CSCI653: High Performance Computing & Simulations

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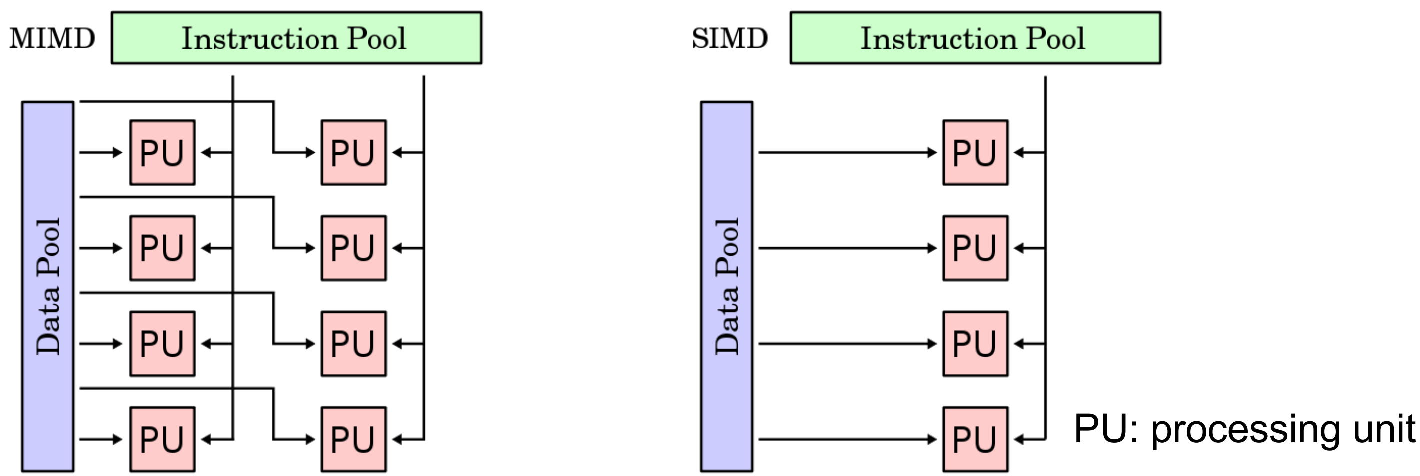
Do "Your" Science Using High Performance Computing

CSCI653 at a Glance: Applications

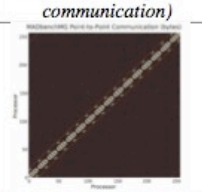
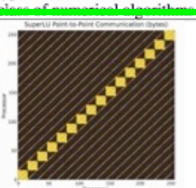
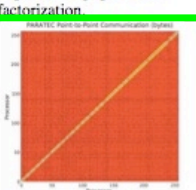
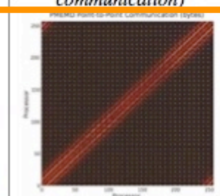
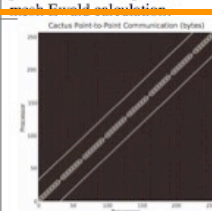
- High performance computing (HPC) with archetypal real-world applications
  > Molecular dynamics (MD): interaction
  > Multiple-instruction multiple-data (MIMD)

  > Quantum dynamics (QD): data parallelism
  > Single-instruction multiple-data (SIMD)
- Hybrid multiscale/multiphysics applications
- Deterministic *vs*. stochastic (to solve intractable) applications
- Data + learning + visualization



The Landscape of Parallel Computing Research: A View from Berkeley Why MD & QD?

7 dwarfs (a dwarf is an algorithmic method that captures a pattern of computation and communication) + 6 combinatorial

Dwarf	*Description*	*Communication Pattern (Figure axes show processors 1 to 256, with black meaning no communication)*	*NAS Benchmark / Example HW*
1. Dense Linear Algebra (e.g., BLAS [Blackford et al 2002], ScaLAPACK [Blackford et al 1996], or MATLAB [MathWorks 2006])	Data are dense matrices or vectors. (BLAS Level 1 = vector-vector; Level 2 = matrix-vector; and Level 3 = matrix-matrix.) Generally, such applications use unit-stride memory accesses to read data from rows, and strided accesses to read data from columns.	 The communication pattern of MadBench, which makes heavy use of ScaLAPACK for parallel dense linear algebra, is typical of a much broader class of numerical algorithms.	Block Triadiagonal Matrix, Lower Upper Symmetric Gauss-Seidel / Vector computers, Array computers
2. Sparse Linear Algebra (e.g., SpMV, OSKI [OSKI 2006], or SuperLU [Demmel et al 1999])	Data sets include many zero values. Data is usually stored in compressed matrices to reduce the storage and bandwidth requirements to access all of the nonzero values. One example is block compressed sparse row (BCSR). Because of the compressed formats, data is generally accessed with indexed loads and stores.	 SuperLU (communication pattern pictured above) uses the BCSR method for implementing sparse LU factorization.	Conjugate Gradient / Vector computers with gather/scatter
3. Spectral Methods (e.g., FFT [Cooley and Tukey 1965])	Data are in the frequency domain, as opposed to time or spatial domains. Typically, spectral methods use multiple butterfly stages, which combine multiply-add operations and a specific pattern of data permutation, with all-to-all communication for some stages and strictly local for others.	 PARATEC: The 3D FFT requires an all-to-all communication to implement a 3D transpose, which requires communication between every link. The diagonal stripe describes BLAS-3 dominated linear-algebra step required for orthogonalization.	Fourier Transform / DSPs, Zalink PDSP [Zarlink 2006]
4. N-Body Methods (e.g., Barnes-Hut [Barnes and Hut 1986], Fast Multipole Method [Greengard and Rokhlin 1987])	Depends on interactions between many discrete points. Variations include particle-particle methods, where every point depends on all others, leading to an $O(N^2)$ calculation, and hierarchical particle methods, which combine forces or potentials from multiple points to reduce the computational complexity to O(N log N) or O(N).	 PMEMD's communication pattern is that of a particle mesh Ewald calculation.	(no benchmark) / GRAPE [Tokyo 2006], MD-GRAPE [IBM 2006]
5. Structured Grids (e.g., Cactus [Goodale et al 2003] or Lattice-Boltzmann Magneto-hydrodynamics [LBMHD 2005])	Represented by a regular grid; points on grid are conceptually updated together. It has high spatial locality. Updates may be in place or between 2 versions of the grid. The grid may be subdivided into finer grids in areas of interest ("Adaptive Mesh Refinement"); and the transition between granularities may happen dynamically.	 Communication pattern for Cactus, a PDE solver using 7-point stencil on 3D block-structured grids.	Multi-Grid, Scalar Penta-diagonal / QCDOC [Edinburg 2006], BlueGeneL
6. Unstructured Grids (e.g., ABAQUS [ABAQUS 2006] or FIDAP [FLUENT 2006])	An irregular grid where data locations are selected, usually by underlying characteristics of the application. Data point location and connectivity of neighboring points must be explicit. The points on the grid are conceptually updated together. Updates typically involve multiple levels of memory reference indirection, as an update to any point requires first determining a list of neighboring points, and then loading values from those neighboring points.		Unstructured Adaptive / Vector computers with gather/scatter, Tera Multi Threaded Architecture [Berry et al 2006]
7. Monte Carlo (e.g., Quantum Monte Carlo [Aspuru-Guzik et al 2005])	Calculations depend on statistical results of repeated random trials. Considered embarrassingly parallel.	Communication is typically not dominant in Monte Carlo methods.	Embarrassingly Parallel / NSF Teragrid

