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

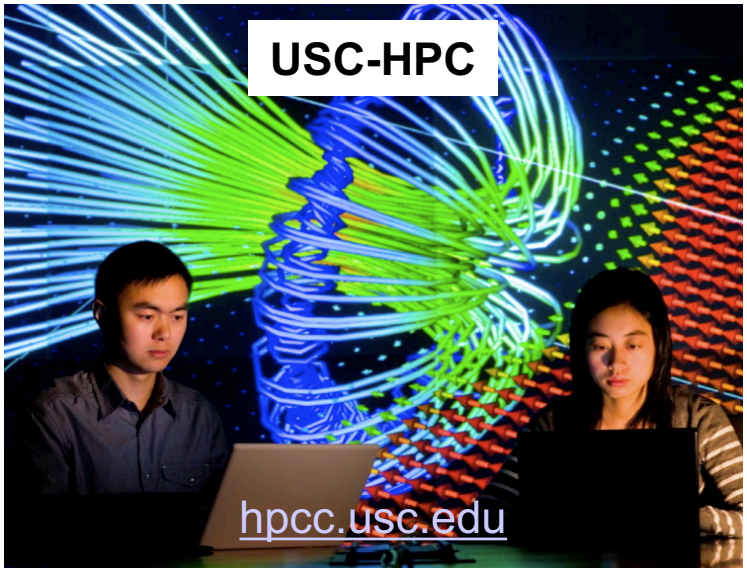
https://www.cs.usc.edu/academic-programs/masters/high-performance-computing-simulations

Computational Sciences at USC

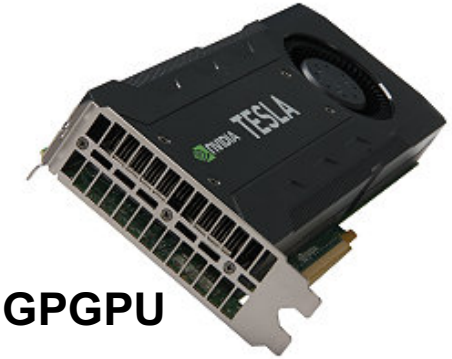
Aiichiro Nakano

Email: anakano@usc.edu

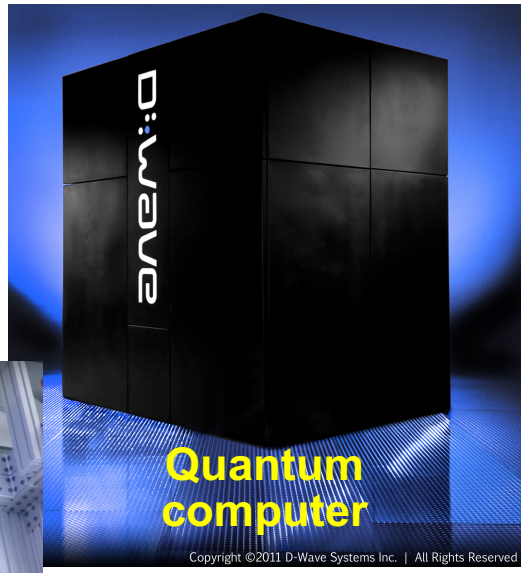
High Performance Computing

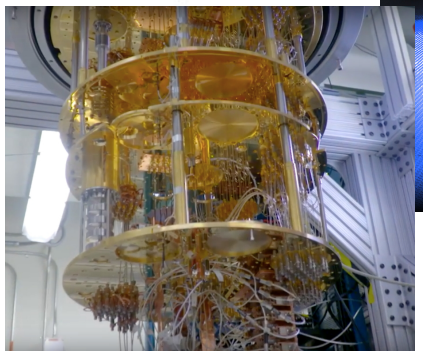


- *USC HPC (Center for High Performance Computing & Communication)*: **13,440 CPU-core GPU-accelerated 0.62 petaflop/s cluster**
- *USC ISI (Information Sciences Institute)*: **1,098-qubit D-Wave quantum computer**

