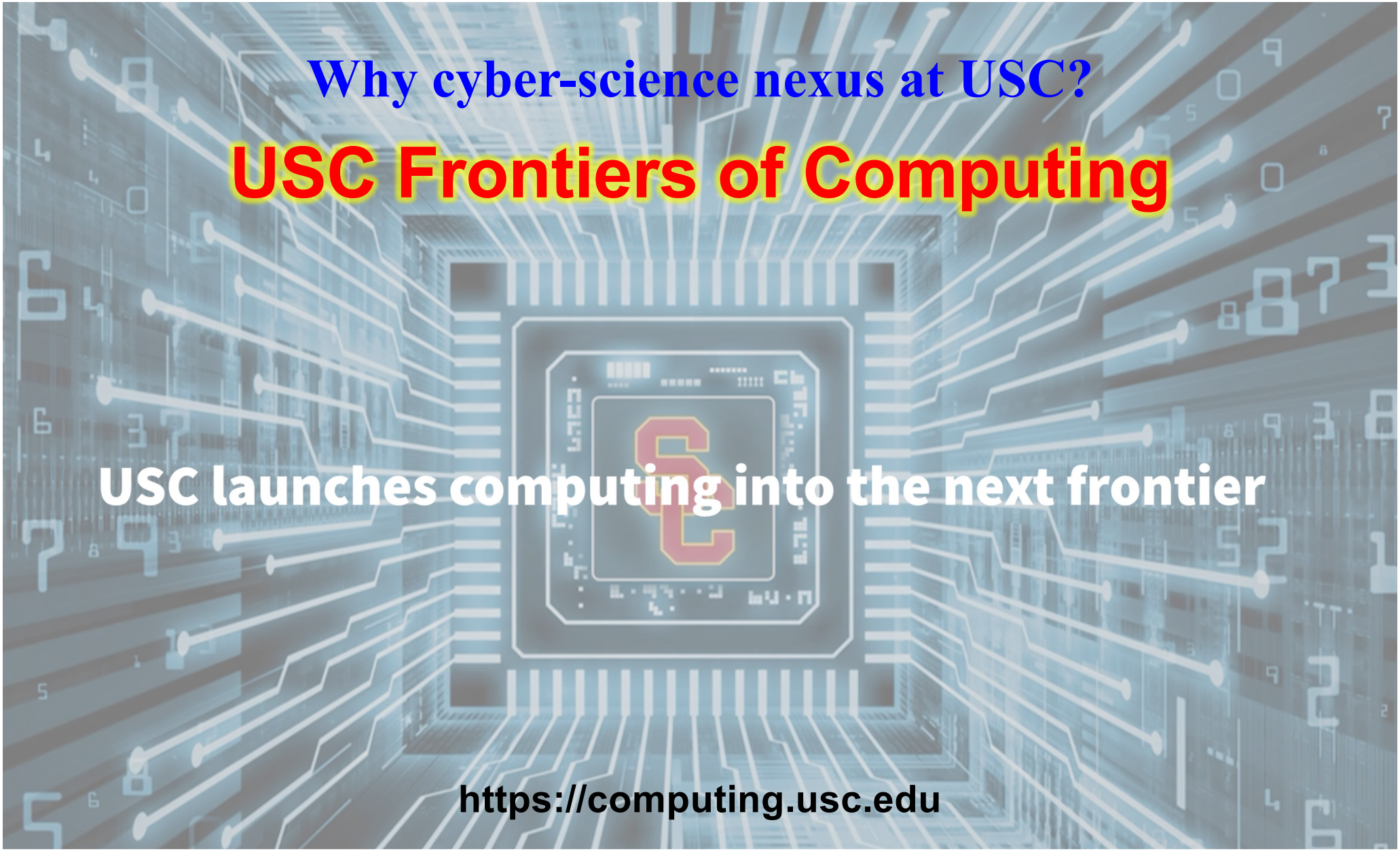
Quantum Computing for Science



Use all to advance science!

Why cyber-science nexus at USC?

USC Frontiers of Computing

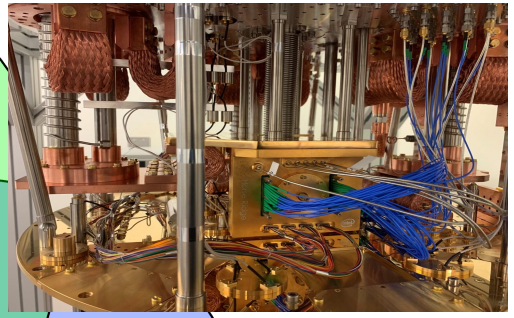


- **$1 billion+, 10 years initiative**
- **New School of Advanced Computing:** https://sac.usc.edu
- **30 senior & 60 junior & mid-level hires**