In performance optimization

MD

QD

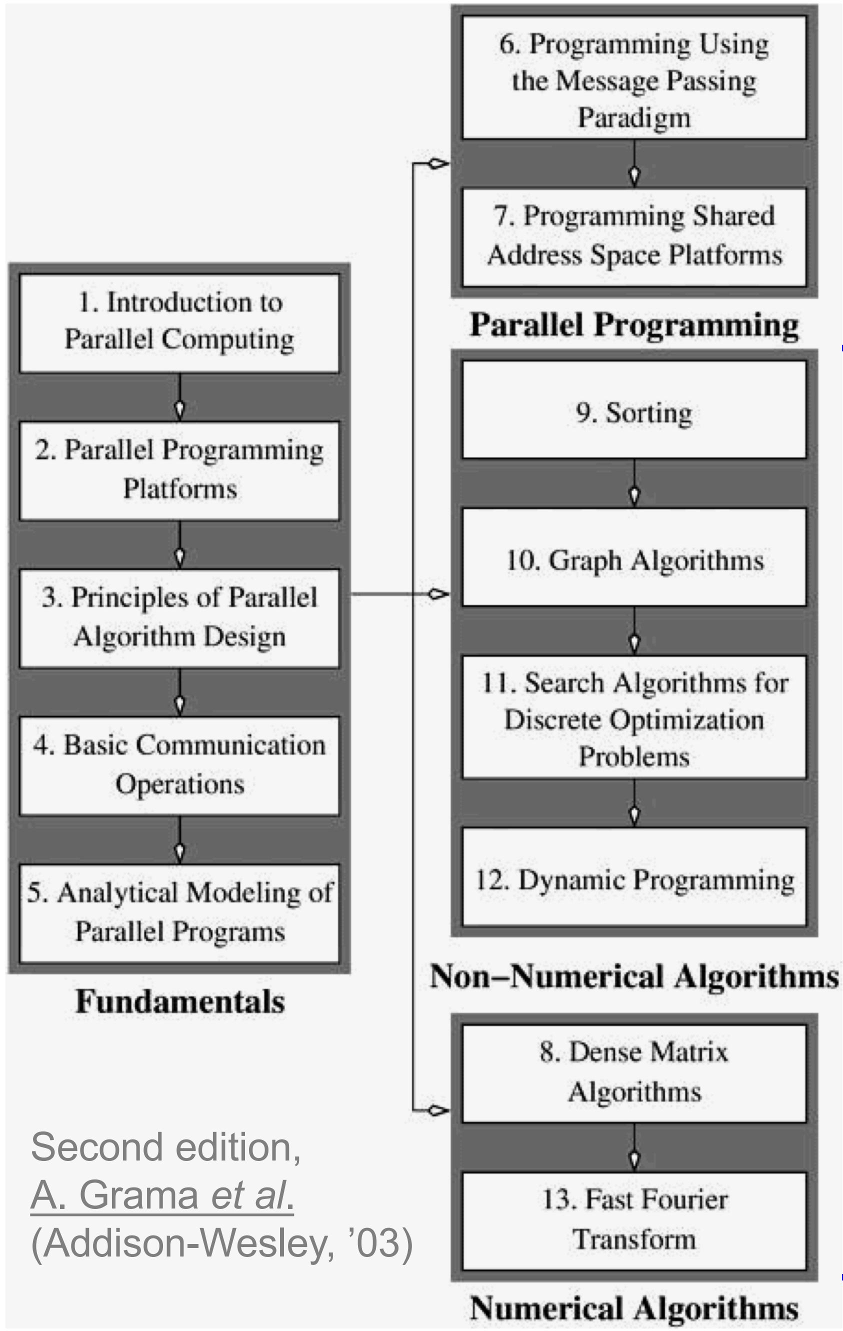
Monte Carlo

https://www2.eecs.berkeley.edu/Pubs/TechRpts/2006/EECS-2006-183.html

CSCI653: Algorithms & Tools

- ***Just one thing*: Divide-conquer-“recombine” (DCR) algorithm; it’s data locality!**
- ***Parallel computing = decomposition (who does what)*: Scalability analysis; performance optimization**
- ***Programming languages*: MPI (distributed memory) + OpenMP (shared memory) + CUDA|OpenMP target| SYCL (heterogeneous accelerator)**

Introduction to Parallel Computing



MPI

OpenMP

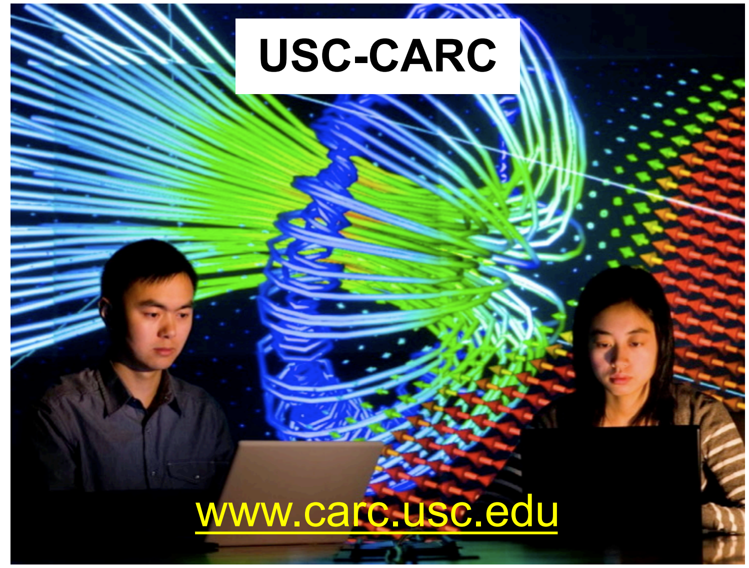
SIMD, MIMD *etc.*

Decomposition

Scalability analysis

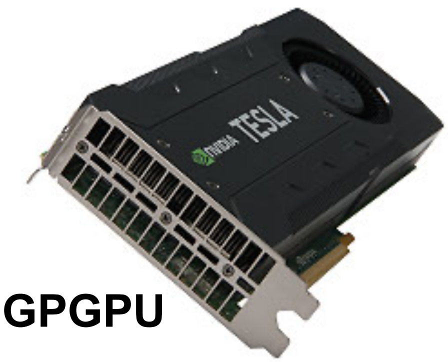
Covered in hardware & MD/QD lectures

High Performance Computing (HPC)

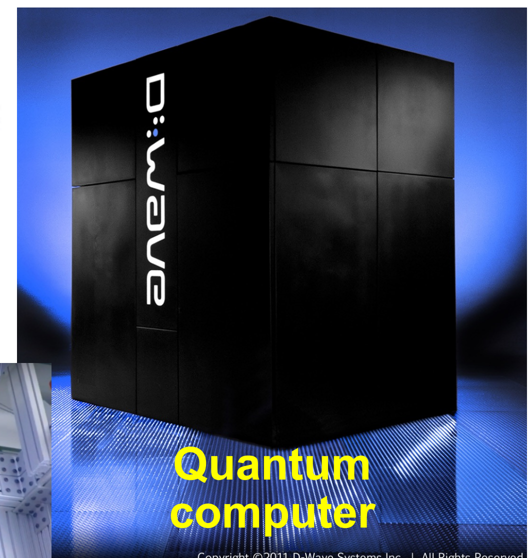


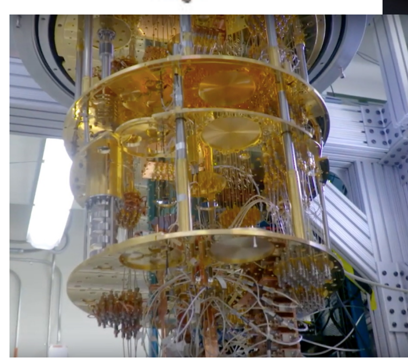
- *USC CARC (Center for Advanced Research Computing)*: **10,000+ CPU cores accelerated by GPUs**
- *USC ISI (Information Sciences Institute)*: **1,098-qubit D-Wave quantum computer**

