Applications of Parallel Computers

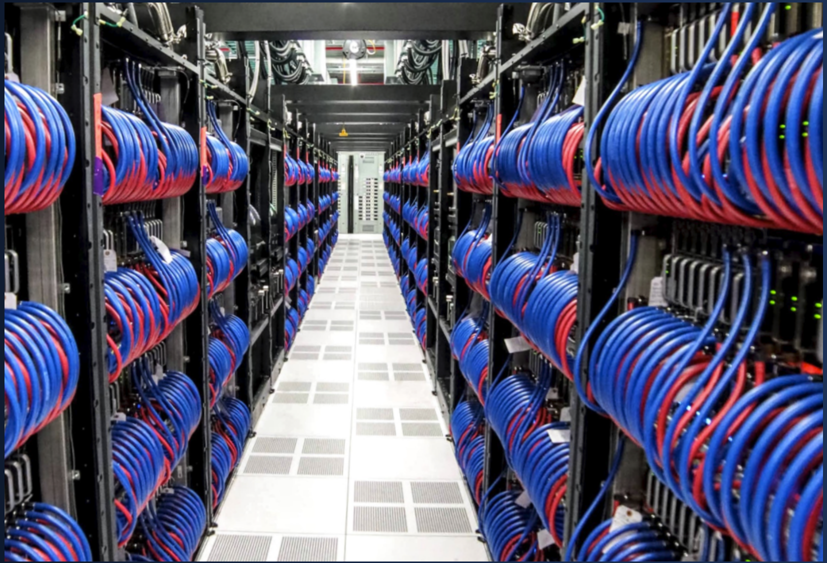
Aydın Buluç

(Guest Lecture for CS61C)

Special thanks to Kathy Yelick for lots of slides

What is a supercomputer?

High speed network connecting fast processors and memory



= 4 x

1 exaflop

(10^{18} ops/sec)

