CyberMAGICS Workshop

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*Now at *University of South Carolina***

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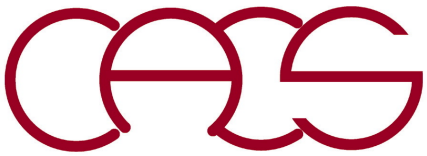
June 5, 2025

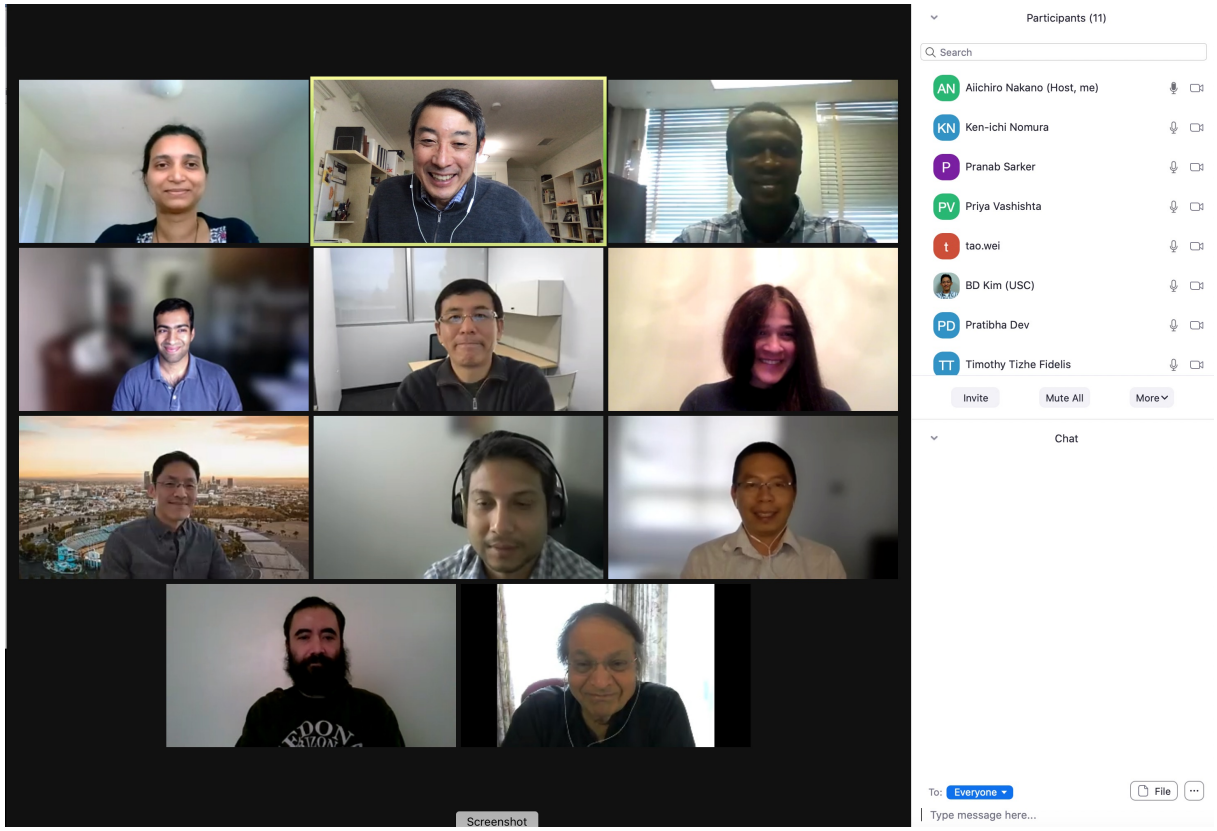


HOWARD UNIVERSITY

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 (2021-26) project

Nakano, Nomura, Vashishta (USC); Dev, Wei (Howard)

Exaflop/s Computing Is Here

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**El Capitan** - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States	11,039,616	1,742.00	2,746.38	29,581
2	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE Cray OS, HPE DOE/SC/Oak Ridge National Laboratory United States	9,066,176	1,353.00	2,055.72	24,607
3	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	9,264,128	1,012.00	1,980.01	38,698
4	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States	2,073,600	561.20	846.84	
5	**HPC6** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, RHEL 8.9, HPE Eni S.p.A. Italy	3,143,520	477.90	606.97	8,461

