CyberMAGICS Workshop

Aiichiro Nakano, Ken-ichi Nomura, Priya Vashishta
Collaboratory for Advanced Computing & Simulations
University of Southern California

Pratibha Dev, Tao Wei
Howard University

Email: anakano@usc.edu

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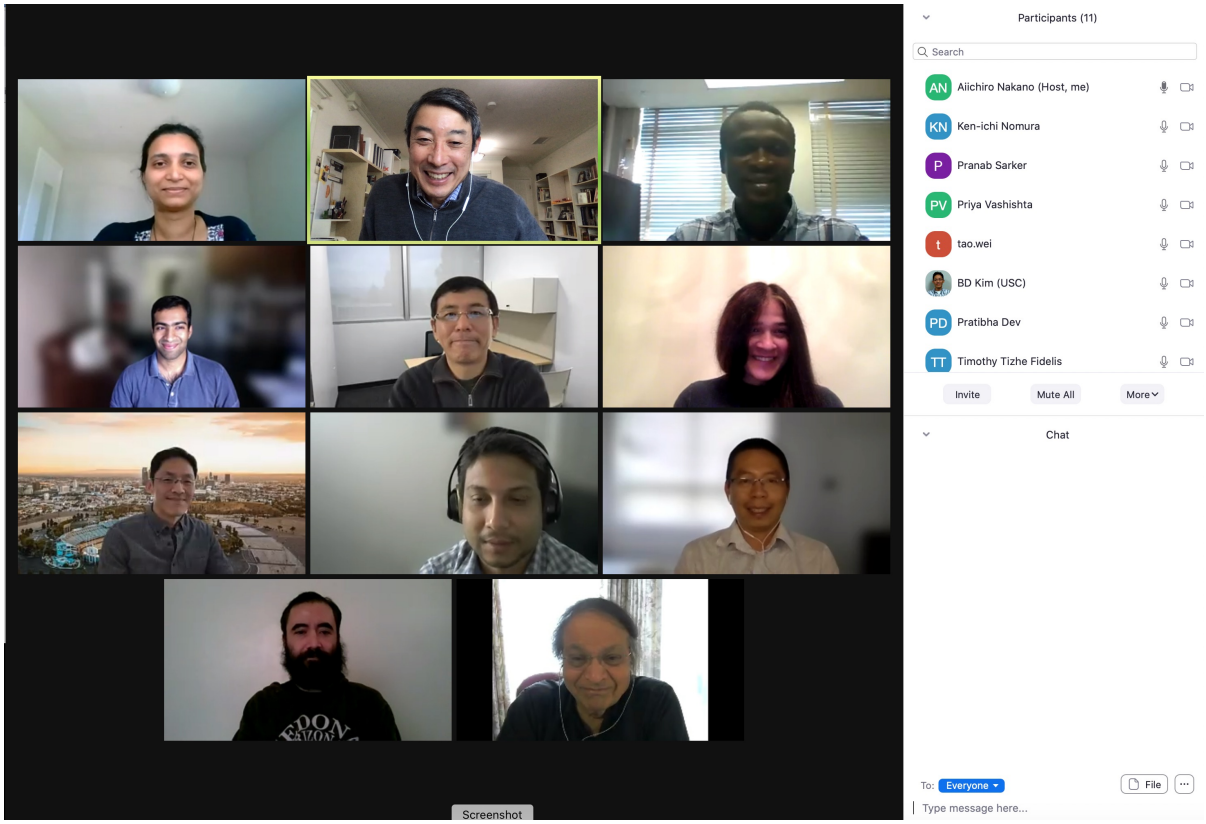
USC-Howard Cybertraining

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)

Exaflop/s Computer Is Here

ORNL's Frontier First to Break the Exaflop Ceiling

May 30, 2022

The 59th edition of the TOP500 revealed the Frontier system to be the first true exascale machine with an HPL score of 1.102 Exaflop/s.