Training Cyber-Science Workforce

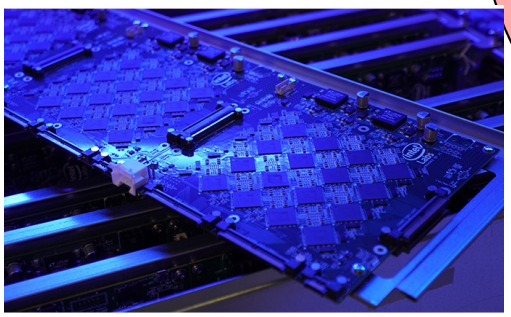
- New generation of computational scientists at the nexus of post-exascale computing, quantum computing & AI
- Unique dual-degree program: Ph.D. in materials science or physics, along with MS in computer science, MS in quantum information science or MS in materials engineering with AI

Horse Ridge II
Quantum computer



Cybertraining on exa + quantum + AI platforms

Neuromorphic
Pohoiki Springs

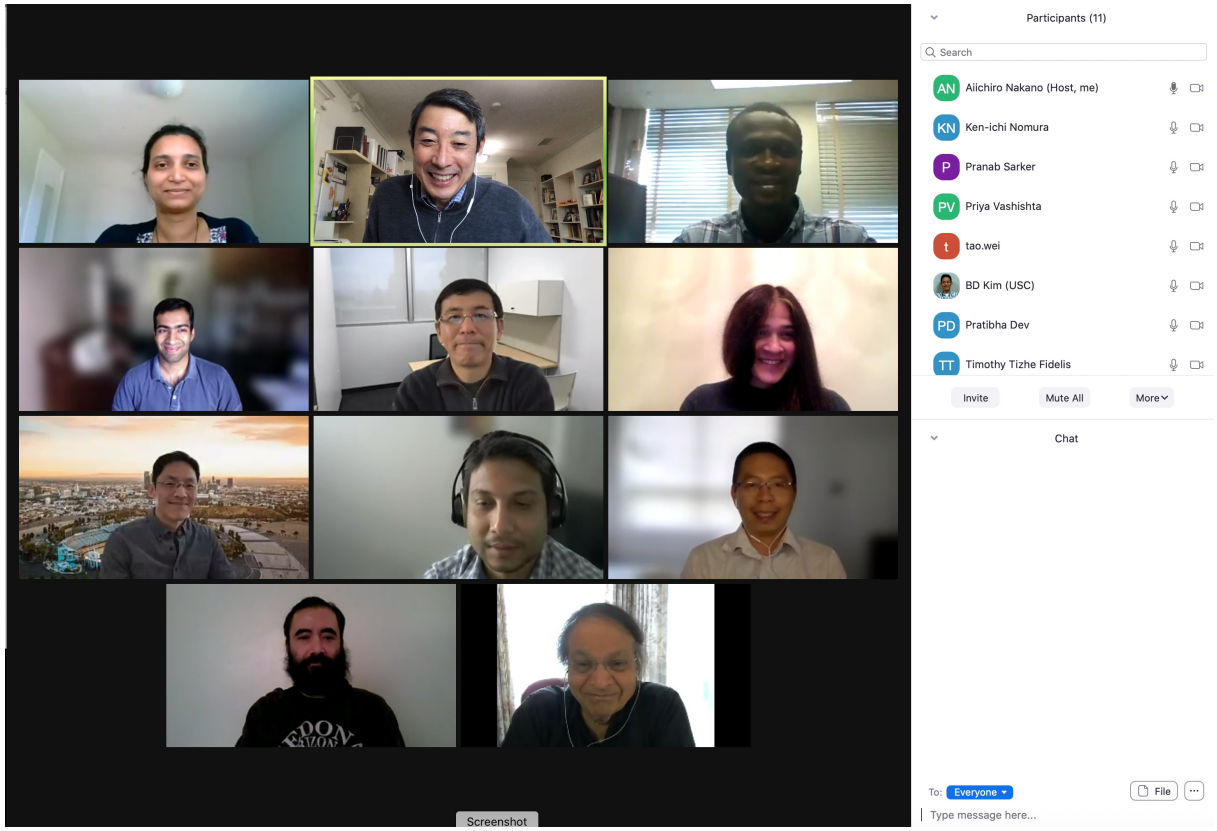


Exascale
Aurora

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

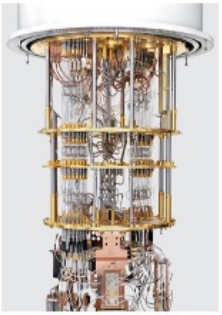
QXMD

Nonadiabatic quantum molecular dynamics

GEARS

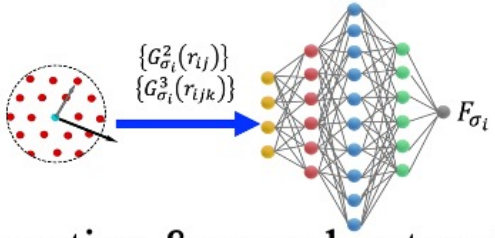
Augmented-reality user interface

MISTIQS



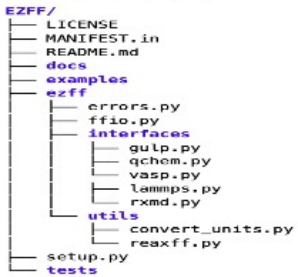
Quantum many-body dynamics on quantum computers

