

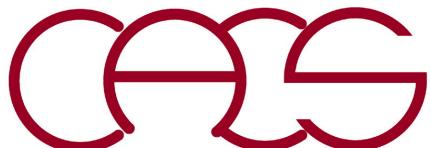
CSCI653: High Performance Computing & Simulations

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Department of Physics & Astronomy
Department of Quantitative & Computational Biology
University of Southern California*

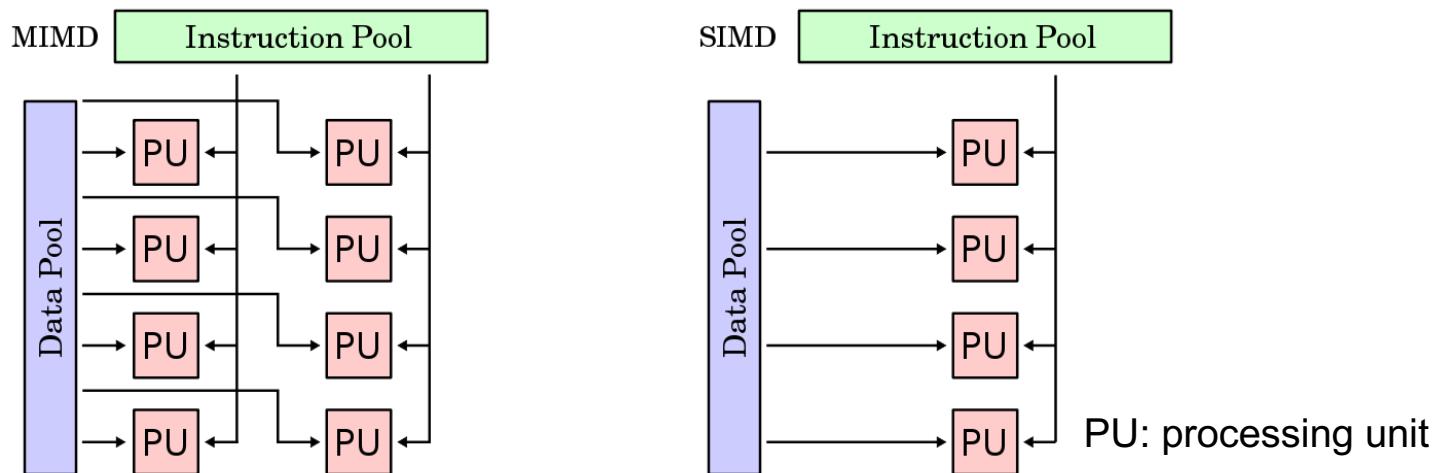
Email: anakano@usc.edu

Do “Your” Science Using High Performance Computing



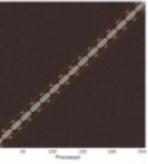
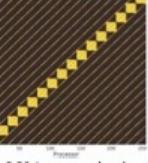
CSCI653 at a Glance: Applications

- 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

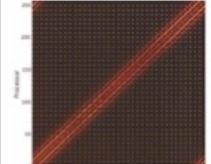
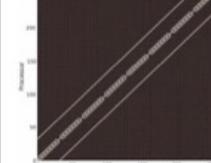
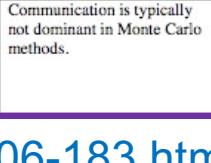


The Landscape of Parallel Computing Research: A View from Berkeley — Why MD & QD?

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.		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.		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.		Fourier Transform / DSPs, Zalink PDSP [Zalink 2006]

In performance optimization

Dwarf	Description	Communication Pattern (Figure axes show processors 1 to 256, with black meaning no communication)	NAS Benchmark / Example HW
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 $O(N^3)$ calculation, and hierarchical particle methods, which combine forces or potentials from multiple points to reduce the computational complexity to $O(N \log N)$ or $O(N)$.		(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.		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.		Embarrassingly Parallel / NSF Teragrid