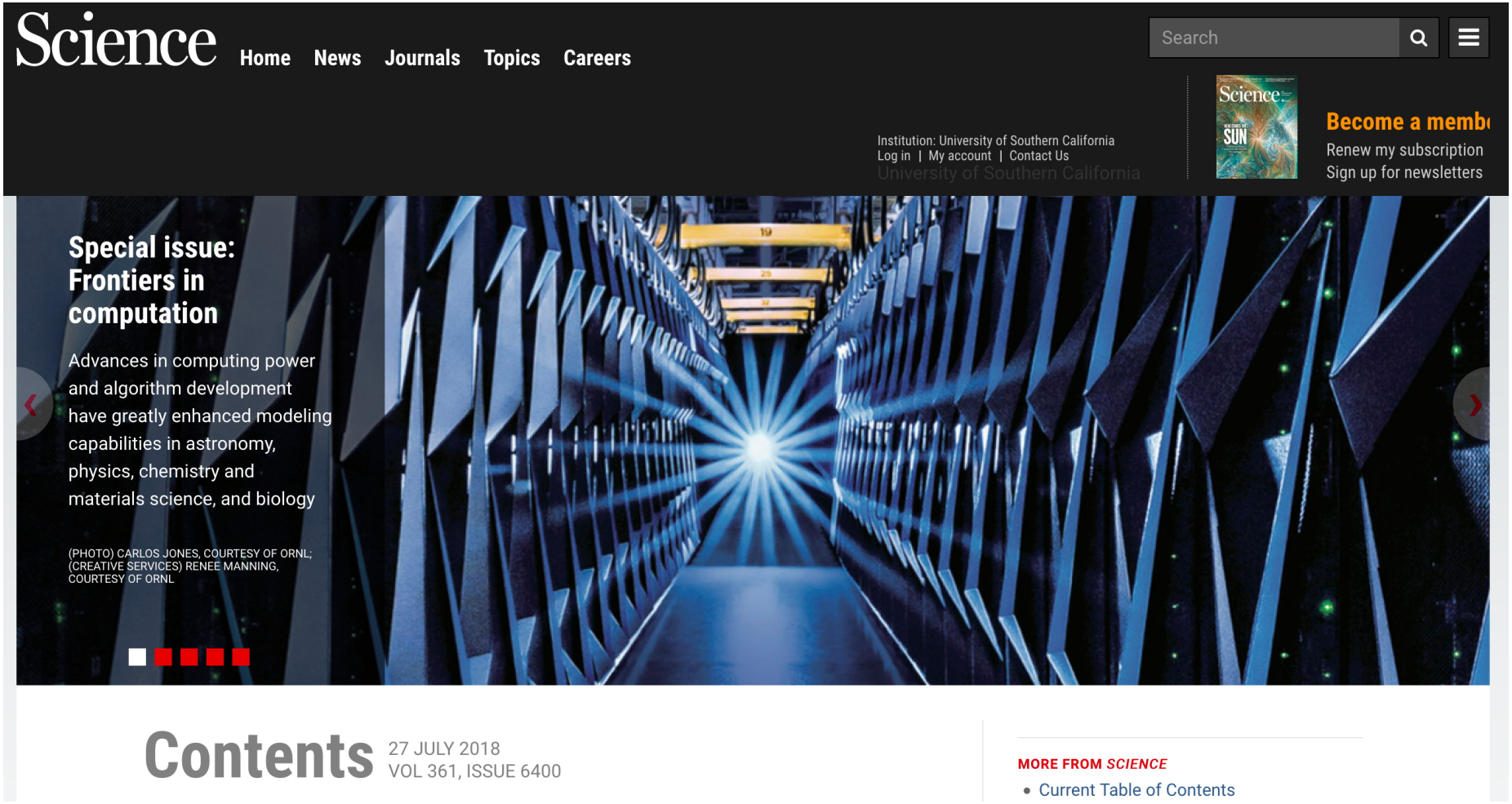


GPGPU





QPU



122 petaflop/s Summit on the cover of *Science* (July 27, ’18)