RXMD-NN



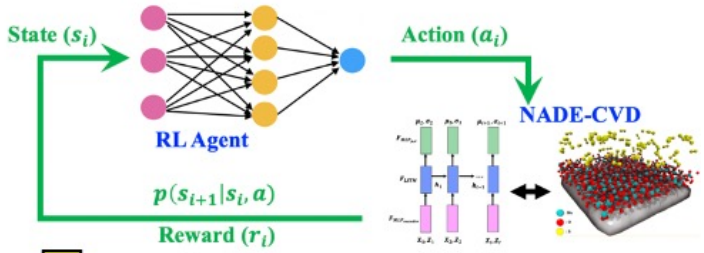
Reactive & neural-network molecular dynamics

EZFF



Easy force-field parameterization & uncertain quantification

MAITAI



AI tools for materials design

https://cybermagics.netlify.app/software

USC-Howard Future Manufacturing

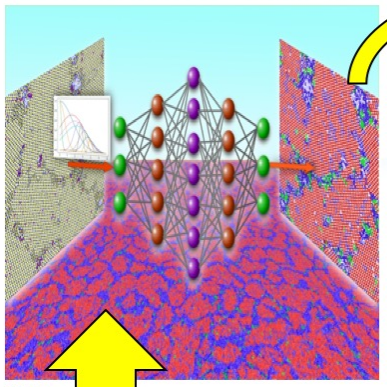
FMRG: Artificial Intelligence Driven Cybermanufacturing of Quantum Material Architectures

$3.75M NSF project (2020-2025)

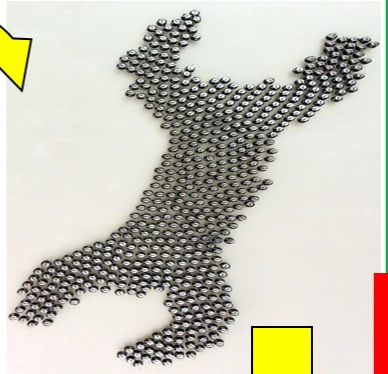
Multidisciplinary Closed-Loop Approach

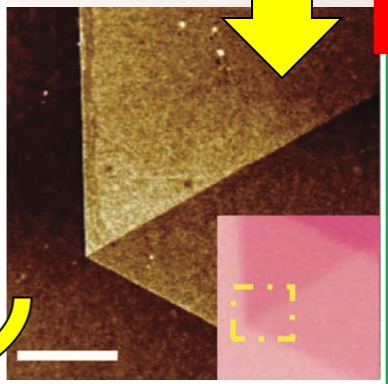
Machine learning & multiscaling (*Kalia*)

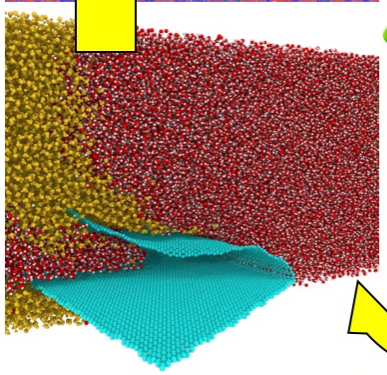
AI-guided self-assembly & collective robotics (*Nagpal*)



Cyber-physical system (*Rawat*)