MD

QD

Monte Carlo

CSCI653: Algorithms & Tools

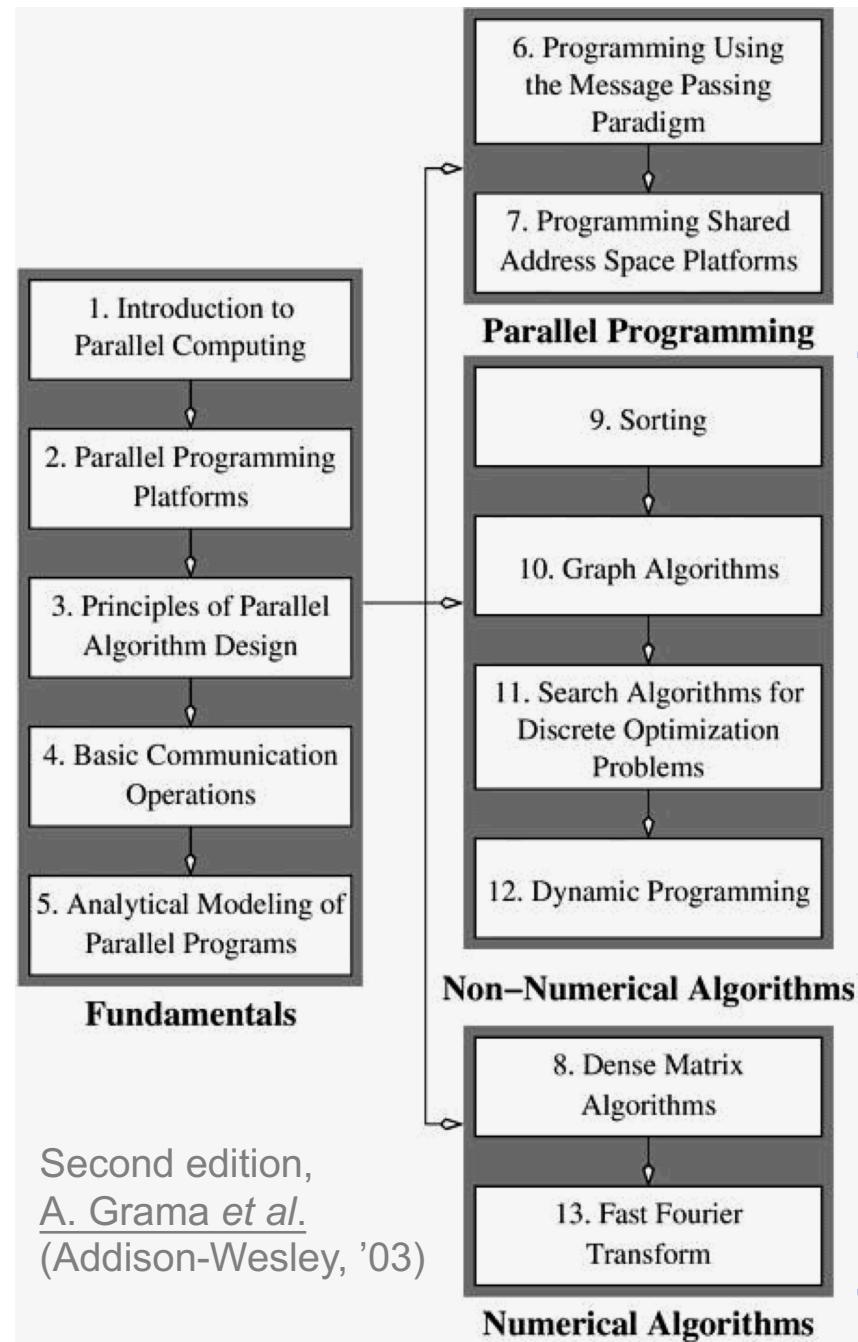
- *Just one thing:* Divide-conquer-“recombine” (DCR) algorithm; it’s data locality!
- *Parallel computing = decomposition (who does what):* Scalability analysis; performance optimization
- *Programming languages:* MPI (distributed memory) + OpenMP (shared memory) + CUDA|OpenMP target| SYCL (heterogeneous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

Introduction to Parallel Computing

SIMD, MIMD
etc.

Decomposition

Scalability
analysis



High Performance Computing (HPC)

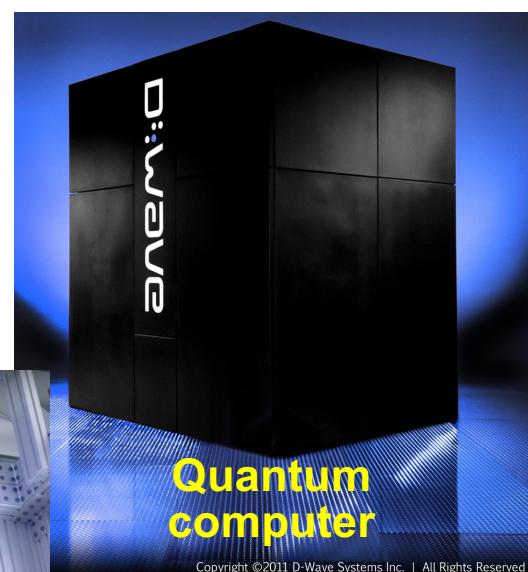


- **USC CARC (Center for Advanced Research Computing):** 10,000+ CPU cores accelerated by GPUs
- **USC ISI (Information Sciences Institute):** 1,098-qubit D-Wave quantum computer

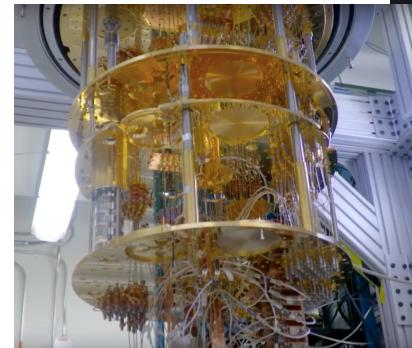
Petaflop/s = 10^{15} mathematical operations per second
Exaflop/s = 10^{18} mathematical operations per second