Computational Sciences at USC

The Nobel Prize in Chemistry 2013

© Nobel Media AB

Martin Karplus

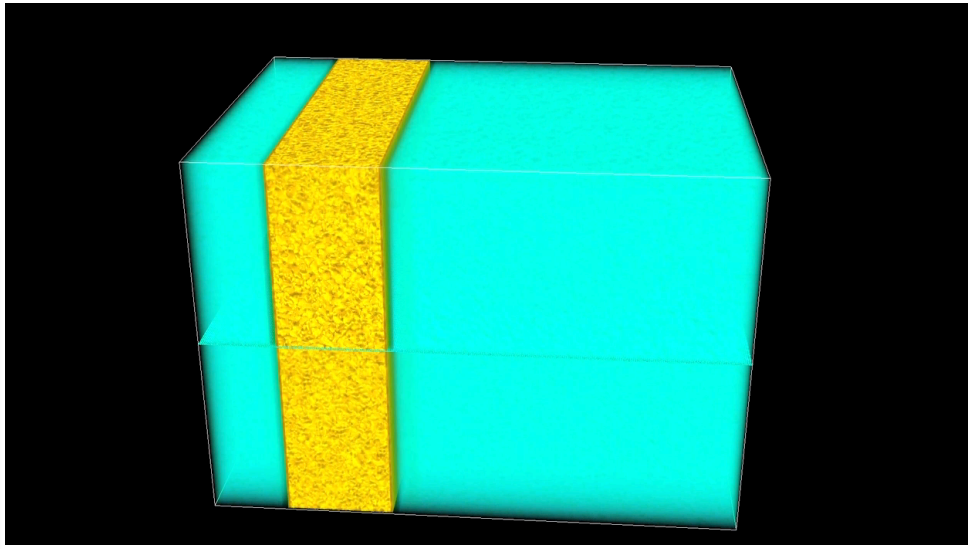
Photo: Keilana via Wikimedia Commons

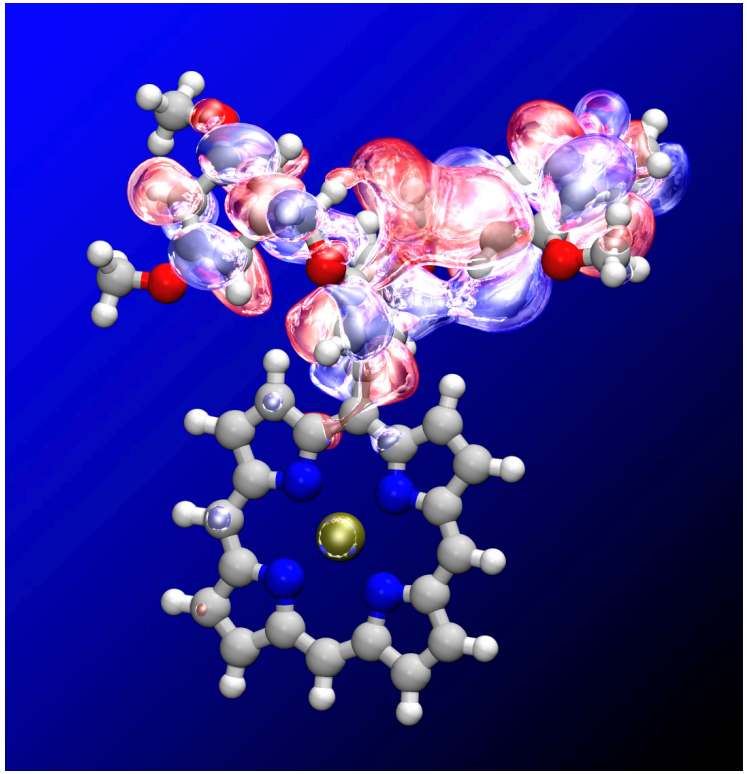
Michael Levitt

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, 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 (2017-2020)**

