

CyberMAGICS Workshop

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

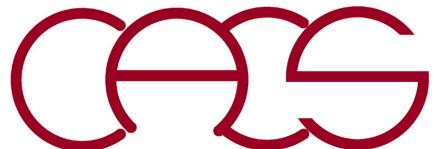
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Supported by National Science Foundation,
Award OAC-2118061

June 30, 2022



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

Participants (11)

Icon	Name	Options
AN	Aichiro Nakano (Host, me)	Speaker Mute
KN	Ken-ichi Nomura	Speaker Mute
P	Pranab Sarker	Speaker Mute
PV	Priya Vashishta	Speaker Mute
t	tao.wei	Speaker Mute
BD	BD Kim (USC)	Speaker Mute
PD	Pratibha Dev	Speaker Mute
TT	Timothy Tizhe Fidelis	Speaker Mute

Chat

To: Everyone

Type message here...

Screenshot

*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 Has Just Arrived!

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

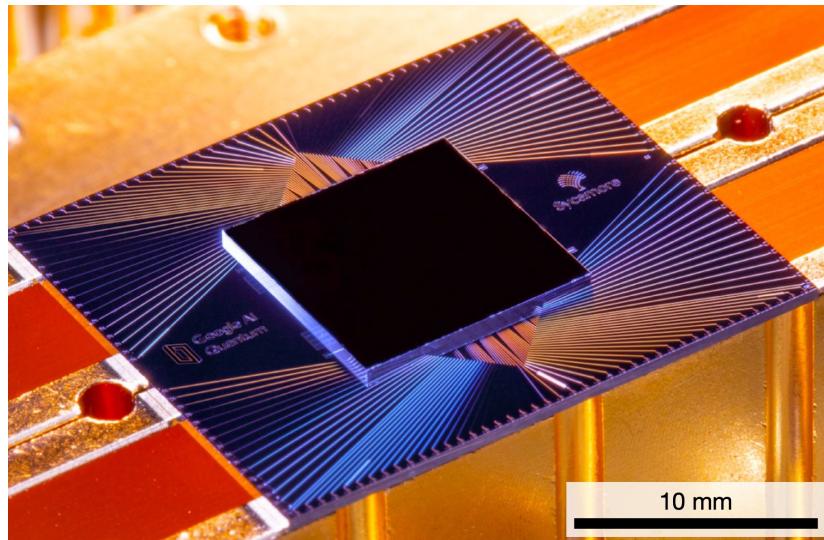
Postexascale Computing for Science



Compute Cambrian explosion



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!