Exaflop/s: 10^{18} floating-point operations per second = 10^{3} Petaflop/s

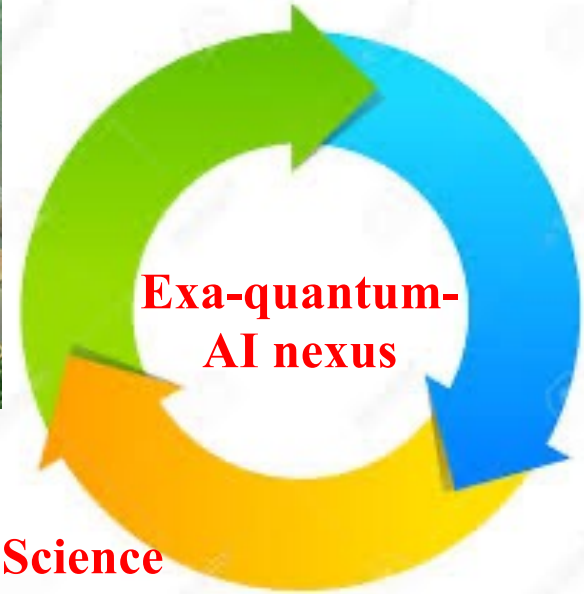
https://www.top500.org

Changing Computing Landscape for Science

Postexascale Computing for Science

Deelman *et al.*: *Science* **387**, 829 ('25)

Compute Cambrian explosion



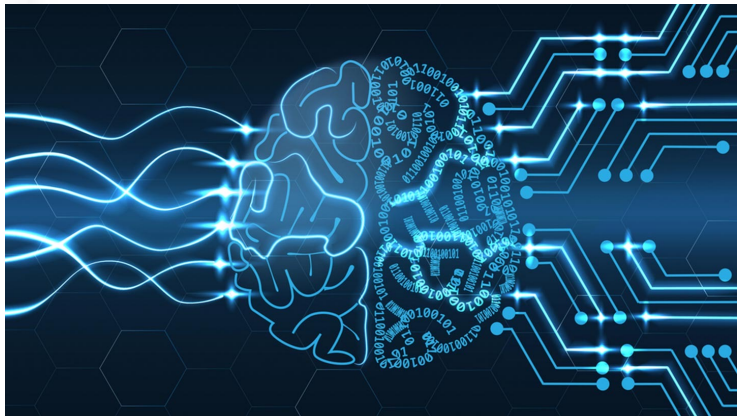
AI for Science

DOE readies multibillion-dollar AI push

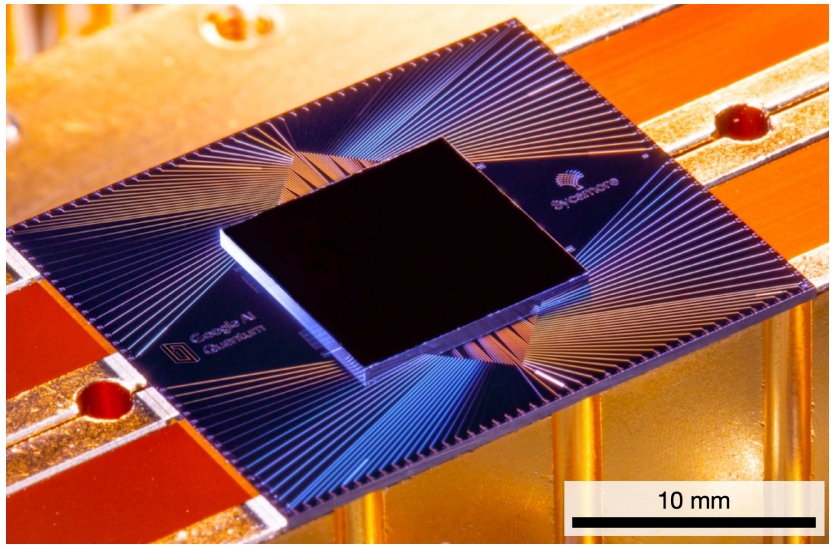
U.S. supercomputing leader is the latest big backer in a globally crowded field

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

Science **366**, 559 ('19)



Quantum Computing for Science

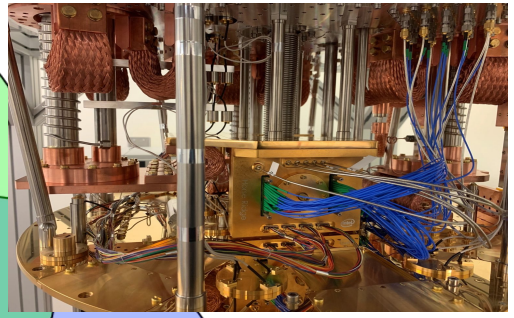


Use all to advance science!