GPGPU



QPU



Current & Future Supercomputing

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



Innovative & Novel Computational Impact on Theory & Experiment

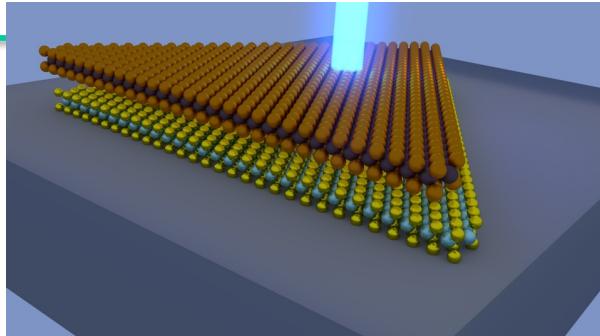
Title: AI-Guided Exascale Simulations of Quantum Materials Manufacturing and Control

PI and Co-PIs: Aiichiro Nakano—PI, Rajiv K. Kalia, Ken-ichi Nomura, Priya Vasishta

- Atomistic simulations on million cores (pre-exascale)



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



Early Science Projects for Aurora

Supercomputer Announced

Metascalable layered materials genome

Investigator: Aiichiro Nakano, University of Southern California

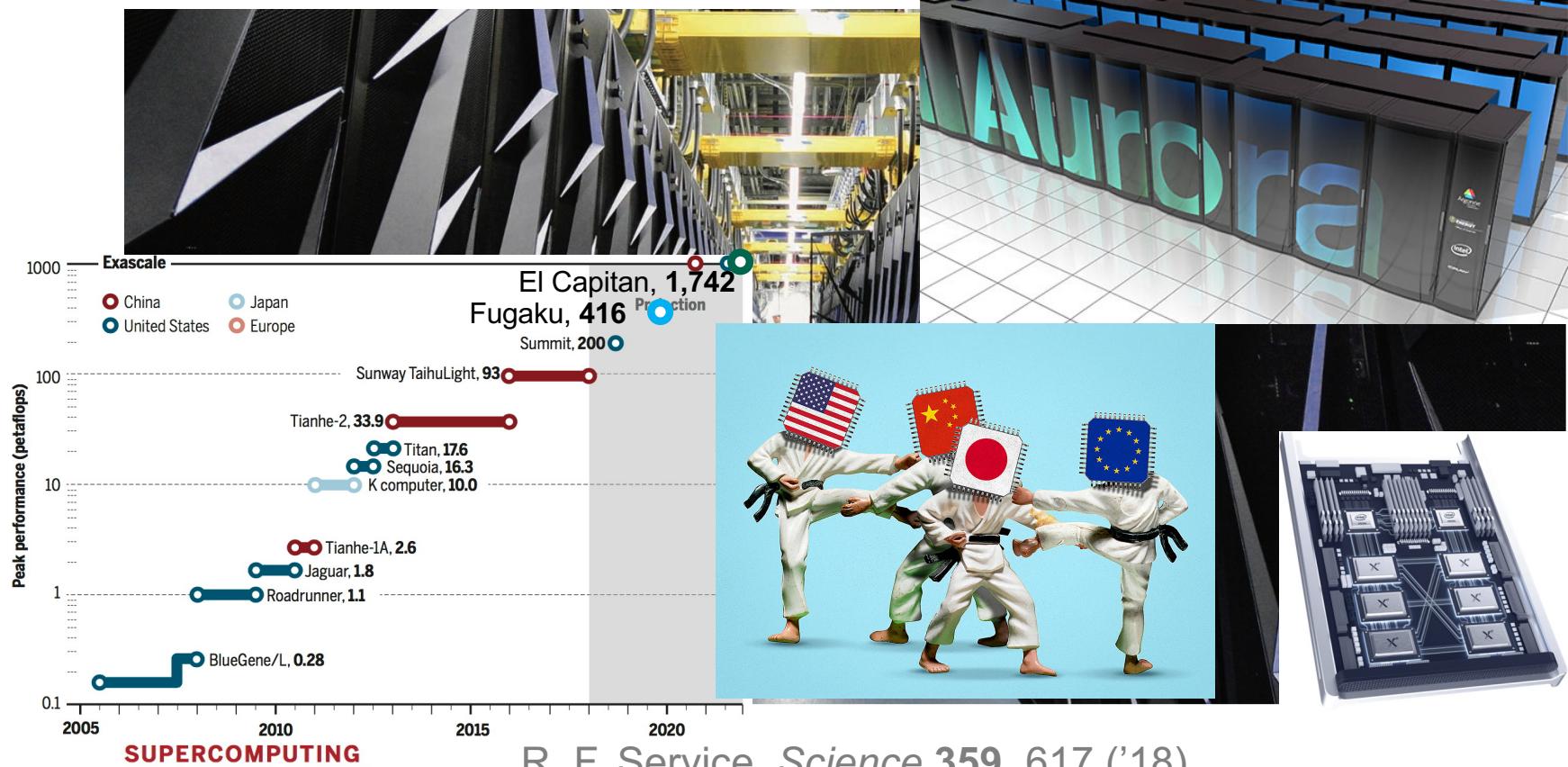


1.01 exaflop/s
Intel Aurora

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)