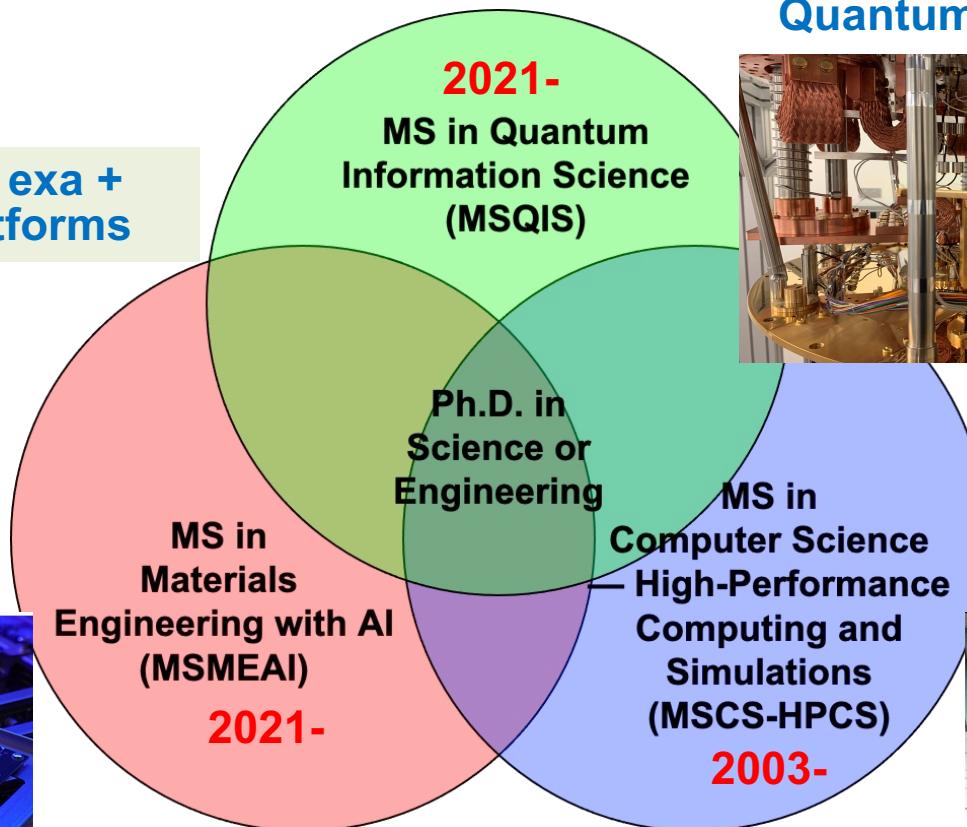
Training Cyber Science Workforce

- New generation of computational scientists at the **nexus of exascale computing, quantum computing & AI**
- Unique dual-degree program: 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

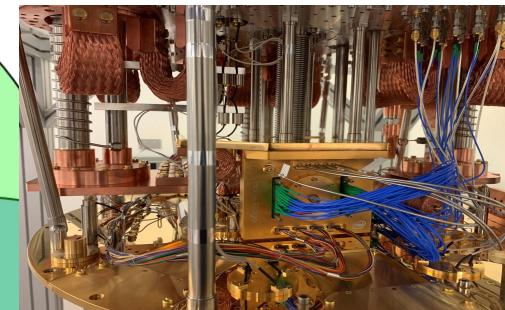
Cybertraining on exa +
quantum + AI platforms



Neuromorphic
Pohoiki Springs



Horse Ridge II
Quantum computer

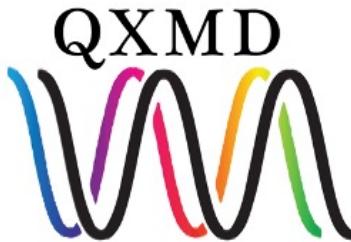


Exascale
Aurora



AIQ-XMaS Software Suite

AI & Quantum-Computing Enabled Exa Quantum Materials Simulator

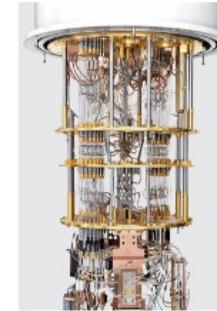


Nonadiabatic quantum molecular dynamics



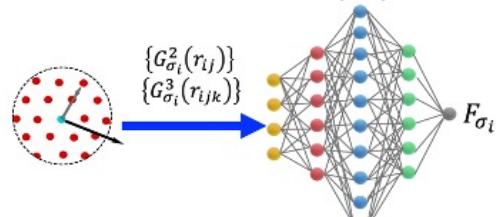
Augmented-reality user interface

MISTIQS



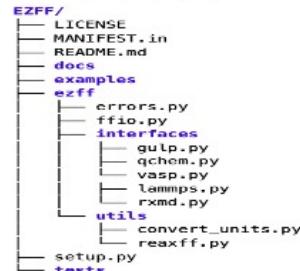
Quantum many-body dynamics on quantum computers

RXMD-NN



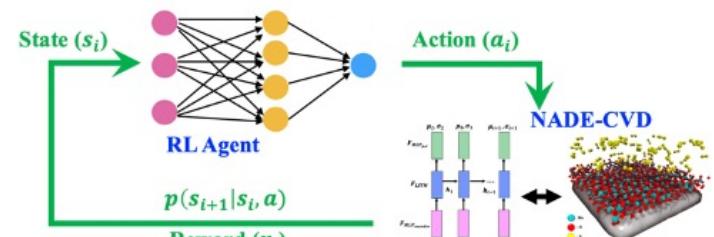
Reactive & neural-network molecular dynamics