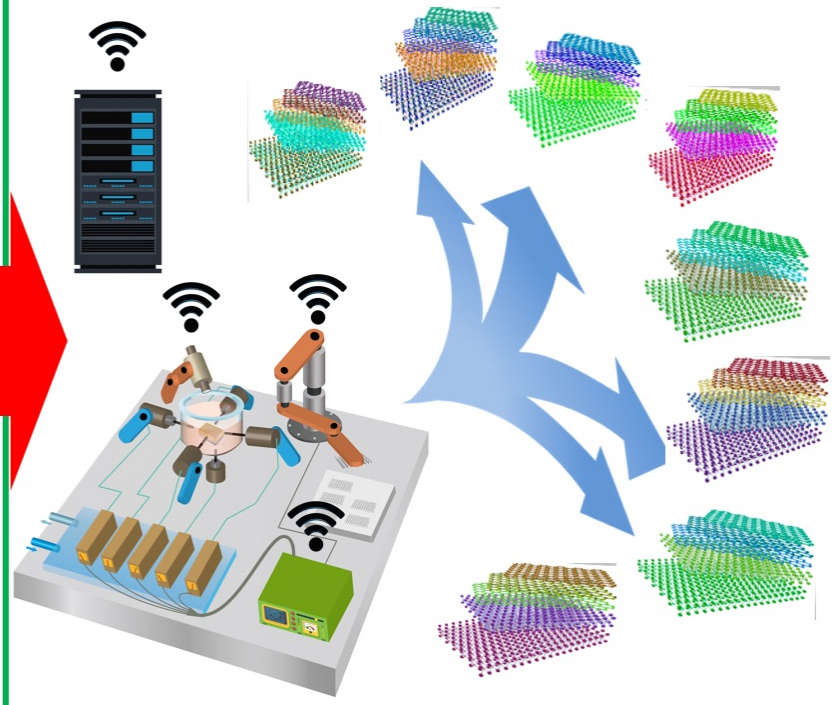


First-principles-based simulations (*Nakano*)

Novel fluidic-folding synthesis (*Wang*)

Future Manufacturing Goal

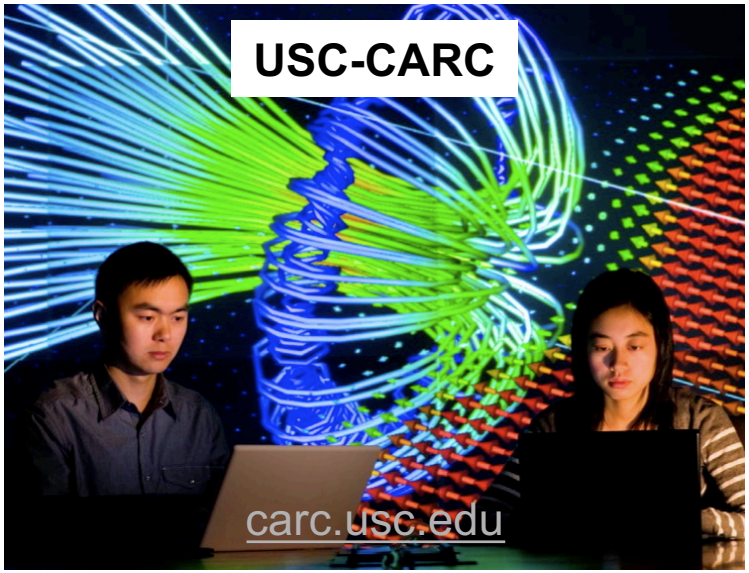
Precisely aligned van der Waals hetero-structures to enable future twistronics



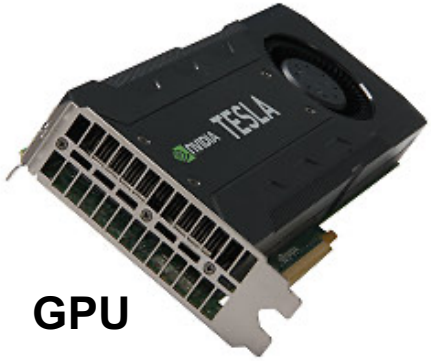
AI- & robotics-guided, scalable manufacturing platform

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

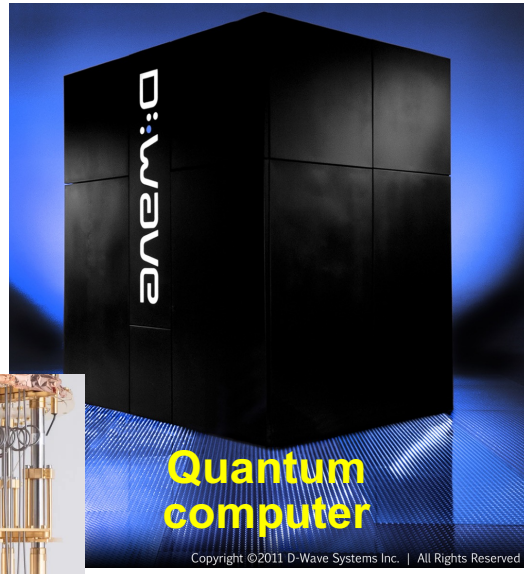
High Performance Computing

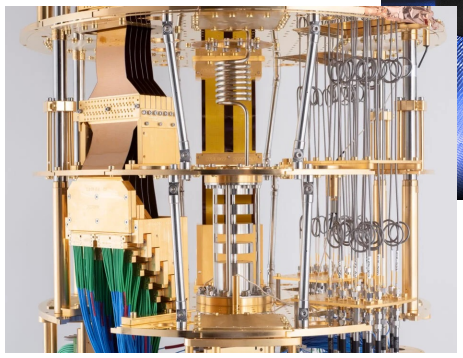


- *USC CARC (Center for Advanced Research Computing)*: **21,000 CPU-cores & 200+ GPUs**
- *USC ISI (Information Sciences Institute)*: **1,098-qubit D-Wave quantum computer**
- *USC-IBM Quantum Innovation Center*: **Cloud access to 100+ qubit IBM quantum computers (2024-)**