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

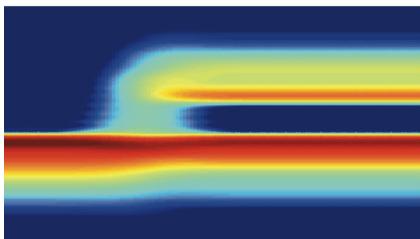
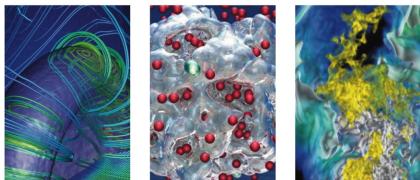
In 1957, the launch of the Sputnik satellite vaulted the Soviet Union to the lead in the space race and galvanized the United States. U.S. supercomputer researchers are today facing their own

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>

BES



NOVEMBER 3-5, 2015

ROCKVILLE, MARYLAND

Exa-leadership

BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

An Office of Science review sponsored jointly by
Advanced Scientific Computing Research and Basic Energy Sciences

16,661-atom QMD

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

*On-demand hydrogen
production from water*

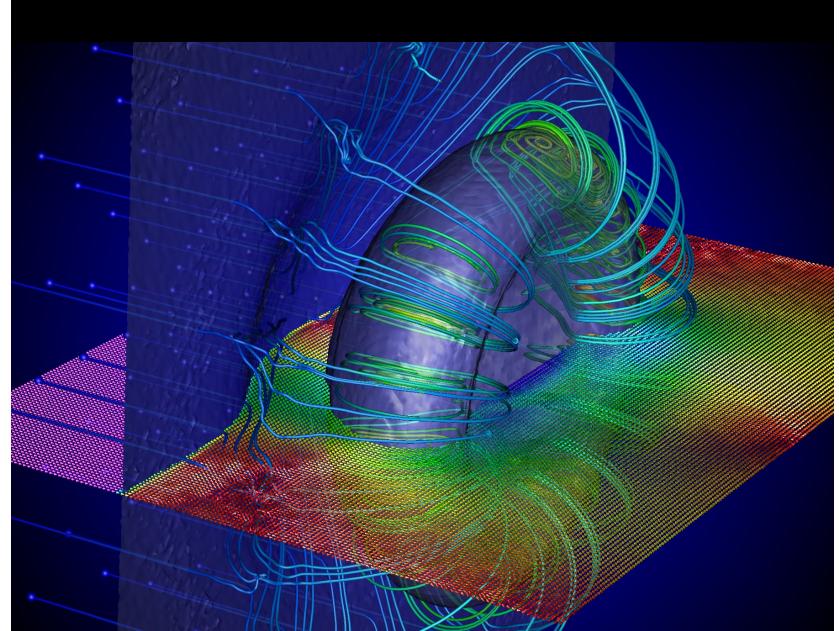
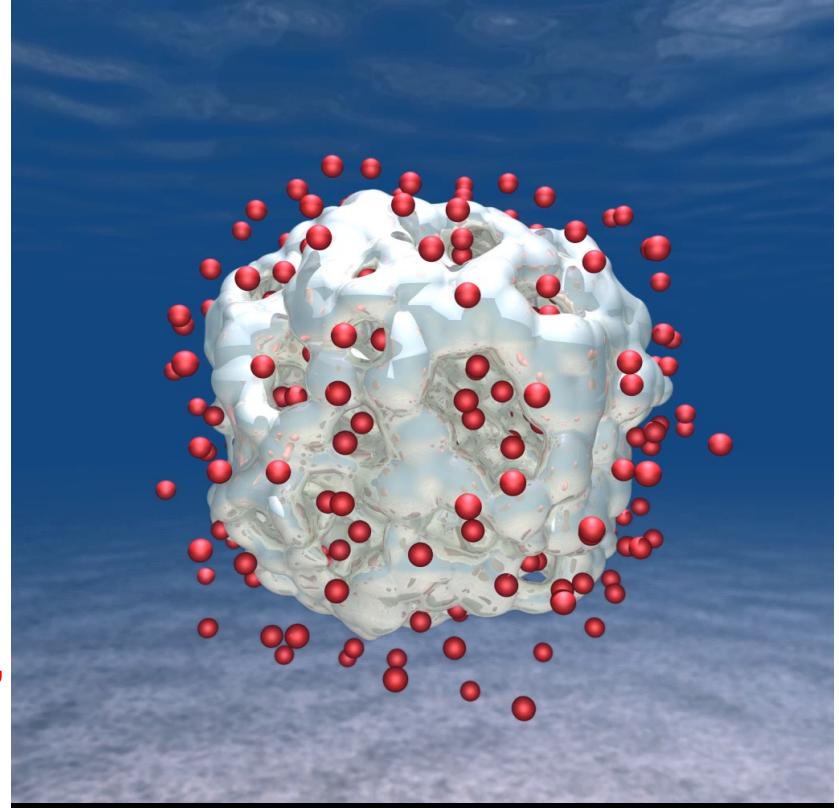
10^9 -atom RMD