Petaflop/s = 10^{15} mathematical operations per second
Exaflop/s = 10^{18} mathematical operations per second



GPGPU





QPU

Current & Future Supercomputing

- **Won two DOE supercomputing awards to develop & deploy metascalable ("design once, scale on future platforms") simulation algorithms**

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

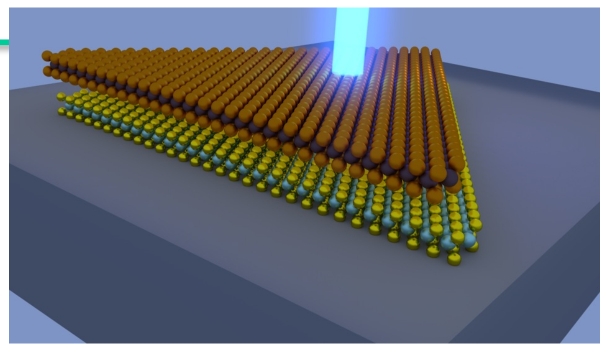
- **Atomistic simulations on million cores (pre-exascale)**

Innovative & Novel Computational Impact on Theory & Experiment

Title: AI-Guided Exascale Simulations of Quantum Materials Manufacturing and Control
PI and Co-PIs: Aiichiro Nakano–PI, Rajiv K. Kalia, Ken-ichi Nomura, Priya Vasishta

786,432-core IBM Blue Gene/Q
281,088-core Intel Xeon Phi
560-node (2,240-GPU) AMD/NVIDIA Polaris

AURORA | EARLY SCIENCE PROGRAM



Early Science Projects for Aurora Supercomputer Announced

Metascalable layered materials genome

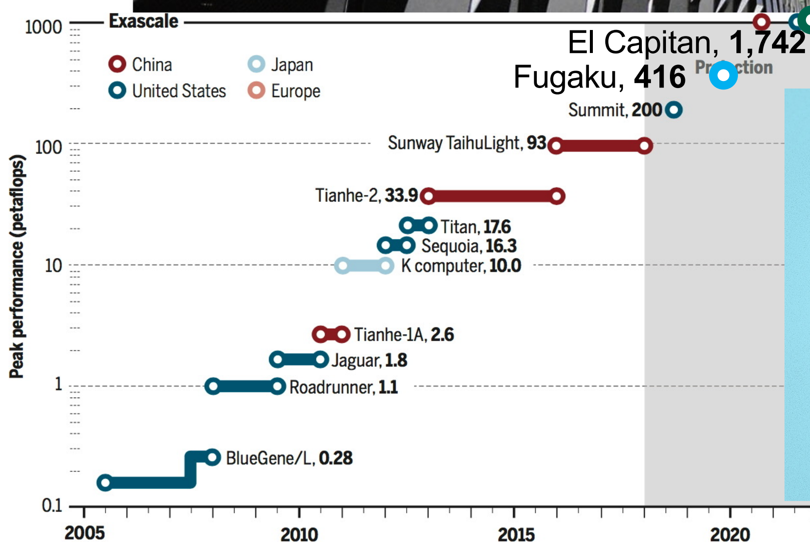
Investigator: Aiichiro Nakano, University of Southern California

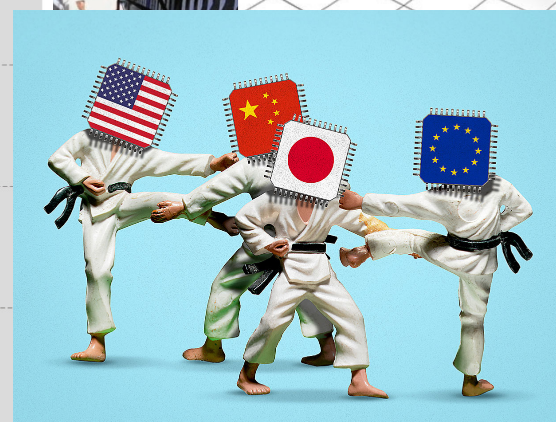
1.01 exaflop/s
Intel Aurora

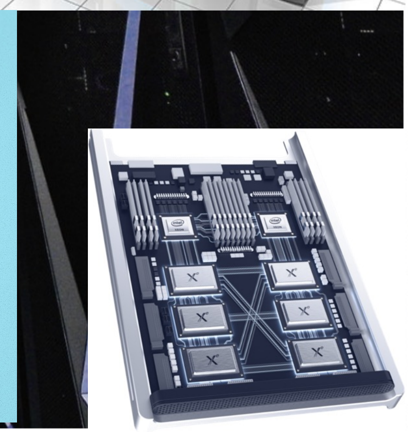
Exaflop/s = 10^{18} mathematical operations per second

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

CACS@Aurora in the Global Exascale Race







R. F. Service, *Science* **359**, 617 ('18)

SUPERCOMPUTING

Design for U.S. exascale computer takes shape

Competition with China accelerates plans for next great leap in supercomputing power

Exa(peta)flop/s = 10^{18} (10^{15}) floating-point operations per second

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.