GPU





QPU

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

Computational Sciences at USC

The Nobel Prize in Chemistry 2013

© Nobel Media AB

Martin Karplus

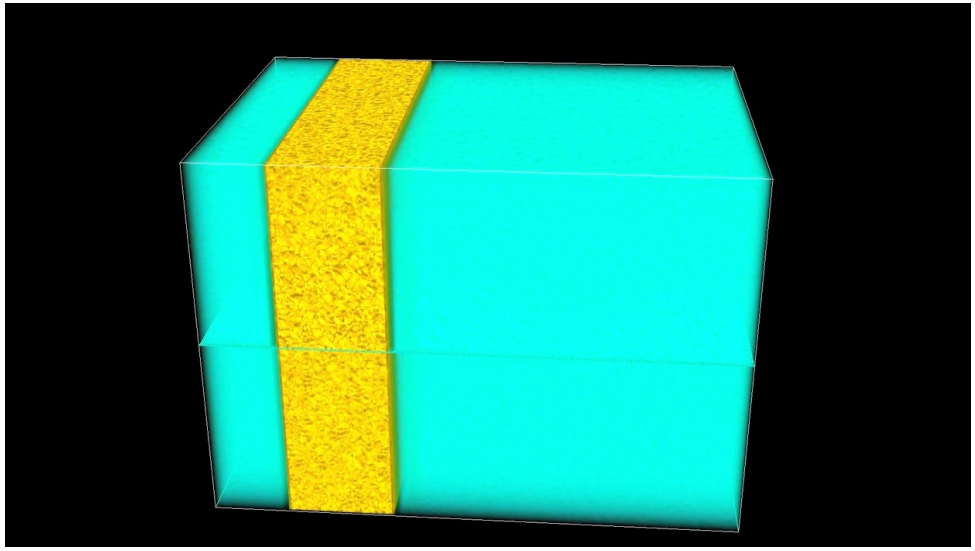
Photo: Keilana via Wikimedia Commons

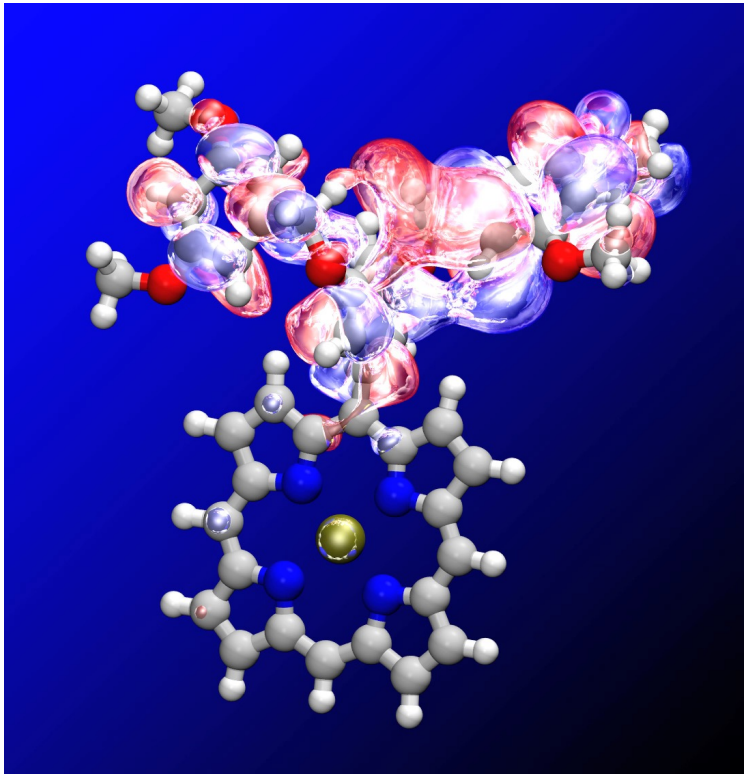
Michael Levitt

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**
- **40 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**

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

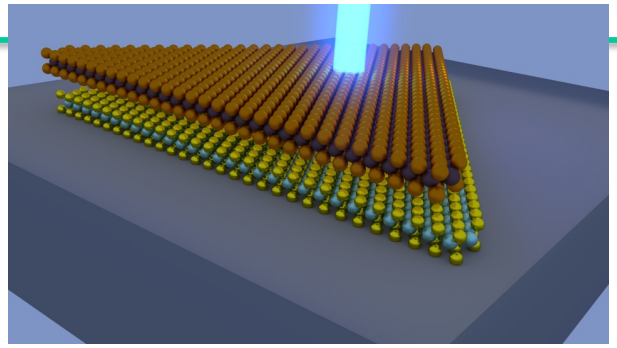
- **Atomistic simulations on million cores (pre-exascale)**