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

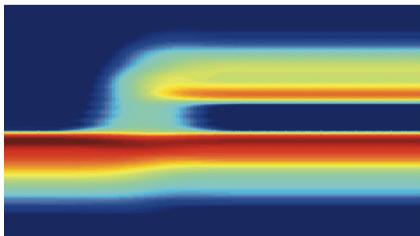
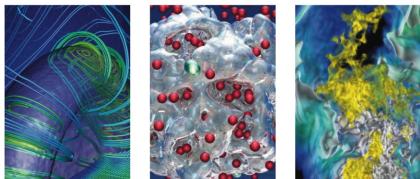
MD



U.S. DEPARTMENT OF
ENERGY



BES



NOVEMBER 3-5, 2015

ROCKVILLE, MARYLAND

BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

An Office of Science review sponsored jointly by
Advanced Scientific Computing Research and Basic Energy Sciences

16,661-atom QMD

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

10⁹-atom RMD

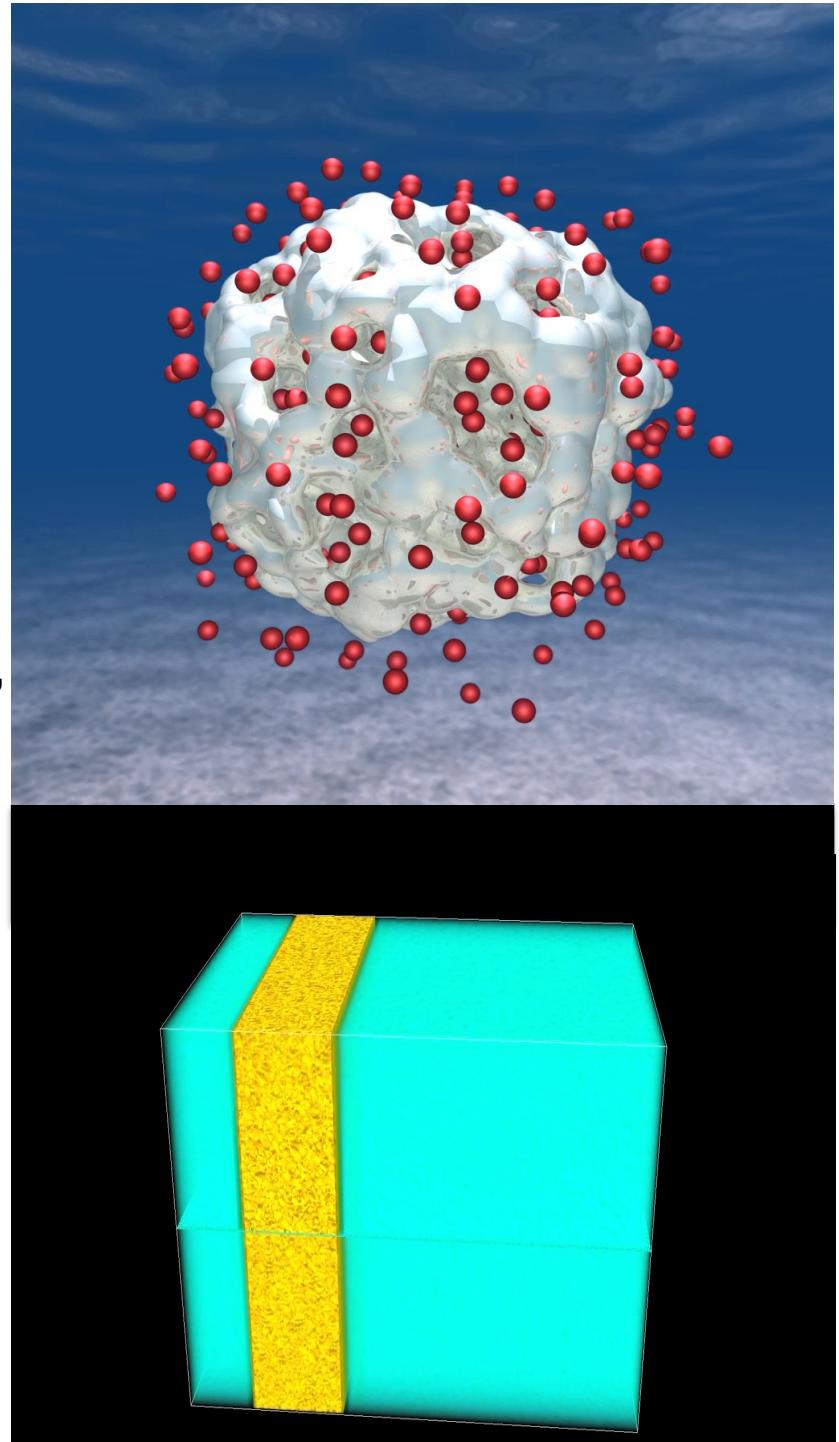
**Shekhar *et al.*,
Phys. Rev. Lett.
111, 184503 ('13)**