https://www.tomshardware.com/news/two-chinese-exascale-supercomputers

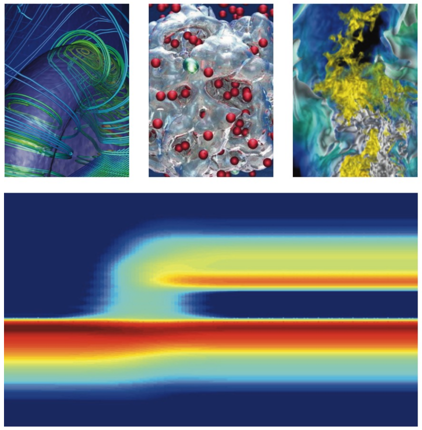
Exa-leadership

BES

BASIC ENERGY SCIENCES

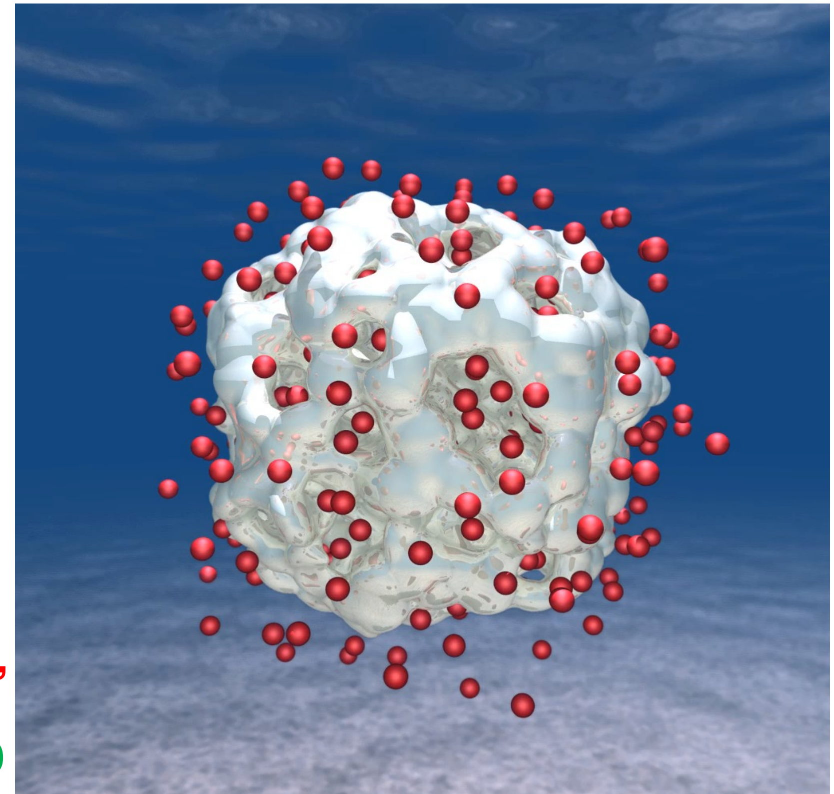
EXASCALE REQUIREMENTS REVIEW

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

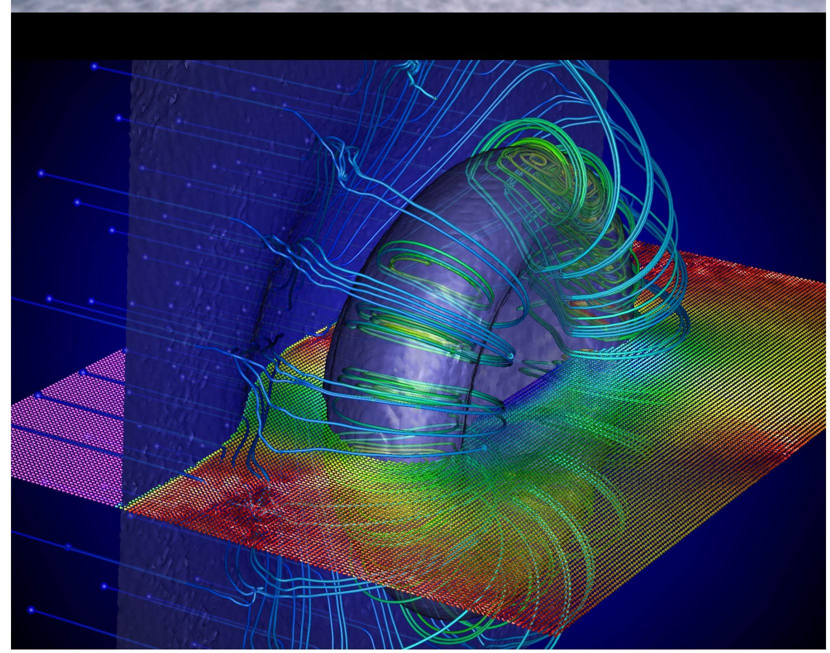
Shimamura *et al.*, *Nano Lett.* 14, 4090 ('14)

QD

On-demand hydrogen production from water

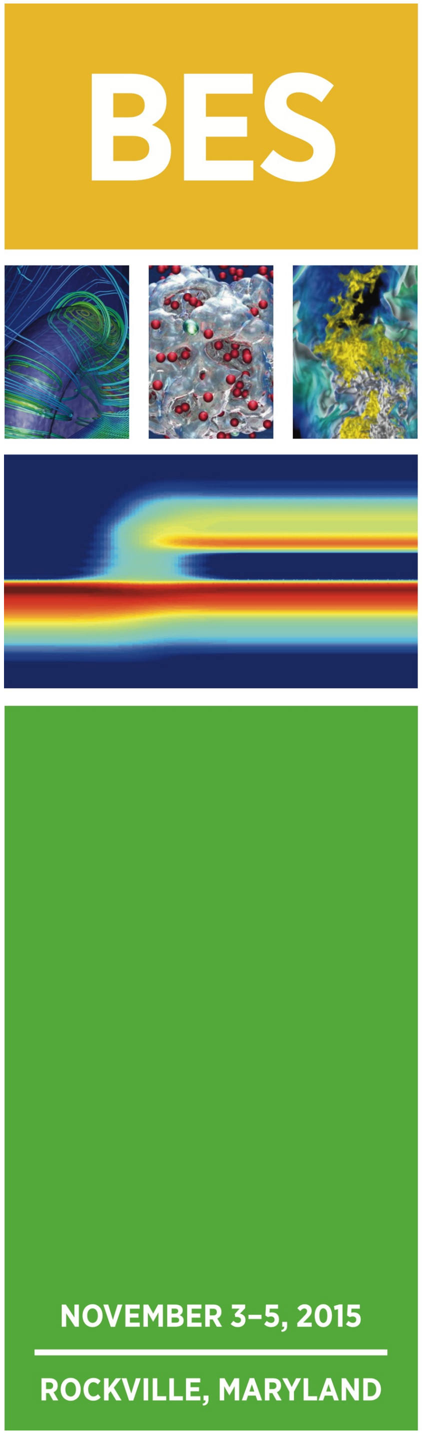
10^9-atom RMD

Shekhar *et al.*, *Phys. Rev. Lett.* 111, 184503 ('13)