The No. 1 spot is now held by the Frontier system at Oak Ridge National Laboratory (ORNL) in the US. Based on the latest HPE Cray EX235a architecture and equipped with AMD EPYC 64C 2GHz processors, the system has 8,730,112 total cores, a power efficiency rating of 52.23 gigaflops/watt, and relies on gigabit ethernet for data transfer.

Exaflop/s: 10^{18} floating-point operations per second

https://www.top500.org

Changing Computing Landscape for Science

Postexascale Computing for Science

Compute Cambrian explosion

AI for Science

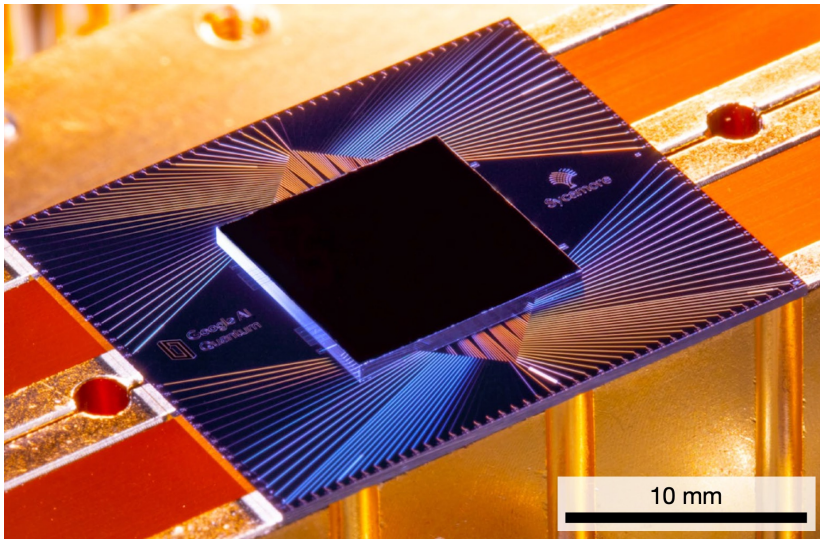
DOE readies multibillion-dollar AI push

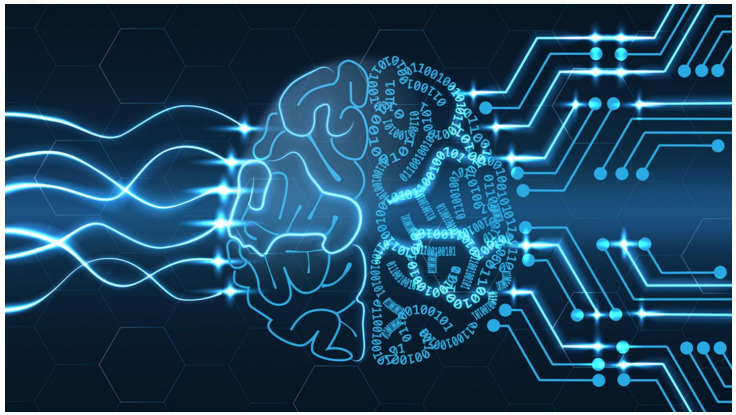
U.S. supercomputing leader is the latest big backer in a globally crowded field

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

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

Quantum Computing for Science



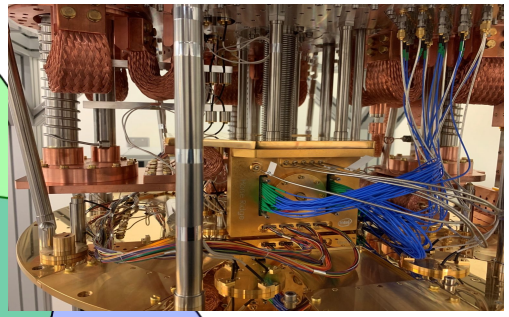


Use all to advance science!