Training Cyber Science Workforce

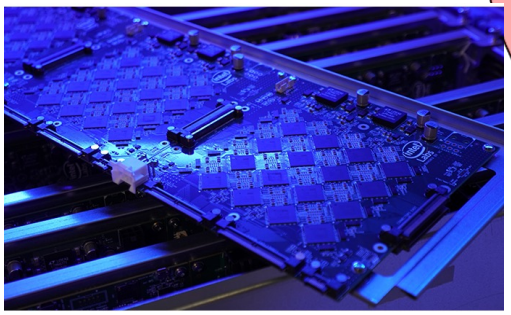
- New generation of computational scientists at the nexus of exascale computing, quantum computing & AI
- Unique dual-degree program at USC: Ph.D. in materials science or physics, along with MS in computer science specialized in high-performance computing & simulations, MS in quantum information science,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

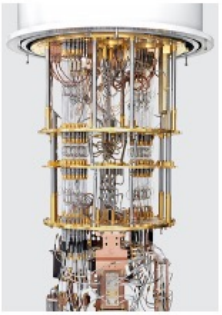
QXMD

Nonadiabatic quantum molecular dynamics

GEARS

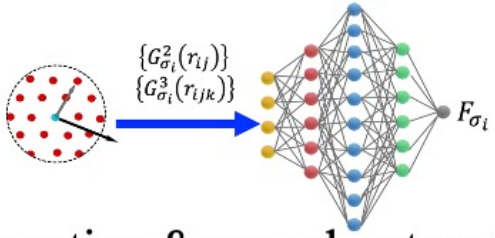
Augmented-reality user interface

MISTIQS



Quantum many-body dynamics on quantum computers

RXMD-NN



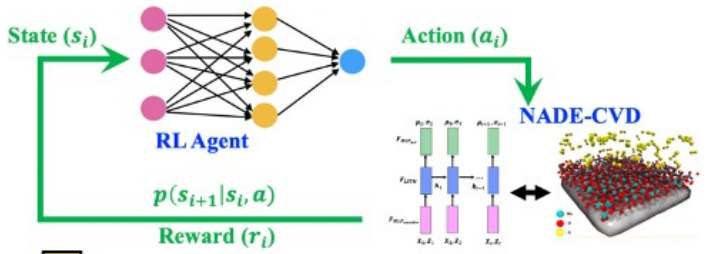
Reactive & neural-network molecular dynamics

EZFF

```
EZFF/
├── LICENSE
├── MANIFEST.in
├── README.md
├── docs
├── examples
├── ezff
│   ├── errors.py
│   ├── ffio.py
│   ├── interfaces
│   │   ├── gulp.py
│   │   ├── qchem.py
│   │   ├── vasp.py
│   │   ├── lammps.py
│   │   └── rxmd.py
│   └── utils
│       ├── convert_units.py
│       └── reaxff.py
├── setup.py
└── tests
```

Easy force-field parameterization & uncertain quantification

MAITAI



AI tools for materials design

You will have a glimpse of QXMD, RXMD, MAITAI

Agenda: June 5-6, 2025

Thursday, June 5, 2025		
Time (PT)	Topic	Instructor
8:00 - 9:00 am	Introduction and logistics	Aiichiro Nakano
9:00 - 9:40 am	Molecular dynamics simulation basics	Priya Vashishta
9:40 – 10:20 am	Density functional theory basics	Pratibha Dev, Tao Wei
10:20 - 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	Nabankur Dasgupta (main), Taufeq Razakh (sub), Anikeya Aditya, Suryakanti Debata
1:30 - 2:30 pm	Reactive molecular dynamics lecture	Ken-ichi Nomura
Friday, June 6, 2025		
Time (PT)	Topic	Instructor
8:00 - 9:30 am	Reactive molecular dynamics hands on: RXMD code	Marco Olguin (main), Tian Sang (sub), Nitish Baradwaj, Pranab Sarker
9:30 - 10:30 am	Machine learning and AI lecture	Ken-ichi Nomura
10:30 am - 11:30 am	Lunch break	
11:30 am - 1:30 pm	Machine learning and AI hands-on	Tian Sang (main), Marco Olguin (sub), Ruru Ma
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 Friday (or simple self-introduction)**

Now, introduction of instructors & group photo