MD

U.S. DEPARTMENT OF ENERGY



BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

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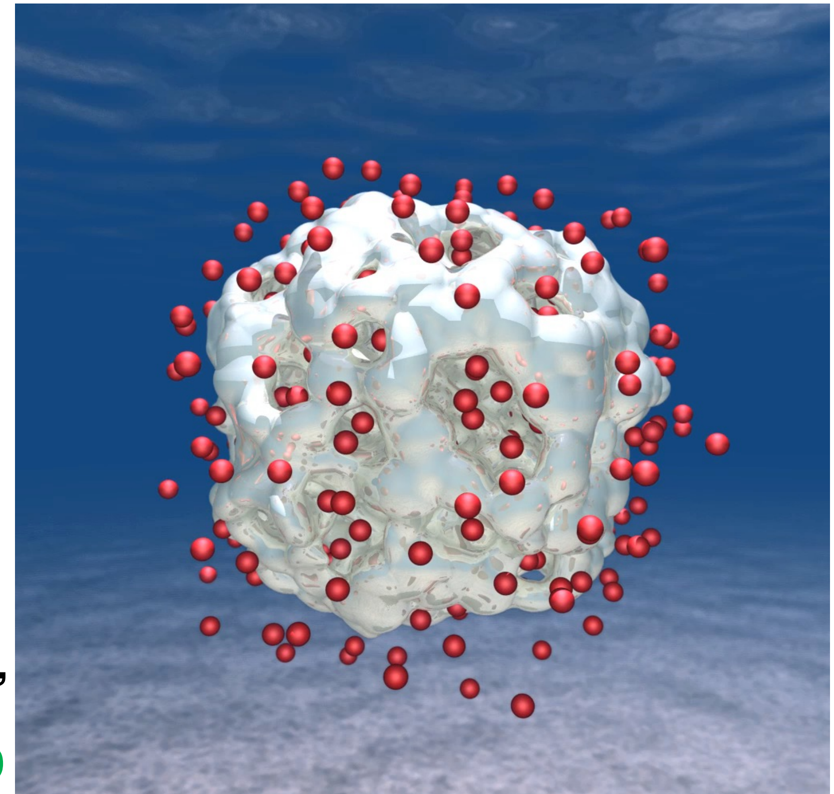
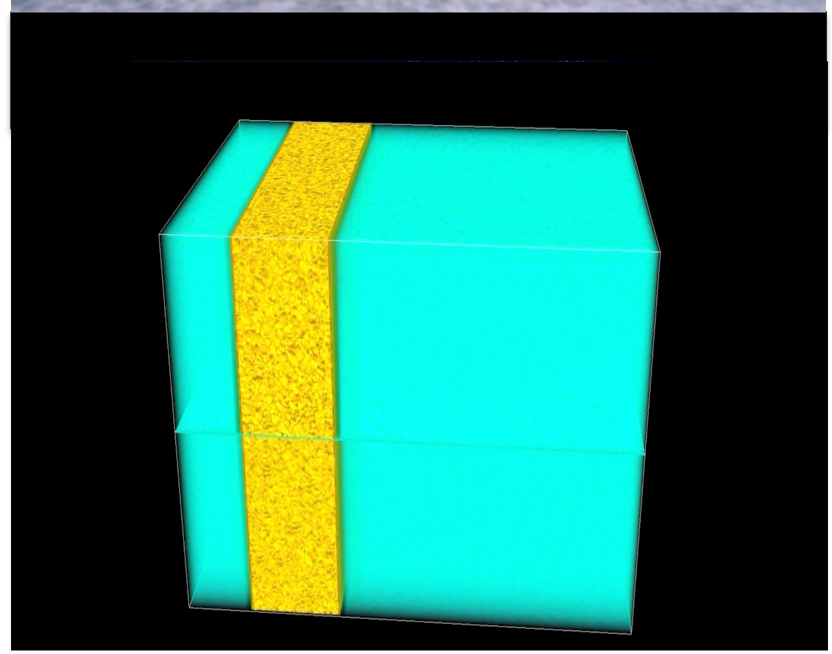


16,661-atom QMD

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



10^9-atom RMD

Shekhar *et al*.,
Phys. Rev. Lett.
111, 184503 ('13)

Fluid dynamics
atom-by-atom

MD

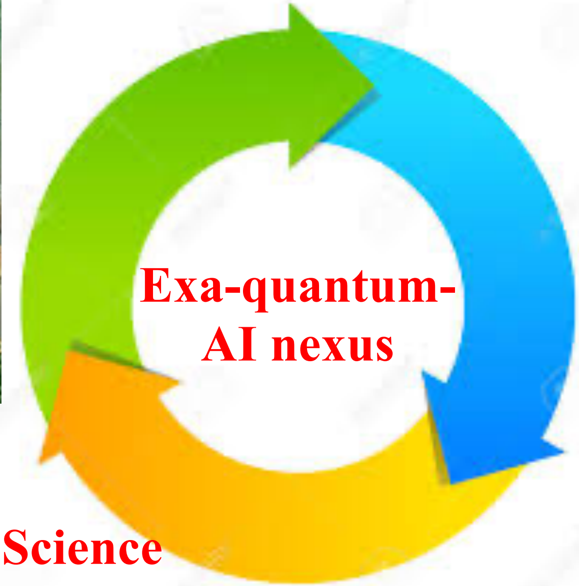
U.S. DEPARTMENT OF
ENERGY

Changing Computing Landscape for Science

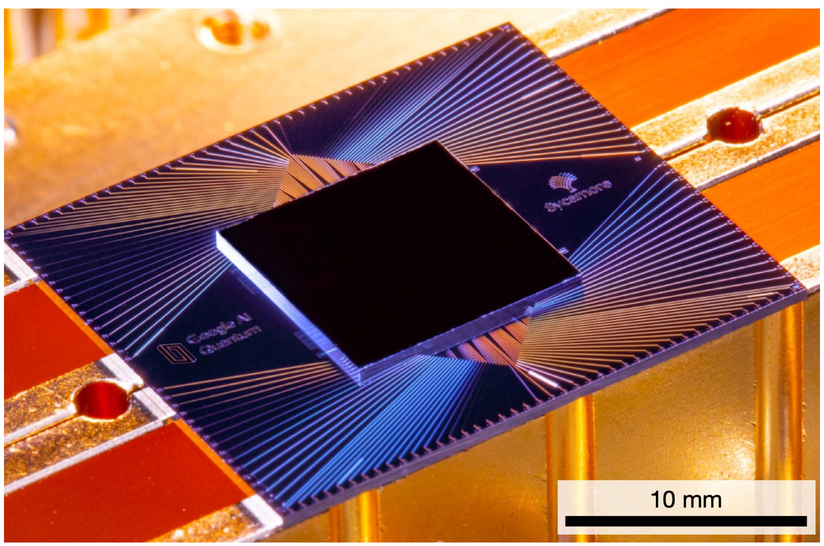
Postexascale Computing for Science

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

Compute Cambrian explosion



Quantum Computing for Science



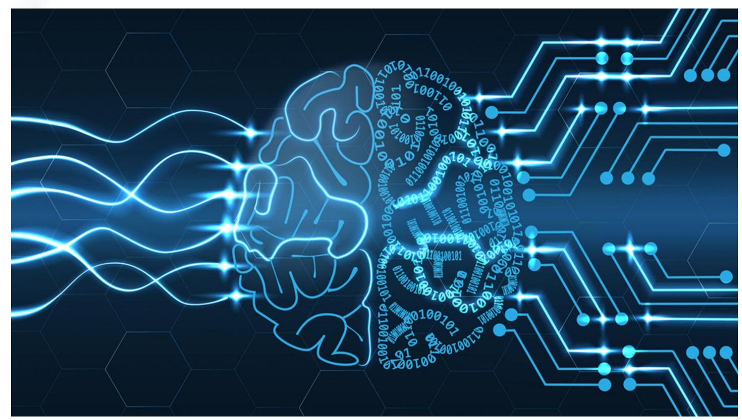
AI for Science

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 ('19)



Use all to advance science!

Glimpse of Compute Cambrian Explosion

ALCF AI Testbed

ALCF AI Testbed Systems are in production and available for allocations to the research community
https://accounts.alcf.anl.gov/#/allocationRequests

8 nodes each with 8 Reconfigurable DataFlow Units (RDU)

SambaNova SN-30

2 CS-2 Wafer scale engines (WSE)

Upgrading to CS-3

Cerebras CS-2

4 nodes each with 16 Intelligent Processing Units (IPUs)

Graphcore Bow Pod64

9 nodes each with 8 GroqChip Tensor streaming processors (TSP)