Training Cyber Science Workforce

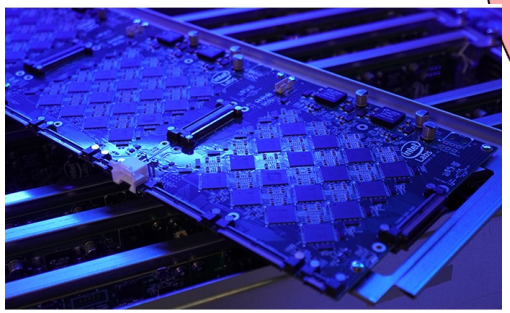
- New generation of computational scientists at the nexus of exascale computing, quantum computing & AI
- Unique dual-degree program at USC: Ph.D. in materials science or physics, along with MS in computer science specialized in high-performance computing & simulations, MS in quantum information science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

Horse Ridge II
Quantum computer



Cybertraining on exa + quantum + AI platforms

Neuromorphic
Pohoiki Springs



Exascale
Aurora

AIQ-XMaS Software Suite

AI & Quantum-Computing Enabled Exa Quantum Materials Simulator

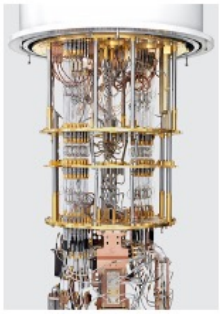
QXMD

Nonadiabatic quantum molecular dynamics

GEARS

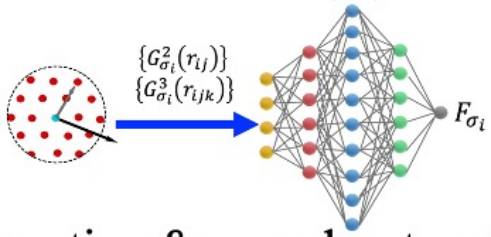
Augmented-reality user interface

MISTIQS



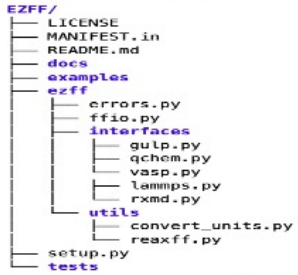
Quantum many-body dynamics on quantum computers

RXMD-NN



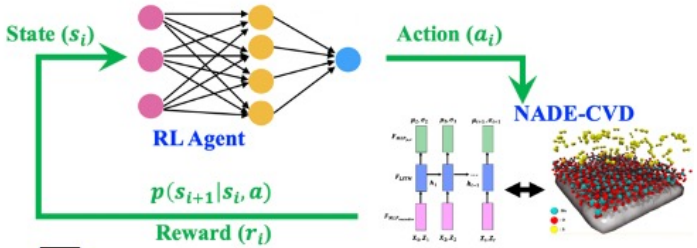
Reactive & neural-network molecular dynamics