EZFF



Easy force-field parameterization & uncertain quantification

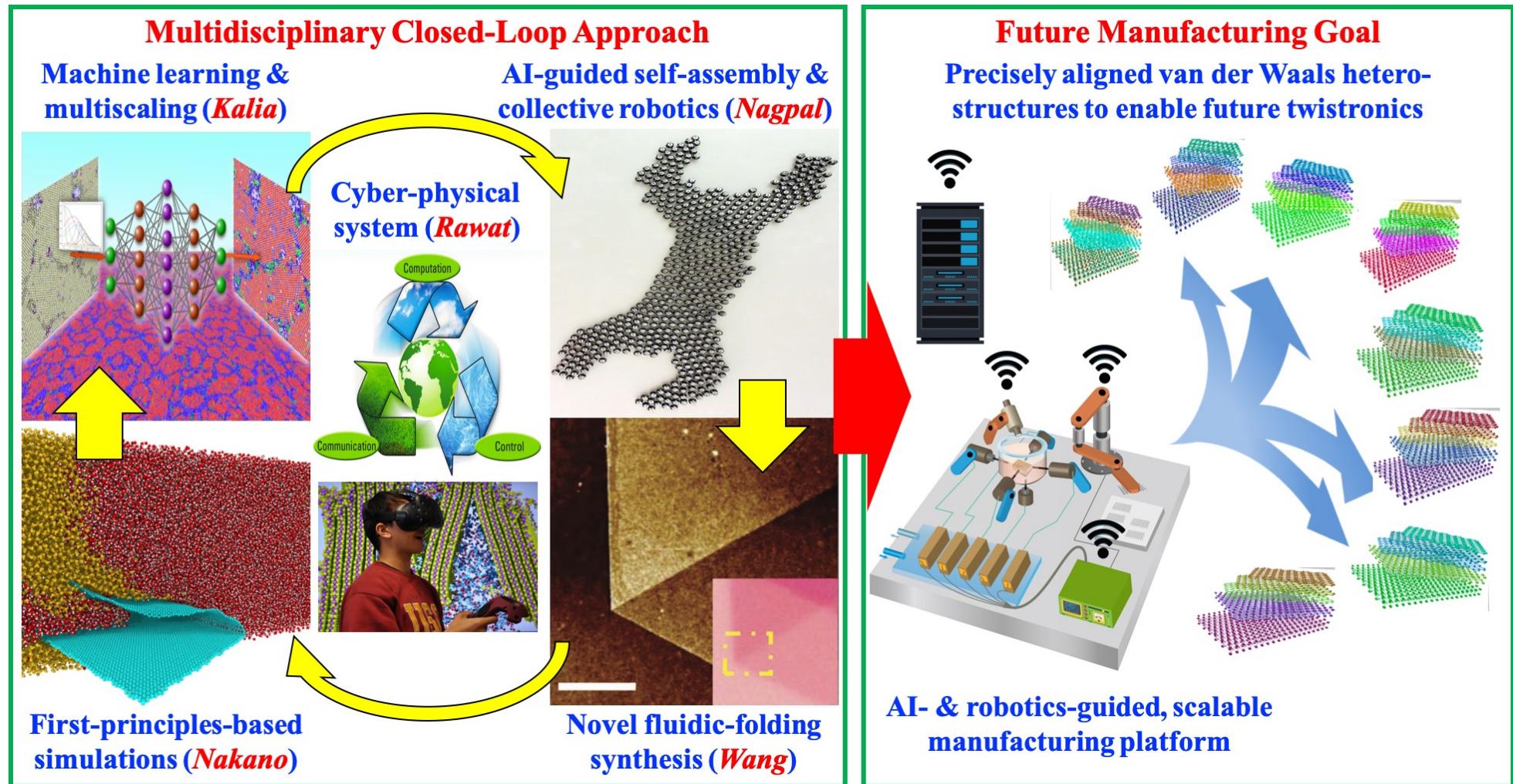
MAITAI



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 30 – July 2, 2022

Thursday, June 30, 2022		
Time (PDT)	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	Reactive molecular dynamics basics	Ken-ichi Nomura
11:00 am - 12:00 pm	Lunch break	
12:00 - 2:00 pm	Reactive molecular dynamics hands on: RXMD code	Ankit Mishra, Nitish Baradwaj
2:00 - 3:00 pm	Machine learning basics	Ken-ichi Nomura
Friday, July 1, 2022		
Time (PDT)	Topic	Instructor
8:00 - 9:00 am	Machine learning hands-on	Ankit Mishra, Nitish Baradwaj
9:00 - 10:00 am	Quantum molecular dynamics basics	Aiichiro Nakano
10:00 - 11:00 am	Quantum molecular dynamics hands-on: QXMD code (part 1)	Thomas Linker, Anikeya Aditya
11:00 am - 12:00 pm	Lunch break	
12:00 - 1:00 pm	Quantum molecular dynamics hands-on: QXMD code (part 2)	Thomas Linker, Anikeya Aditya
1:00 - 3:00 pm	Quantum computing basics and hands-on	Aiichiro Nakano, Shogo Fukushima
Saturday, July 2, 2022		
Time (PDT)	Topic	Instructor
9:00 - 11:00 am	Participant presentations	All participants
11:00 - 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**