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

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



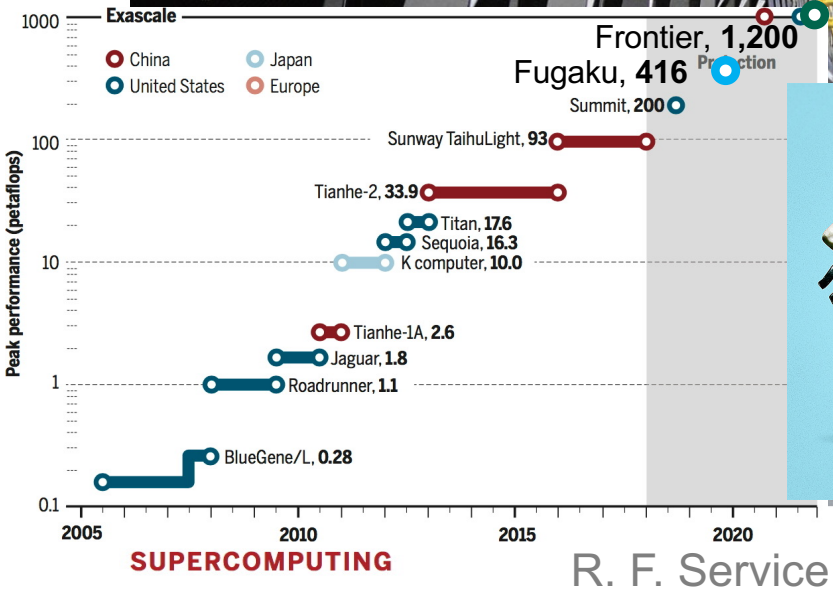
Early Science Projects for Aurora Supercomputer Announced
Metascalable layered materials genome
Investigator: Aiichiro Nakano, University of Southern California

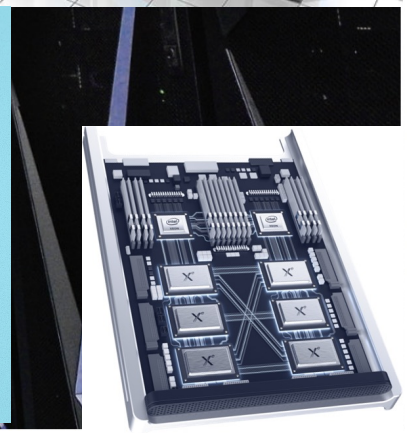
1.01 exaflop/s
Intel Aurora

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





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.

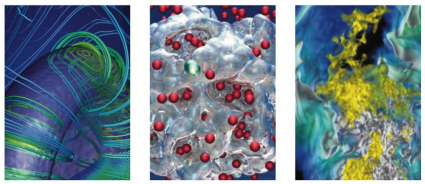
https://www.tomshardware.com/news/two-chinese-exascale-supercomputers