EZFF



Easy force-field parameterization & uncertain quantification

MAITAI

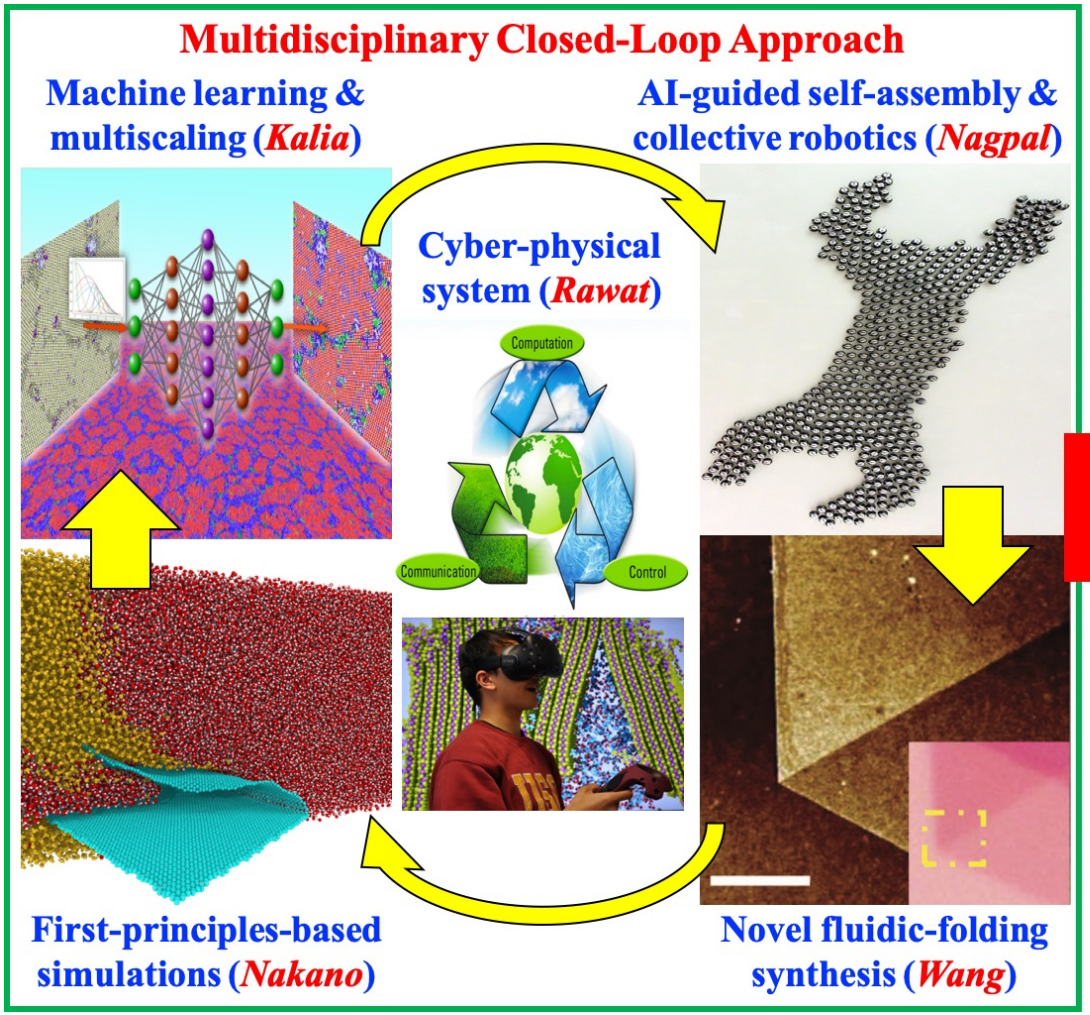


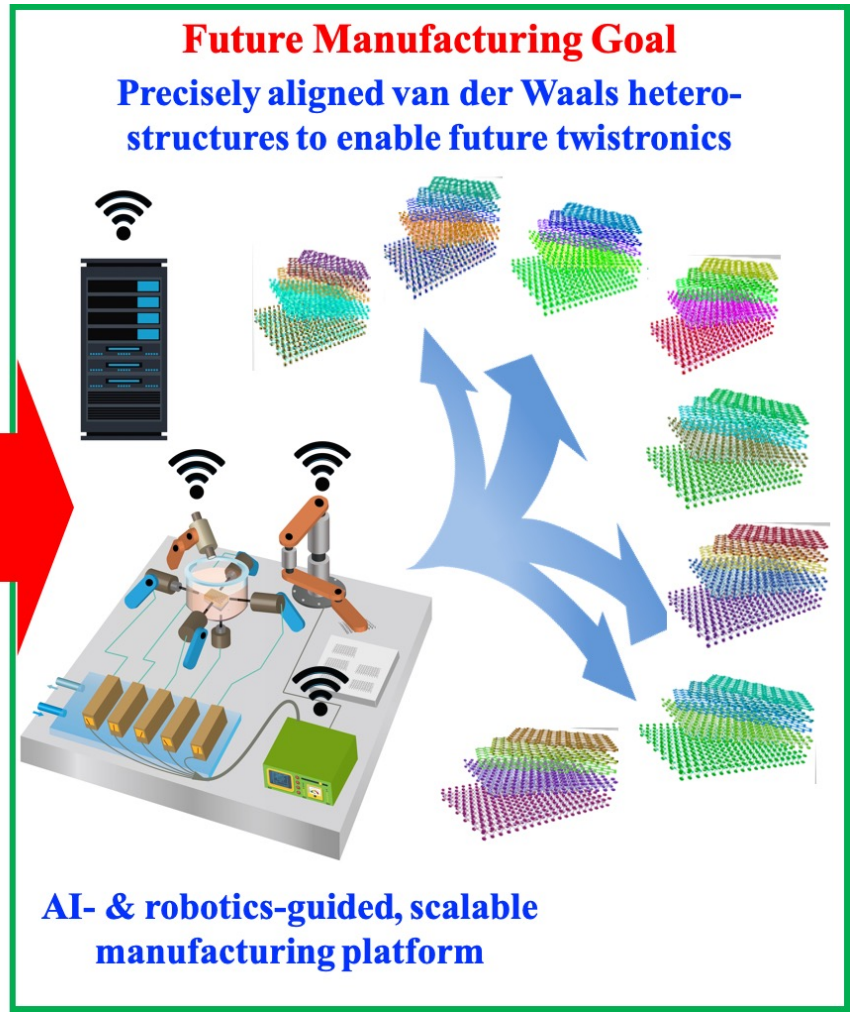
AI tools for materials design

USC-Howard Future Manufacturing

FMRG: Artificial Intelligence Driven Cybermanufacturing of Quantum Material Architectures

$3.75M NSF project (2020-2025)





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

Agenda: June 29 – July 1, 2023

Thursday, June 29, 2023		
Time(PDT)	Topic	Instructor
8:00 am - 9:00 am	Introduction and logistics	Aiichiro Nakano
9:00 am - 10:00 am	Molecular dynamics simulation basics	Priya Vashishta
10:00 am - 11:00 am	Reactive molecular dynamics basics	Ken-ichi Nomura
11:00 am - 12:00 pm	Lunch break	
12:00 pm - 1:30 pm	Reactive molecular dynamics hands on: RXMD code	Nitish Baradwaj, Ruru Ma, Tian Sang, Pranab Sarker, Hind Aljaddani
1:30 pm - 2:30 pm	Machine learning basics	Ken-ichi Nomura
Friday, June 30, 2023		
Time(PDT)	Topic	Instructor
8:00 am - 10:00 am	Machine learning hands-on	Anikeya Aditya, Nitish Baradwaj, Taufeq Razakh, Liqiu Yang
10:00 am - 11:00 am	Quantum molecular dynamics basics	Aiichiro Nakano
11:00 am - 12:00 pm	Lunch break	
12:00 pm - 1:30 pm	Quantum molecular dynamics hands-on: QXMD code	Anikeya Aditya, Ayu Irie, Himani Mishra, Liqiu Yang, Jingxin Zhang
1:30 pm - 2:30 pm	Quantum computing basics and hands-on	Aiichiro Nakano
Saturday, July 1, 2023		
Time(PDT)	Topic	Instructor
9:00 am - 11:00 am	Participant presentations	Workshop Attendees
11:00 am - 11:15 am	Closing remarks	Pratibha Dev, Tao Wei

https://cybermagics.netlify.app/workshop-schedule.html

Logistics

- **Workshop courseware (lecture notes & Jupyter notebooks) is available at**
  https://cybermagics.netlify.app/workshop-resources.html
- **Hands on training will use cloud resources**
  1. **Google Colab (QXMD, RXMD, AI–machine learning)**
     https://colab.research.google.com
  2. **IBM Quantum (quantum computing)**
     https://quantum-computing.ibm.com
- **Please ask questions any time during the lectures & hands-on sessions using Zoom chat or speak up**
- **You are welcome to make a few-slides research presentation on Saturday (or simple self-introduction)**

Now, introduction of instructors & group photo