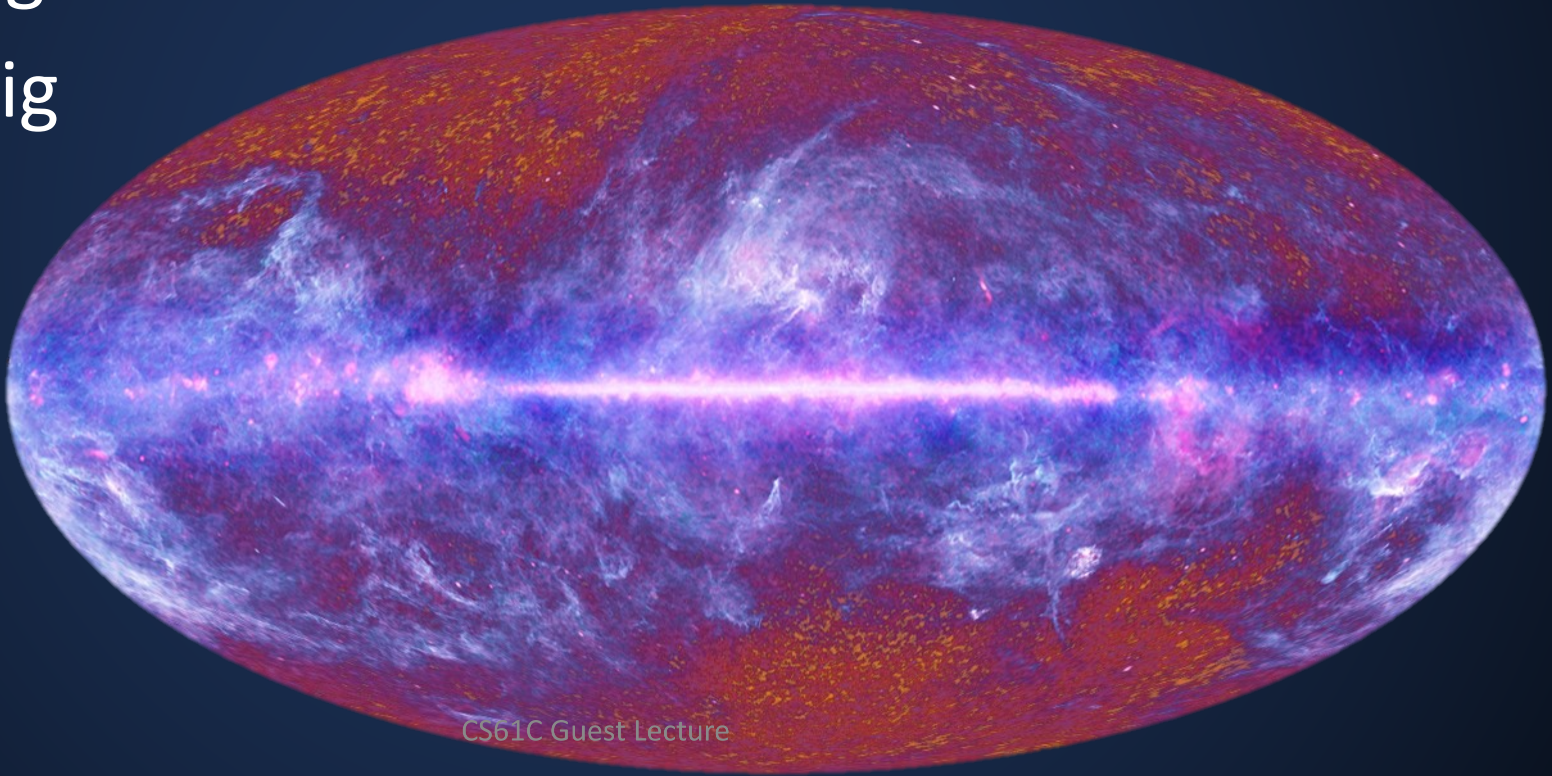
63,000 seats

(each with 3.5 TF laptop)

Supercomputers are used in science

For things that are:

- too big



Supercomputers are used in science

For things that are:

- too big
- too small

Supercomputers are used in science

For things that are:

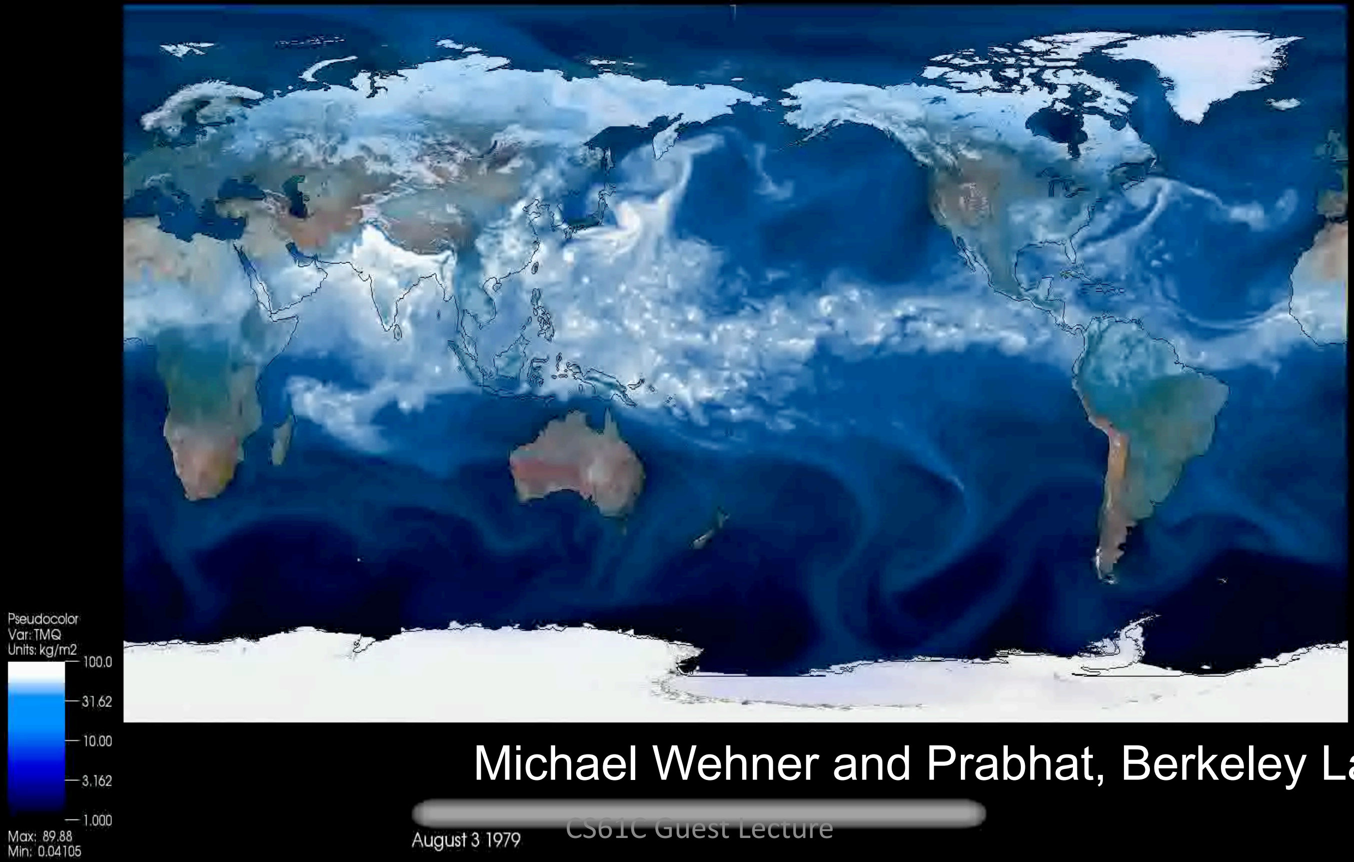
- too big
- too small
- too fast

Supercomputers are used in science

For things that are:

