

CyberMAGICS Workshop

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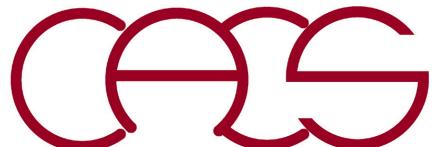
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*Now at *University of South Carolina*



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Award OAC-2118061**

June 25, 2024



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*

The screenshot shows a video conference interface with 11 participants. The participants are arranged in a grid layout. The participants listed in the interface are:

- Aichiro Nakano (Host, me)
- Ken-ichi Nomura
- Pranab Sarker
- Priya Vashishta
- tao.wei
- BD Kim (USC)
- Pratibha Dev
- Timothy Tizhe Fidelis

***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 Computing 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.



1.21 Exaflop/s as of June 2024

<https://www.top500.org>

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.



Second exaflop/s computer (1.01 Exaflop/s), Aurora, arrived at Argonne National Laboratory in June 2024

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

Changing Computing Landscape for Science

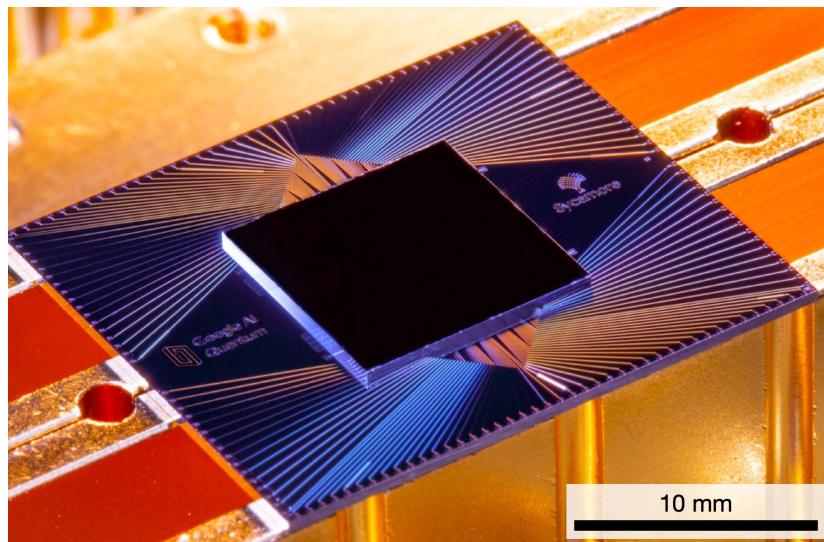
Postexascale Computing for Science



Compute Cambrian explosion



Quantum Computing for Science



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)



Use all to advance science!