Groq

Coming Soon !
Sambanova SN40L
Inference/Finetuning

NSF https://nairrpilot.org

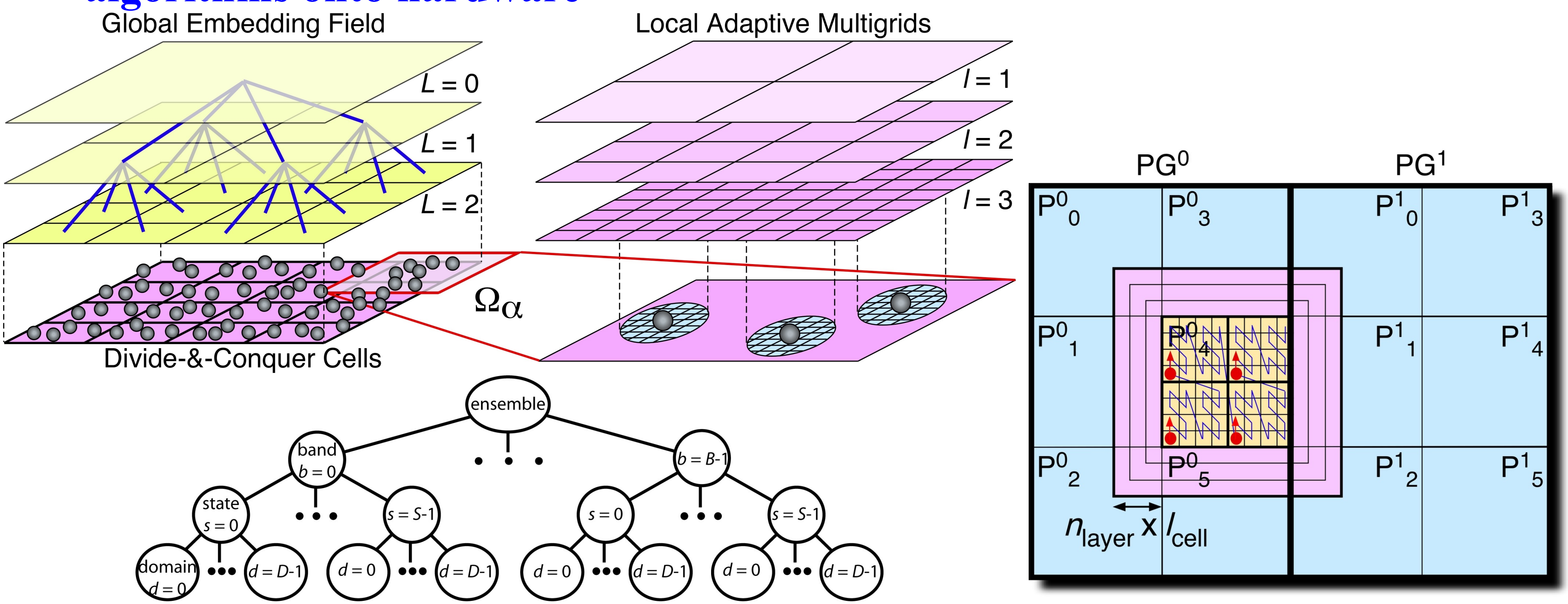
Argonne NATIONAL LABORATORY

https://extremecomputingtraining.anl.gov/agenda-2025/

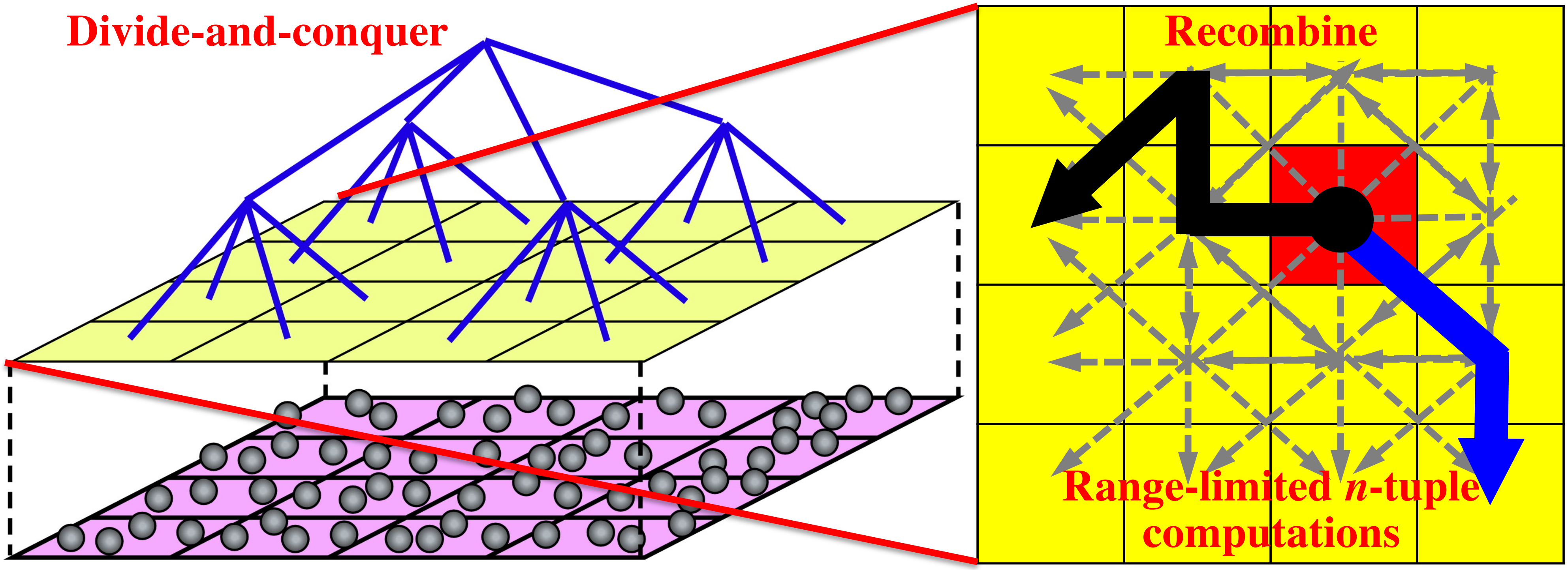
A Metascalable Dwarf

A metascalable (or "design once, scale on new architectures") parallel-computing framework for broad applications (*e.g*. equation solvers, constrained optimization, search, visualization and graphs)

- **Divide-conquer-"recombine" (DCR) algorithms based on spatial locality to design linear-scaling algorithms**
- **Space-time-ensemble parallel (STEP) approach based on temporal locality to predict long-time dynamics**
- **Tunable hierarchical cellular decomposition (HCD) to map these scalable algorithms onto hardware**



Divide-Conquer-Recombine (DCR) Engines



M. Kunaseth *et al*., *ACM/IEEE SC13*

- **Lean divide-&-conquer density functional theory (LDC-DFT) algorithm minimizes the prefactor of $O(N)$ computational cost**

  F. Shimojo *et al*., *J. Chem. Phys.* **140**, 18A529 ('14); S. Tiwari *et al*., *HPCAsia* Best Paper ('20)

- **Extended-Lagrangian reactive molecular dynamics (XRMD) algorithm eliminates the speed-limiting charge iteration**

  K. Nomura *et al*., *Comput. Phys. Commun*. **192**, 91 ('15); K. Liu *et al*., *IEEE/ACM ScalA18*

N. Romero *et al*., *IEEE Computer* **48(11)**, 33 ('15)

But ...