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

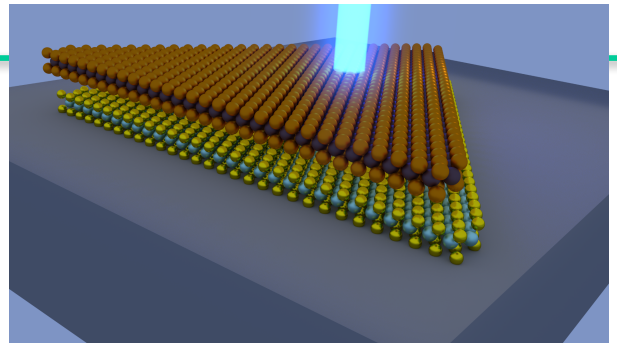
- **NAQMD & RMD simulations on full 800K cores**

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

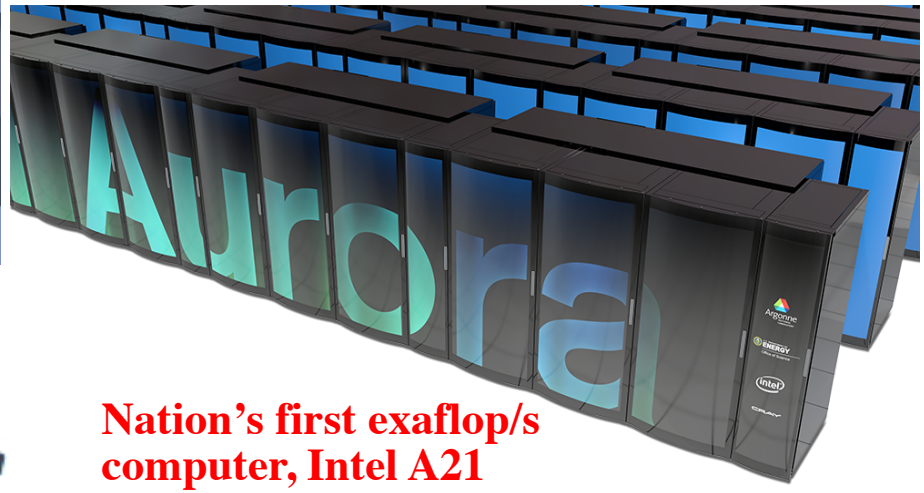


AURORA | EARLY SCIENCE PROGRAM

Early Science Projects for Aurora Supercomputer Announced

Metascalable layered materials genome

Investigator: Aiichiro Nakano, University of Southern California



Nation's first exaflop/s computer, Intel A21 (2021)

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

CACS@A21 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

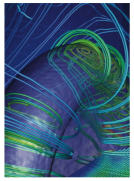
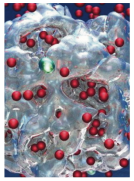
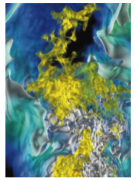
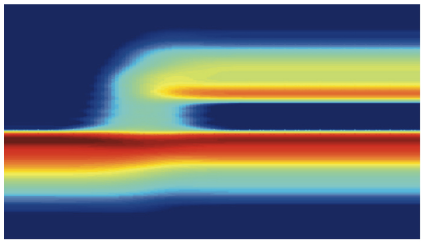
By **Robert F. Service**

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.