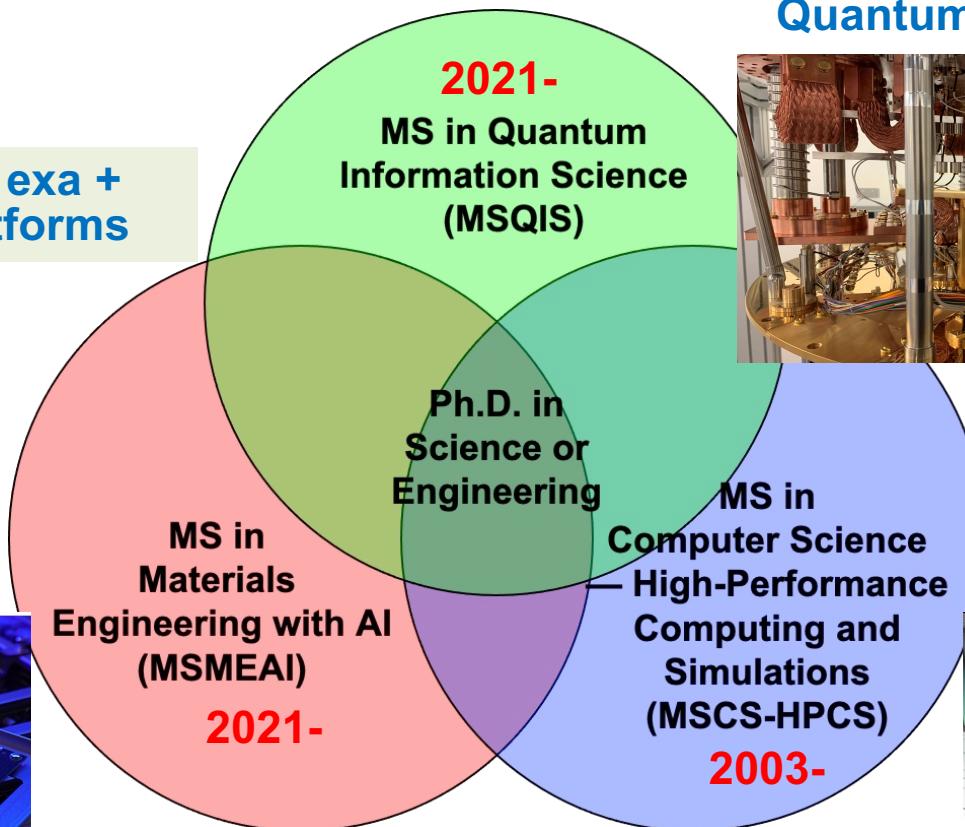
Training Cyber Science Workforce

- 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

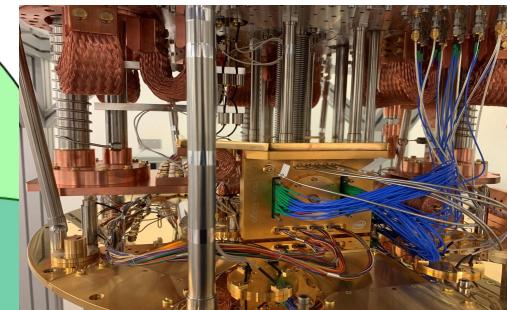
Cybertraining on exa +
quantum + AI platforms



Neuromorphic
Pohoiki Springs



Horse Ridge II
Quantum computer

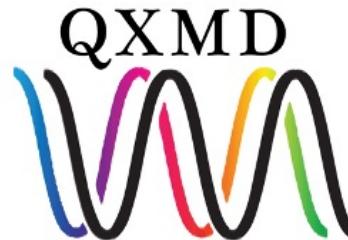


Exascale
Aurora



AIQ-XMaS Software Suite

AI & Quantum-Computing Enabled Exa Quantum Materials Simulator

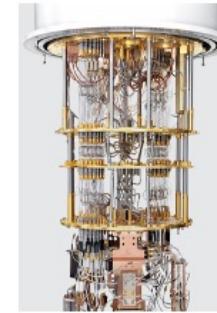


Nonadiabatic quantum molecular dynamics

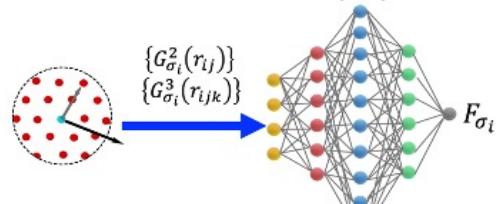
GEARS



MISTIQS

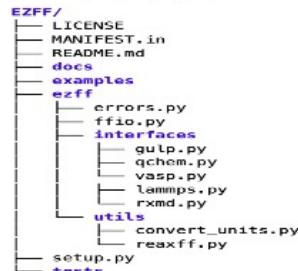


RXMD-NN



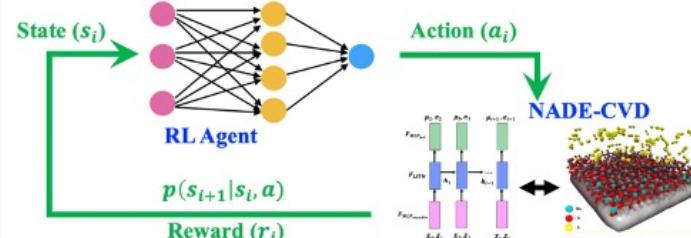
Reactive & neural-network molecular dynamics