- **High performance computing (HPC) is at a historic crossroads, where traditional modeling & simulation applications may not survive**

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

- **Computers are increasingly more *heterogeneous* by integrating different functional units, focusing on *low-precision* arithmetic to serve market-dominating AI applications**
- **Light-matter dynamics is a challenging *multiscale/multiphysics problem* involving multiple field & particle equations of different computational characteristic for light, electron, & atoms, extending over electron/atom-to-device scales**

General matrix-matrix multiply (GEMM) performance on Aurora GPU

	One Tile	Full Node	Scaling
DGEMM **64 bits**	15 TFlop/s	179 TFlop/s	11.9
SGEMM **32 bits**	22 TFlop/s	258 TFlop/s	11.7
HGEMM **16 bits**	263 TFlop/s	2606 TFlop/s	9.9
BF16GEMM	273 TFlop/s	2645 TFlop/s	9.7
TF32GEMM	110 TFlop/s	1311 TFlop/s	11.9
I8GEMM **8 bits**	577 TFlop/s	5394 TFlop/s	9.4

To GEMM, or not to GEMM?

cf. **Low-precision arithmetic in DeepSeek** *arXiv*:**2412.19437v1** ('24)

Multiscale/multiphysics/heterogeneity/low-precision challenge

Paradigm Shift: DCR/MSA

- **Solved the multiscale/multiphysics/heterogeneity/low-precision challenge by harnessing heterogeneity & low-precision arithmetic**
- ***Divide-conquer-recombine (DCR) algorithms*** **divide a problem into not only spatial but also physical subproblems of different computational characteristics, which are solved using appropriate methods on best-matching hardware units before recombined into a total solution**
- ***Metamodel-space algebra (MSA)*** **lets subproblems to reside in respective hardware units, while minimizing communication & precision requirements**
- **DCR/MSA delineates subproblems with** ***small dynamic ranges & minimal mutual information*** **with** ***parameterized precision*****, which map well onto AI accelerators that support a spectrum of hybrid precision modes**

Hardware supports precision/speed trade-off

Aurora allows 1|2|3 BF16 values to be accumulated in FP32 to provide varying precision/speed

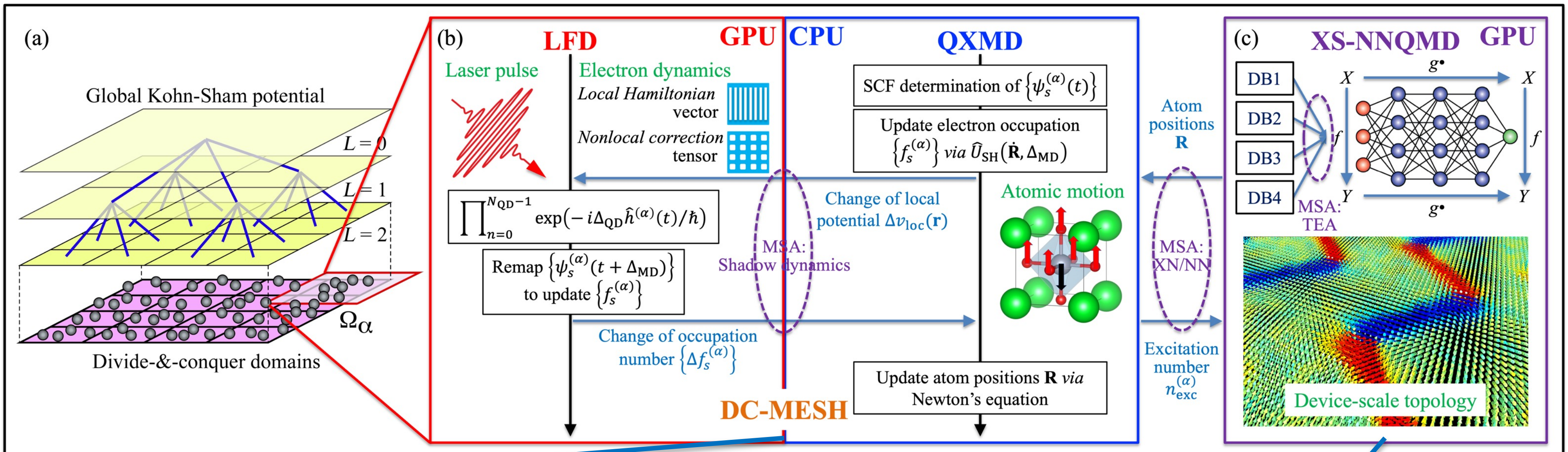
Metascalable (i.e., design-once, scale-to-future) algorithm-hardware co-design opportunities in the post-exascale era

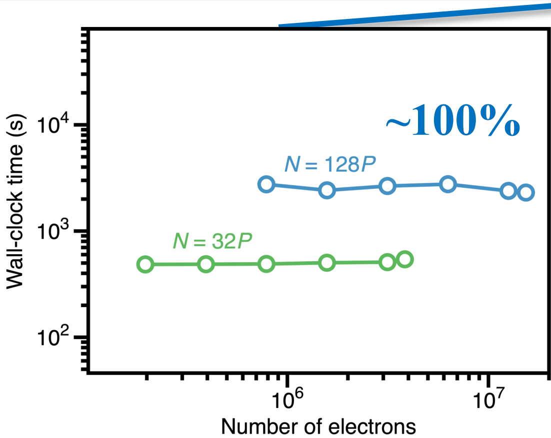
"Multiscale light-matter dynamics in quantum materials: from electrons to topological superlattices"
T. Razakh *et al*. ('25)

Exa Multiscale Light-Matter Dynamics

- ***Breaking the Exaflop/s barrier***: **On 60,000 GPUs of Aurora: 1.87 Exaflop/s; 152× & 3,780× improvements of time-to-solution over state-of-the-art for 15.4M-electron DC-MESH NAQMD & 1.2T-atom excited XS-NNQMD; nearly perfect parallel efficiency**

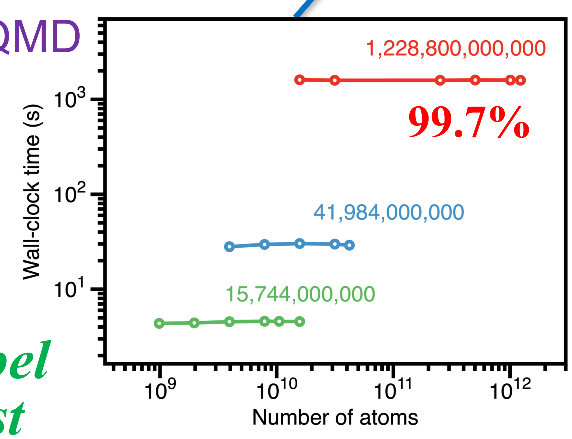
Exaflop/s = 10^{18} mathematical operations per second





DC-MESH NAQMD

XS-NNQMD



2025 Gordon Bell prize (aka Nobel prize of supercomputing) finalist

T. Razakh *et al.* ('25)

Quantum Dynamics on Quantum Computers

- **We have simulated nontrivial quantum dynamics on publicly available IBM's Q16 Melbourne & Rigetti's Aspen NISQ computers, *i.e.*, ultrafast control of emergent magnetism by THz radiation in 2D material** L. Bassman *et al.*, *Phys. Rev. B* **101**, 184305 ('20)

COMPUTING SCIENCES RESEARCH
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APRIL 12, 2022

Miguel
USC sociology
→ BS-physics

Lindsay
UChicago BS-CS
USC PhD-physics

M. Mercado *et al.*, *Phys. Rev. B* **110**, 075116 ('24)

Now What? Physics in 100 Years

- **Increasingly, the development of algorithms will become a central focus of theoretical physics. ... Triumphs of creative understanding such as universality (suppression of irrelevant details), symmetry (informed iteration), and topology (emergence of discrete from continuous) are preadapted to algorithmic thinking.**
- **The work of designing algorithms can be considered as a special form of teaching, aimed at extremely clever but literal-minded and inexperienced students—that is, computers—who cannot deal with vagueness. At present those students are poorly motivated and incurious, but those faults are curable. Within 100 years they (computers) will become the colleagues and ultimately the *successors* of their human teachers, with a distinctive style of thought adapted to their talents.**
- **Two developments will be transformative: naturalized artificial intelligence and expanded sensoria.**

F. Wilczek, *Phys. Today* **69(4)**, 32 ('16)
https://aiichironakano.github.io/cs653/Wilczek-PhysicsIn100Years-PhysToday16.pdf

Rise of generative science using generative AI

T. Taniguchi, *Royal Soc. Open Sci.* **12**, 241678 ('25)
https://aiichironakano.github.io/cs653/Taniguchi-GenerativeScience-RSOS25.pdf

To sum:

HPC for science (previous CSCI 653)

→

AI + quantum + post-exa nexus:
Survive the compute Cambrian explosion
by finding your niche!