BES

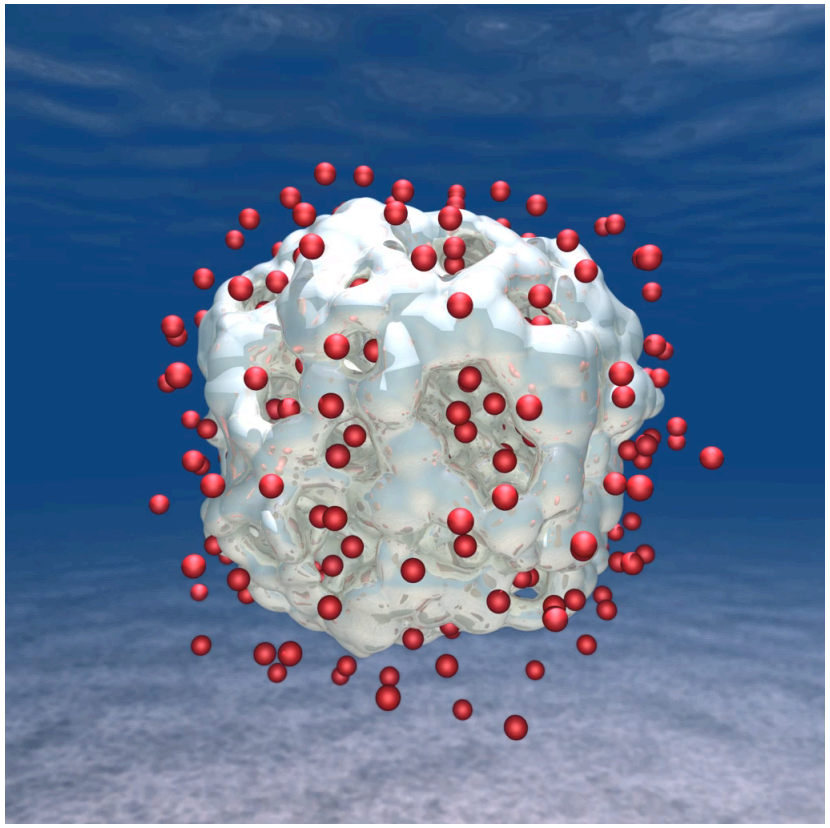
BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

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

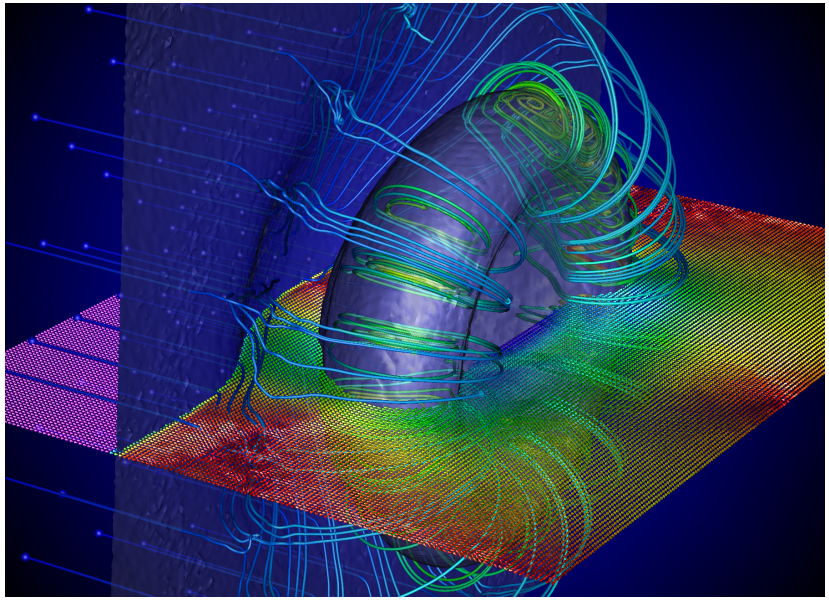
NOVEMBER 3–5, 2015

ROCKVILLE, MARYLAND



16,661-atom QMD

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



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/

Simulation + Data + Learning

- Master of Science in Computer Science (General)

Apart from the general Master of Science in Computer Science, the CS Department also offers the degree with the following specializations:

- Data Science
- Game Development
- Computer Security
- Computer Networks
- Software Engineering
- Intelligent Robotics
- Multimedia and Creative Technologies
- High Performance Computing and Simulation

Aurora/A21 Early Science Program: Simulation ('17) + Data-Learning ('18)

Early Science Projects for Aurora Supercomputer Announced

Author: By Laura Wolf, Argonne Leadership Computing Facility

January 30, 2017

ALCF Selects Data and Learning Projects for Aurora Early Science Program

June 28, 2018

June 28, 2018 — The Argonne Leadership Computing Facility (ALCF), a U.S. Department of Energy (DOE) Office of Science User Facility, has selected 10 data science and machine learning projects for its Aurora Early Science Program (ESP). Set to be the nation's first exascale system upon its expected 2021 arrival, Aurora will be capable of performing a quintillion calculations per second.