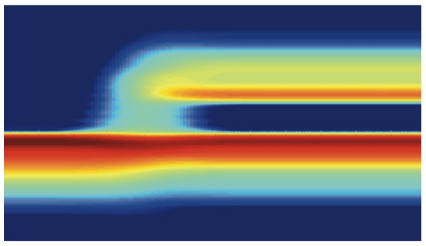
Exa-leadership

BES

BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW





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

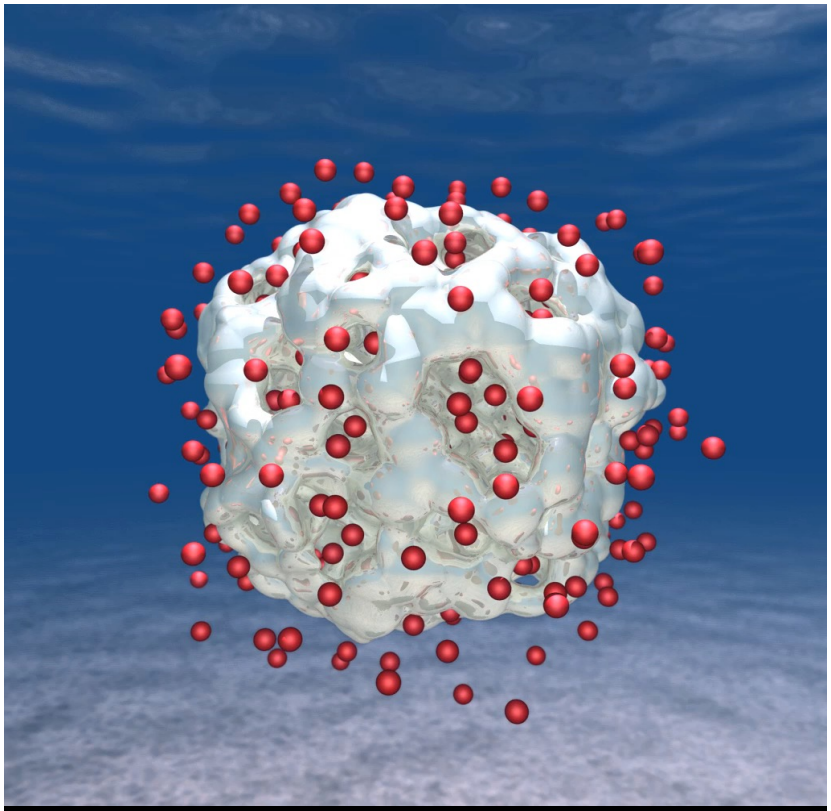
NOVEMBER 3–5, 2015

ROCKVILLE, MARYLAND

16,661-atom QMD

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

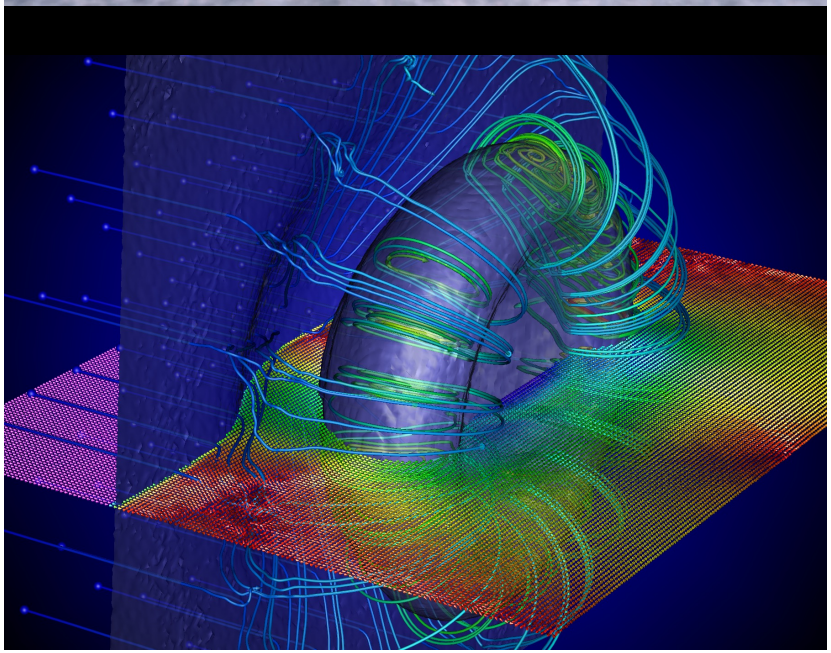
On-demand hydrogen production from water