*Fluid dynamics
atom-by-atom*

MD



U.S. DEPARTMENT OF
ENERGY



Changing Computing Landscape for Science

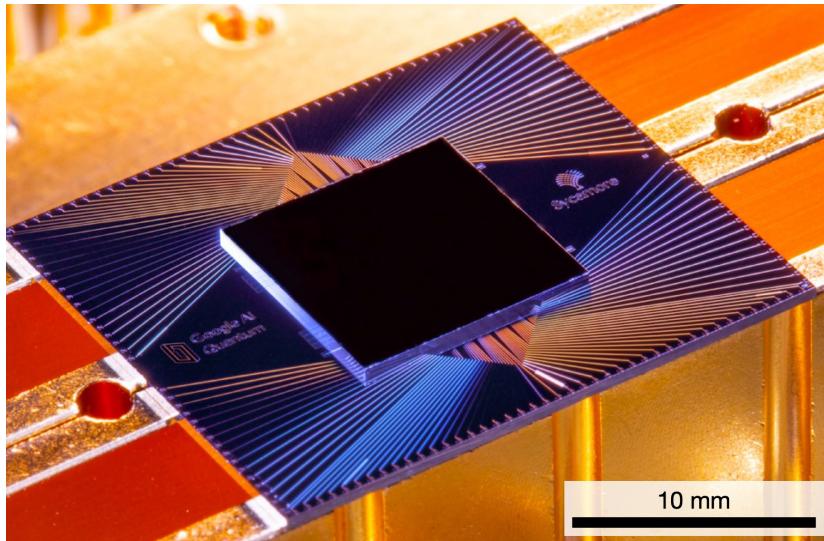
Postexascale Computing for Science

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>



SambaNova SN-30

8 nodes each with 8
Reconfigurable
DataFlow Units (RDU)



Cerebras CS-2

2 CS-2 Wafer scale
engines (WSE)

Upgrading to CS-3



Graphcore Bow Pod64

4 nodes each
with 16 Intelligent
Processing Units
(IPUs)



Groq

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



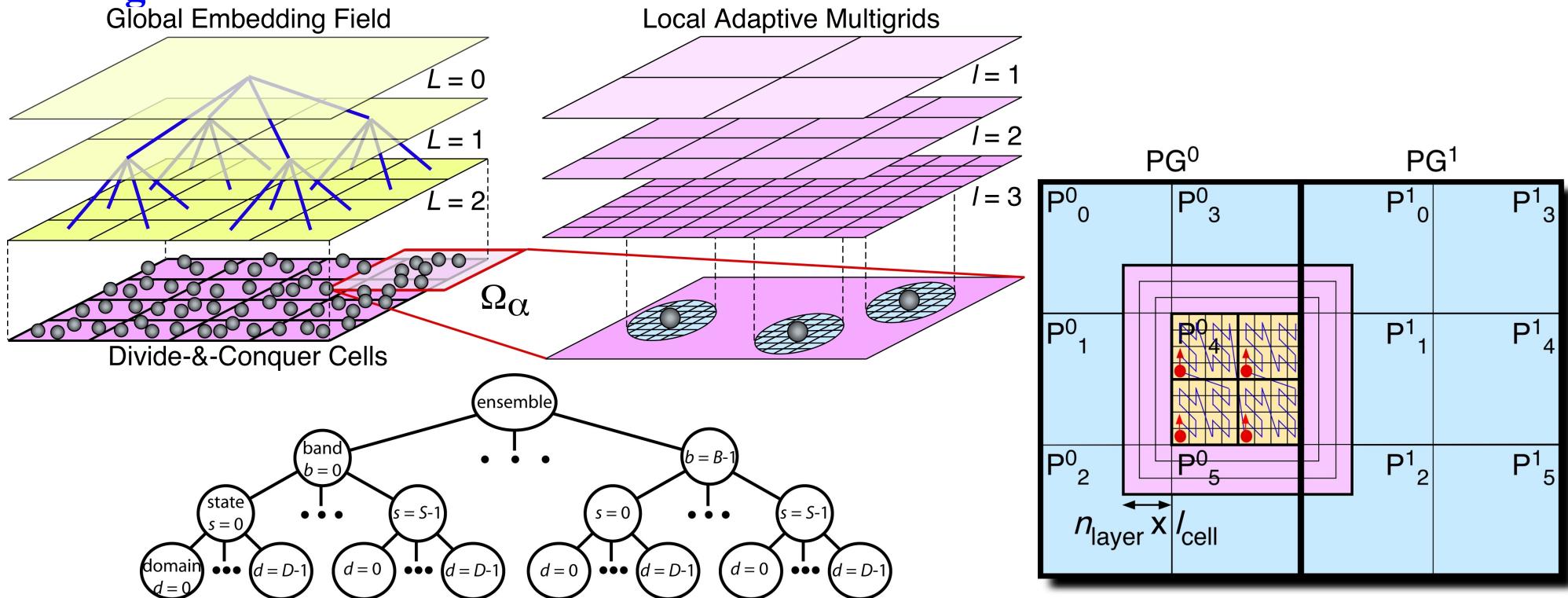
*Coming Soon !
Sambanova SN40L
Inference/Finetuning*