https://www.alcf.anl.gov/projects/aurora-esp

https://www.hpcwire.com/off-the-wire/alcf-selects-data-and-learning-projects-for-aurora-early-science-program

MSCS-HPCS Requirement

A total of **32** units

1. Required Core Courses in Computer Science: 3 courses
   - CSCI570 (analysis of algorithms)
   - 2 from: CS561 (AI), CS 571 (Web), CS585 (database)
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)

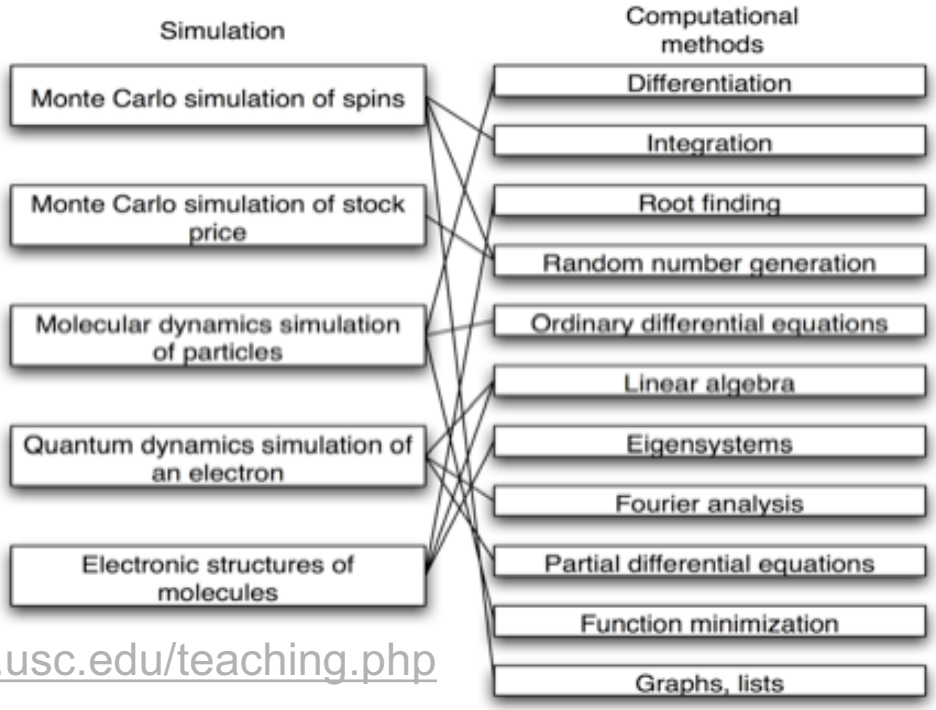
   (b) Computational Science/Engineering Application Track