10^9-atom RMD

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

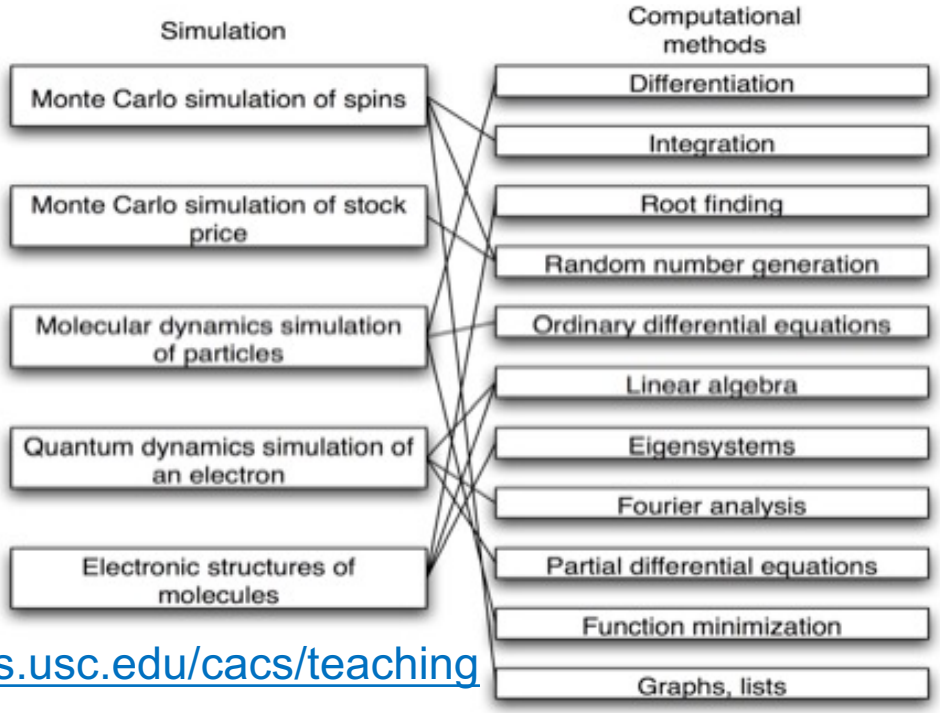
Fluid dynamics atom-by-atom

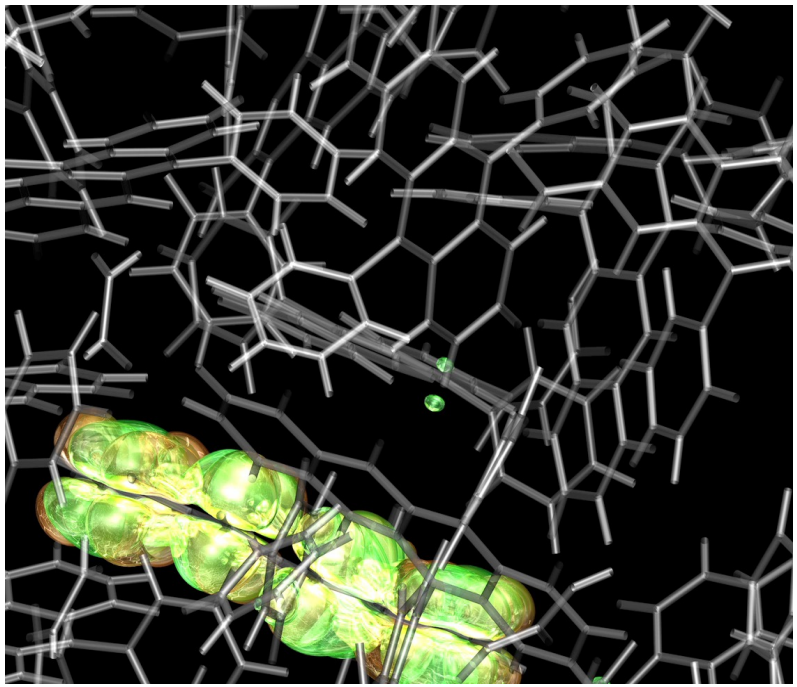


U.S. DEPARTMENT OF ENERGY

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

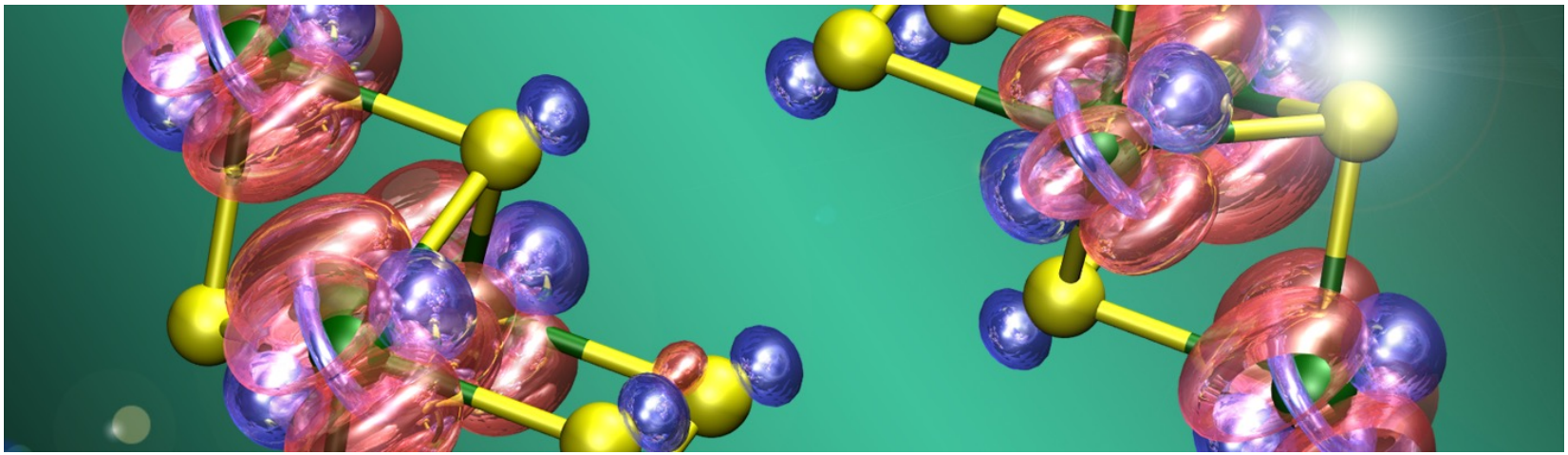
Additional HPCS Course

Detailed lecture notes are available at a USC course home page

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

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.

- **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/services/education/workshops
https://www.carc.usc.edu/services/education/office-hours-and-consultations

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) 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