NSF <https://nairrpilot.org>

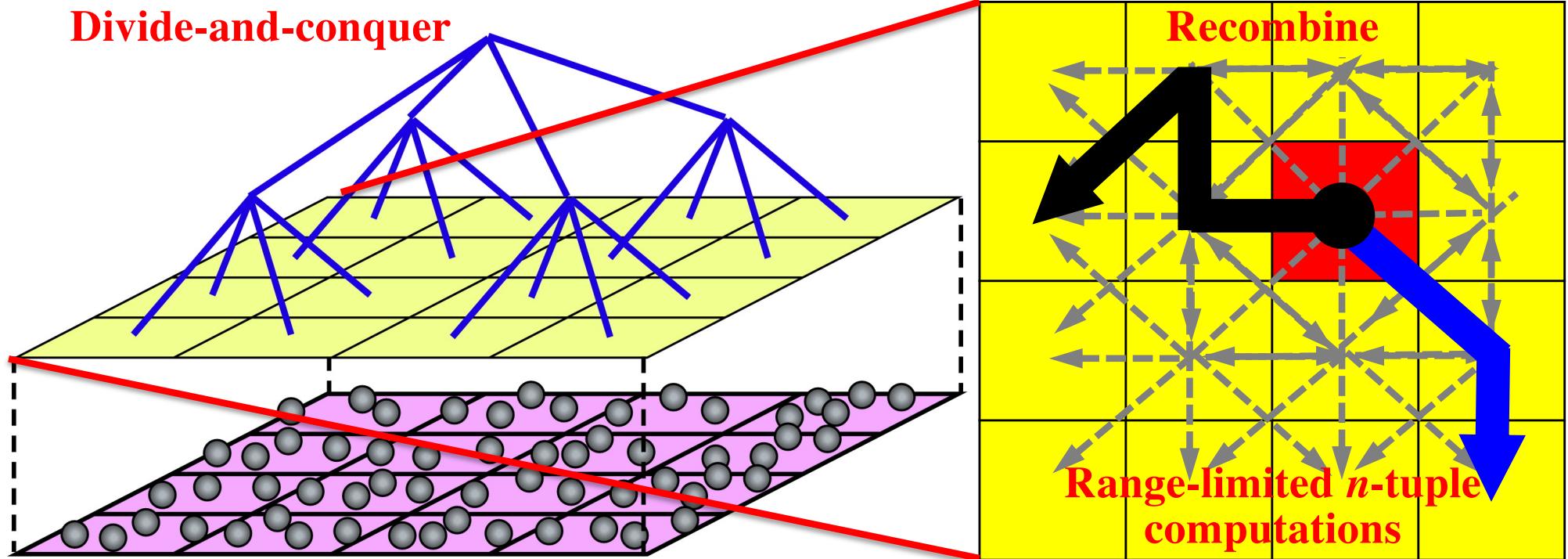
A Metascalable Dwarf

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

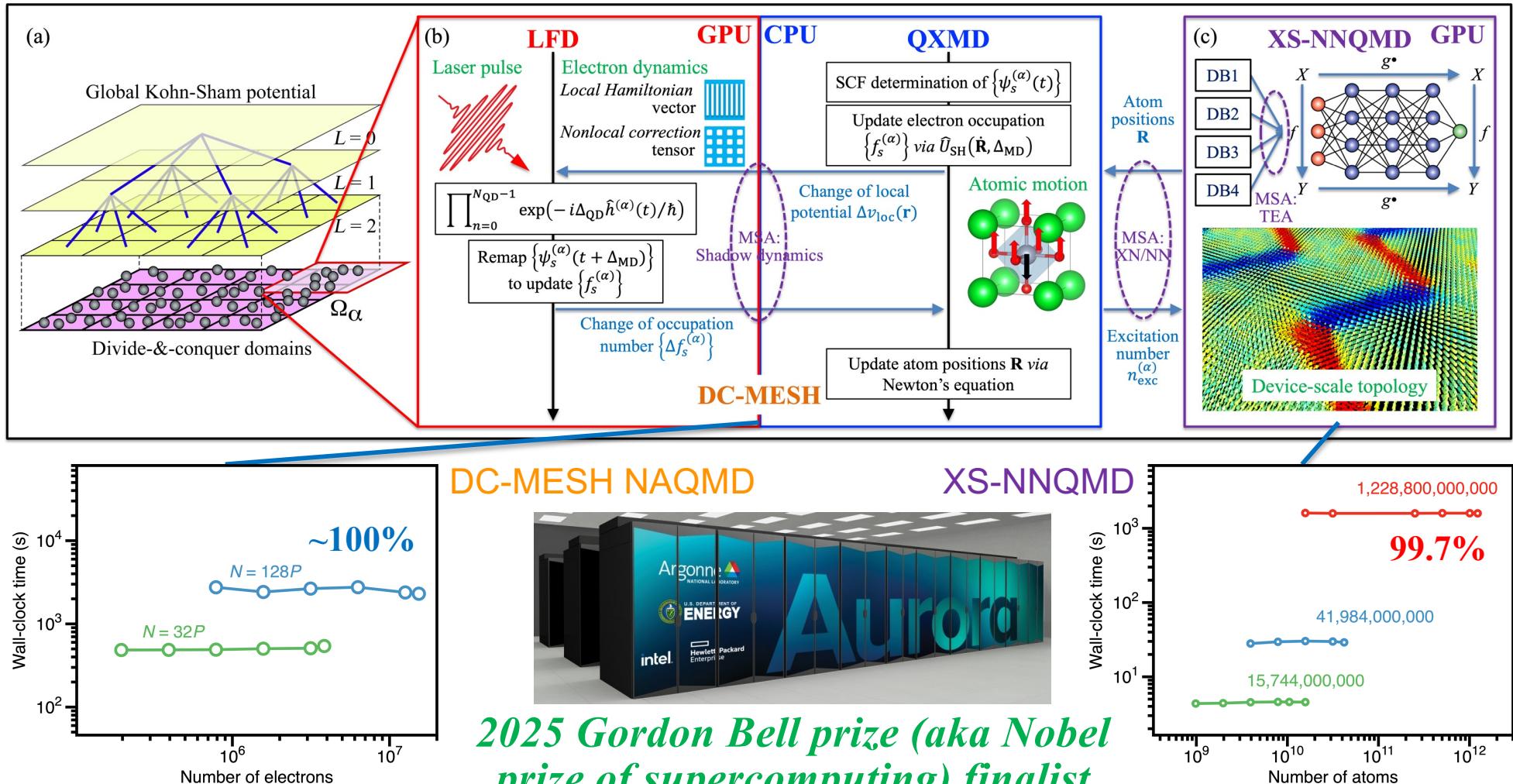
Aurora allows 1|2|3 BF16 values to be accumulated in FP32 to provide varying precision/speed