How?

Use Final Project Publications!

Computer Physics Communications 239 (2019) 265–271

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

PAR^2: Parallel Random Walk Particle Tracking Method for solute transport in porous media☆

Calogero B. Rizzo[a,*], Aiichiro Nakano[b], Felipe P.J. de Barros[a]

Computer Physics Communications 244 (2019) 324–328

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

WaterAlignment: Identification of displaced water molecules in molecular docking using Jonker and Volgenant shortest path augmentation for linear assignment☆

Dab Brill[c,e,*], Jason B. Giles[e], Ian S. Haworth[e], Aiichiro Nakano[a,b,c,d,f]

Computational Materials Science 173 (2020) 109429

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Boltzmann machine modeling of layered MoS_2 synthesis on a quantum annealer

Jeremy Liu[a,b], Ankith Mohan[a], Rajiv K. Kalia[c], Aiichiro Nakano[c], Ken-ichi Nomura[c,*], Priya Vashishta[c], Ke-Thia Yao[a]

buildings

Buildings **9**, 44 (2019)

MDPI

Article

Adaptive Kinetic Architecture and Collective Behavior: A Dynamic Analysis for Emergency Evacuation

Angella Johnson [1,*], Size Zheng [2], Aiichiro Nakano [3], Goetz Schierle [1] and Joon-Ho Choi [1]

Computer Physics Communications 247 (2020) 106873

sDMD: An open source program for discontinuous molecular dynamics simulation of protein folding and aggregation☆

Size Zheng[a,*], Leili Javidpour[b], Muhammad Sahimi[c], Katherine S. Shing[c], Aiichiro Nakano[c]

Quantum Science & Technology **6**, 014007 (2021)

Domain-specific compilers for dynamic simulations of quantum materials on quantum computers

Lindsay Bassman[5,1], Sahil Gulania[2], Connor Powers[1], Rongpeng Li[3], Thomas Linker[1], Kuang Liu[1], T K Satish Kumar[4], Rajiv K Kalia[1], Aiichiro Nakano[1] and Priya Vashishta[1]

Phys. Chem. Chem. Phys. **24**, 10378 (2022)

Probing the presence and absence of metal-fullerene electron transfer reactions in helium nanodroplets by deflection measurements†

John W. Niman,[a] Benjamin S. Kamerin,[a] Thomas H. Villers,[a] Thomas M. Linker,[b] Aiichiro Nakano[b] and Vitaly V. Kresin[*a]

More Final Project Publications

Article https://doi.org/10.1038/s43588-022-00370-6

Fast multi-source nanophotonic simulations using augmented partial factorization

Ho-Chun Lin, Zeyu Wang & Chia Wei Hsu

Nature Computational Science | Volume 2 | December 2022 | 815–822

"30,000,000 times faster than existing methods"

Article https://doi.org/10.1038/s41467-024-47685-8

Scalable computation of anisotropic vibrations for large macromolecular assemblies

Jordy Homing Lam[1,2,3], Aiichiro Nakano[1,4,5] & Vsevolod Katritch[1,2,3,6]

Nature Communications | (2024)15:3479

"250 times faster than existing methods"

https://github.com/jhmlam/Inching

JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING

J. Chem. Inf. Model. 2024, 64, 7027–7034

pubs.acs.org/jcim Article

Exploring the Global Reaction Coordinate for Retinal Photoisomerization: A Graph Theory-Based Machine Learning Approach

Goran Giudetti,[⊥] Madhubani Mukherjee,[⊥] Samprita Nandi, Sraddha Agrawal, Oleg V. Prezhdo, and Aiichiro Nakano*

Cite This: https://doi.org/10.1021/acs.jcim.4c00325 Read Online

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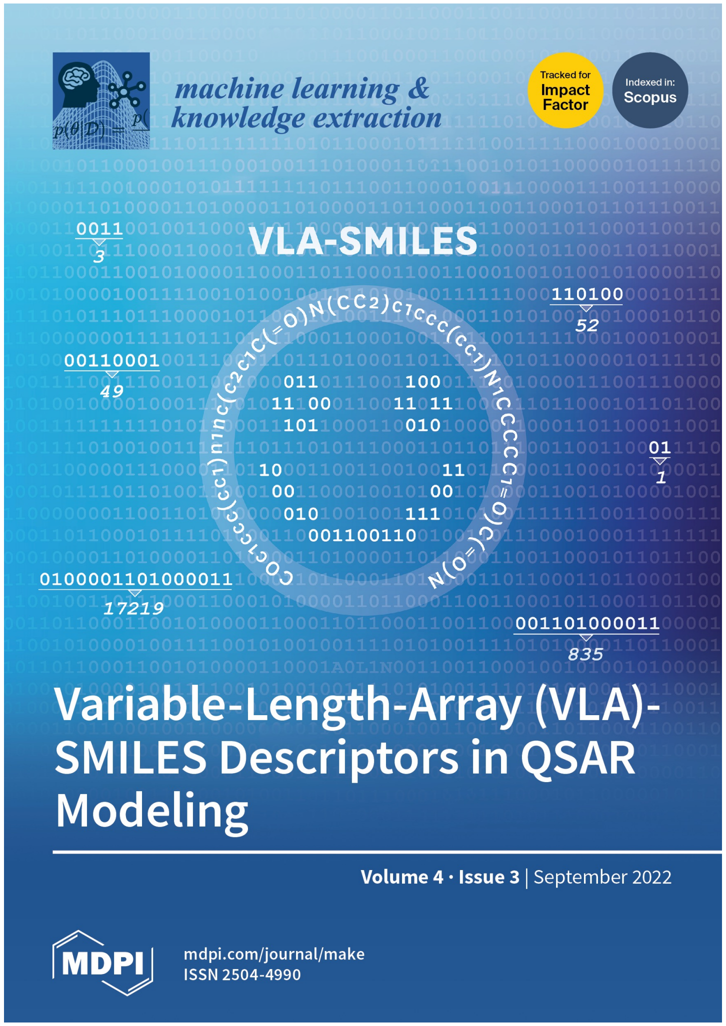

Dielectric polymer property prediction using recurrent neural networks with optimizations

Antonina L. Nazarova, L. Yang, K. Liu, A. Mishra, R. K. Kalia, K. Nomura, A. Nakano, P. Vashishta, and P. Rajak

Journal of Chemical Information and Modeling **61**, 2175 ('21)

VLA-SMILES: Variable-Length-Array SMILES Descriptors in Neural Network-Based QSAR Modeling

Antonina L. Nazarova [1,*,†] and Aiichiro Nakano [2,*]

Journal of Machine Learning and Knowledge Extraction **4**, 715 (2022)

Self-introduction:
Recruit a team member!
(Team project is encouraged)

Before that, assignment 1 =
initiate final project