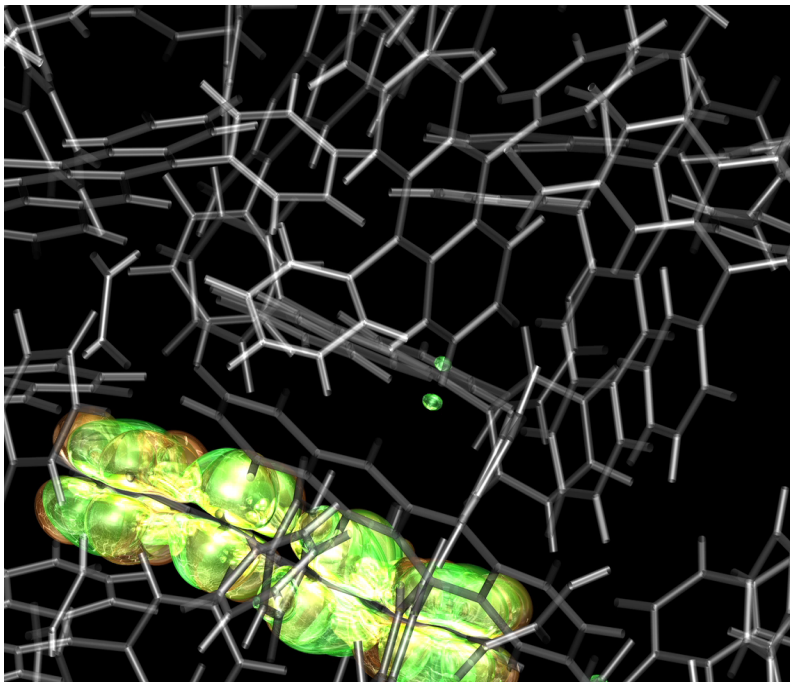
   AME535 (comp fluid dynamics), CE529 (finite element), CHE502 (numerical transport),
   EE553 (comp optimization), EE653 (multithreaded arch), EE657 (parallel processing),
   EE659 (network), Math501 (numerical analysis), MAS575 (atomistic simulation),
   Phys516 (computational physics), PTE582 (fluid flow), ...

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

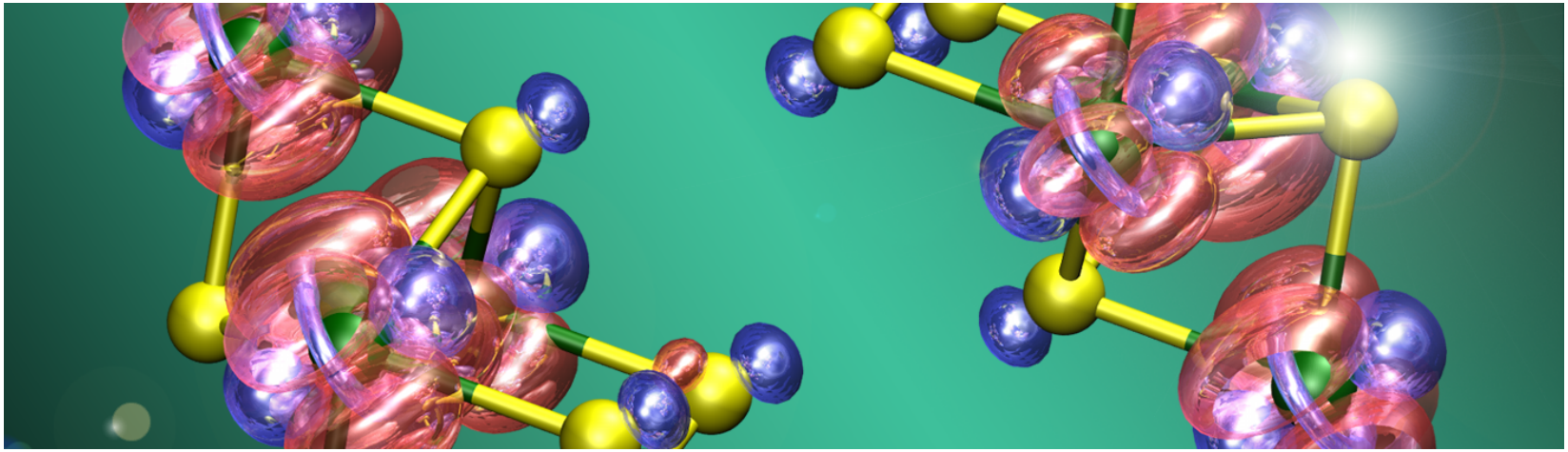
Additional HPCS Course

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".



http://cacs.usc.edu/education/cs699-lecture.html

HPC Tutorials & Office Hours

Series of tutorials + office hours (T, 2:30-5 pm, LVL 3M) at the USC Center for High Performance Computing (HPC):

- **CUDA computing on GPU**
- **Parallel MATLAB**
- **...**

http://hpcc.usc.edu/support/hpcc-computing-workshops
http://hpcc.usc.edu/officehours

Students registered by the end of this week will get an HPC account

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