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., ACM Gordon Bell prize finalist ('25)

Exa Multiscale Light-Matter Dynamics

- Breaking the Exaflop/s barrier:* On 60,000 GPUs of Aurora: **1.87 Exaflop/s**; **152 \times** & **3,780 \times** 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



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 \('20\)](#)



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Lindsay Bassman Awarded Prestigious Marie Curie Fellowship

APRIL 12, 2022



*Lindsay
UChicago BS-CS
USC PhD-physics*

*Miguel
USC sociology
→ BS-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



 ELSEVIER



PAR²: 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



 ELSEVIER



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



 ELSEVIER



Boltzmann machine modeling of layered MoS₂ 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)

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 Gulania², Connor Powers¹ , Rongpeng Li³, Thomas Linker¹ , Kuang Liu¹, T K Satish Kumar⁴, Rajiv K Kalia¹, Aiichiro Nakano¹  and Priya Vashishta¹ 

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 , Aiichiro Nakano   & Vsevolod Katritch  

Nature Communications | (2024)15:3479

“250 times faster than existing methods”

<https://github.com/jhmlam/lncing>



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,¹ Madhubani Mukherjee,¹ Samprita Nandi, Sraddha Agrawal, Oleg V. Prezhdo, and Aiichiro Nakano*



Cite This: <https://doi.org/10.1021/acs.jcim.4c00325>



Read Online

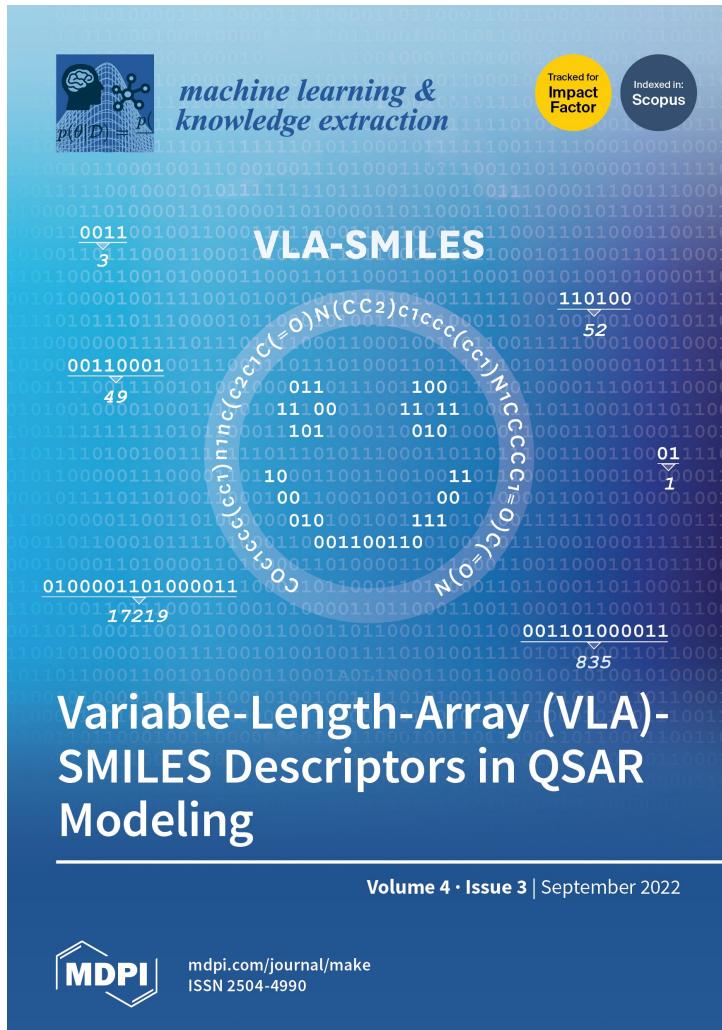
Journal Cover



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)

**Assignment 1 =
initiate your final project**