EZFF



Easy force-field parameterization & uncertain quantification

MAITAI

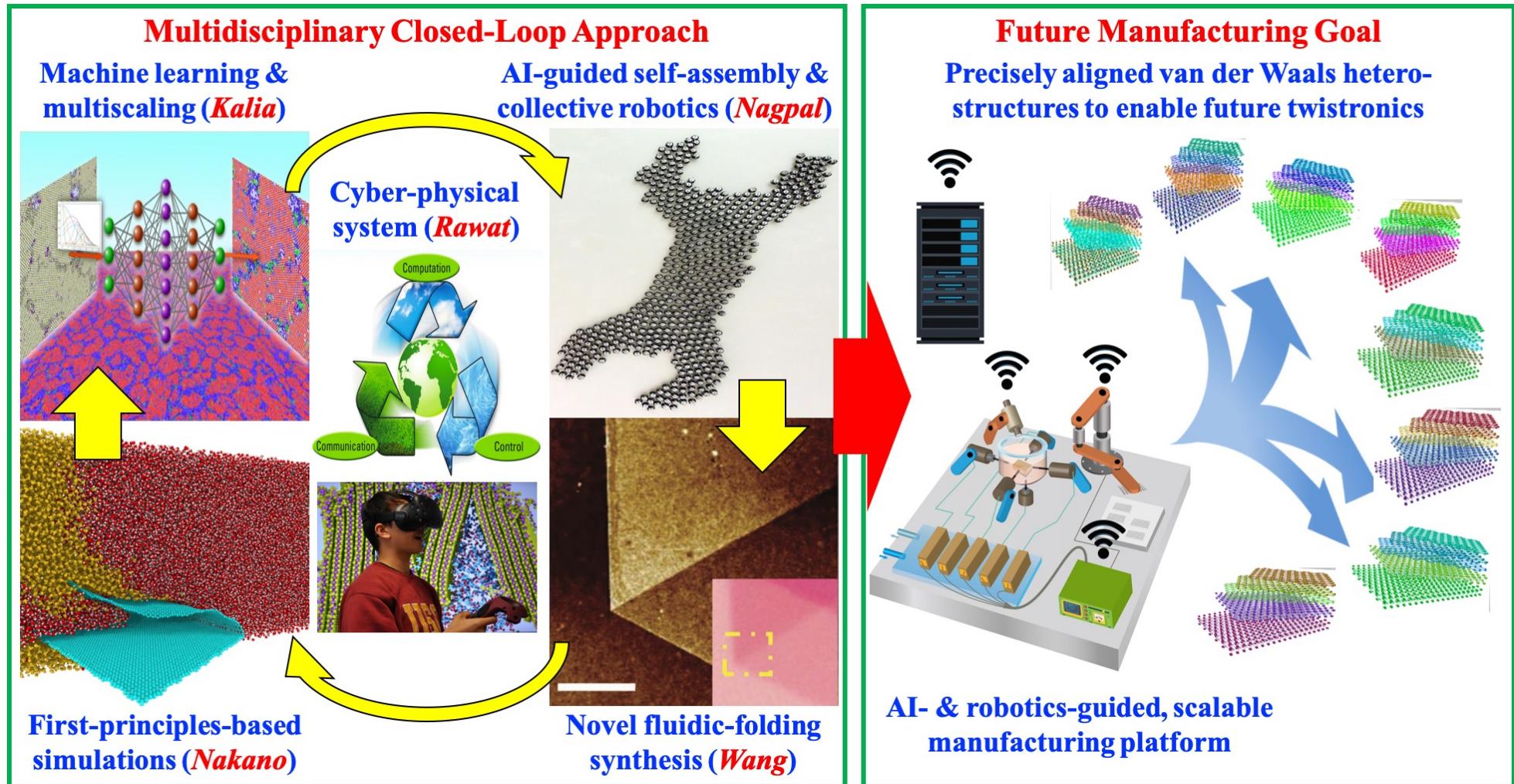


AI tools for materials design

You will have a glimpse of QXMD, RXMD, MAITAI

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 25-26, 2024

Tuesday, June 25, 2024		
Time (PT)	Topic	Instructor
8:00 - 9:00 am	Introduction and logistics	Aiichiro Nakano
9:00 - 10:00 am	Molecular dynamics simulation basics	Priya Vashishta
10:00 - 11:00 am	Quantum molecular dynamics lecture	Aiichiro Nakano
11:00 am - 12:00 pm	Lunch break	
12:00 - 1:30 pm	Quantum molecular dynamics hands on: QXMD code	Anikeya Aditya (main), Taufeq Razakh (sub), Hinata Hokyo, Logan Yamamoto
1:30 - 2:30 pm	Reactive molecular dynamics lecture	Ken-ichi Nomura
Wednesday, June 26, 2024		
Time (PT)	Topic	Instructor
8:00 - 9:30 am	Reactive molecular dynamics hands on: RXMD code	Nitish Baradwaj (main), Jingxin Zhang (sub), Pranab Sarker, Tyler Zheng
9:30 - 10:30 am	Machine learning and AI basics	Ken-ichi Nomura
10:30 am - 11:30 am	Lunch break	
11:30 am - 1:30 pm	Machine learning and AI hands-on	Ruru Ma (main), Tian Sang (sub), Taufeq Razakh
1:30 - 2:30 pm	Participant presentations	Pratibha Dev, Tao Wei

1. QXMD

2. RXMD

3. MAITAI

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

Logistics

- **Workshop courseware (lecture slides & Jupyter notebooks) is available at**
<https://cybermagics.netlify.app/workshop-resources.html>
- **Hands on training will use cloud resources**
Google Colab (QXMD, RXMD, AI–machine learning)
<https://colab.research.google.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 Wednesday (or simple self-introduction)**

Now, introduction of instructors & group photo