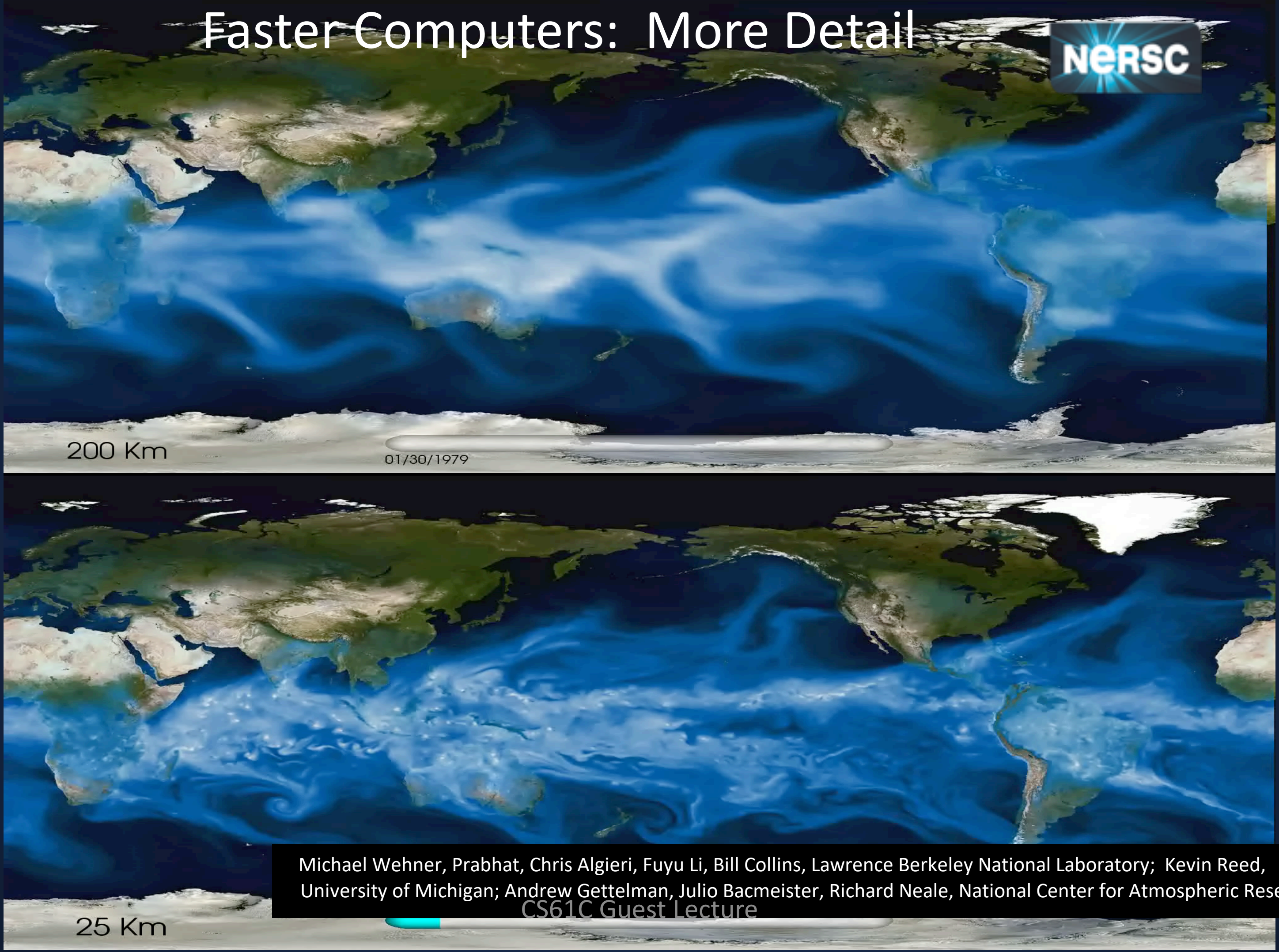
- too big
- too small
- too fast
- too slow

Simulations Show the Effects of Climate Change in Hurricanes



Michael Wehner and Prabhat, Berkeley Lab

Faster Computers: More Detail



Michael Wehner, Prabhat, Chris Algieri, Fuyu Li, Bill Collins, Lawrence Berkeley National Laboratory; Kevin Reed, University of Michigan; Andrew Gettelman, Julio Bacmeister, Richard Neale, National Center for Atmospheric Research

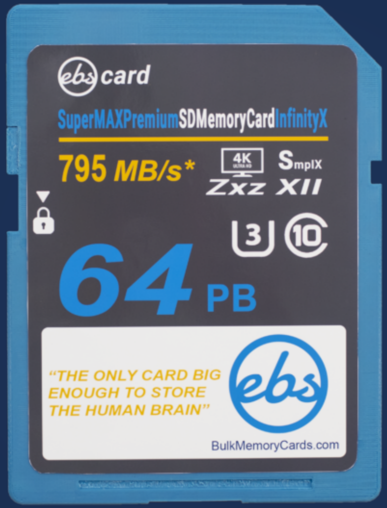
Supercomputers are used in science

For things that are:

- too big
- too small
- too fast
- too slow
- too complex

Sequencers read the genome in fragments, with errors

The need for memory



What if the memory requirements are > 100TB for the science problem that needs to be solved?

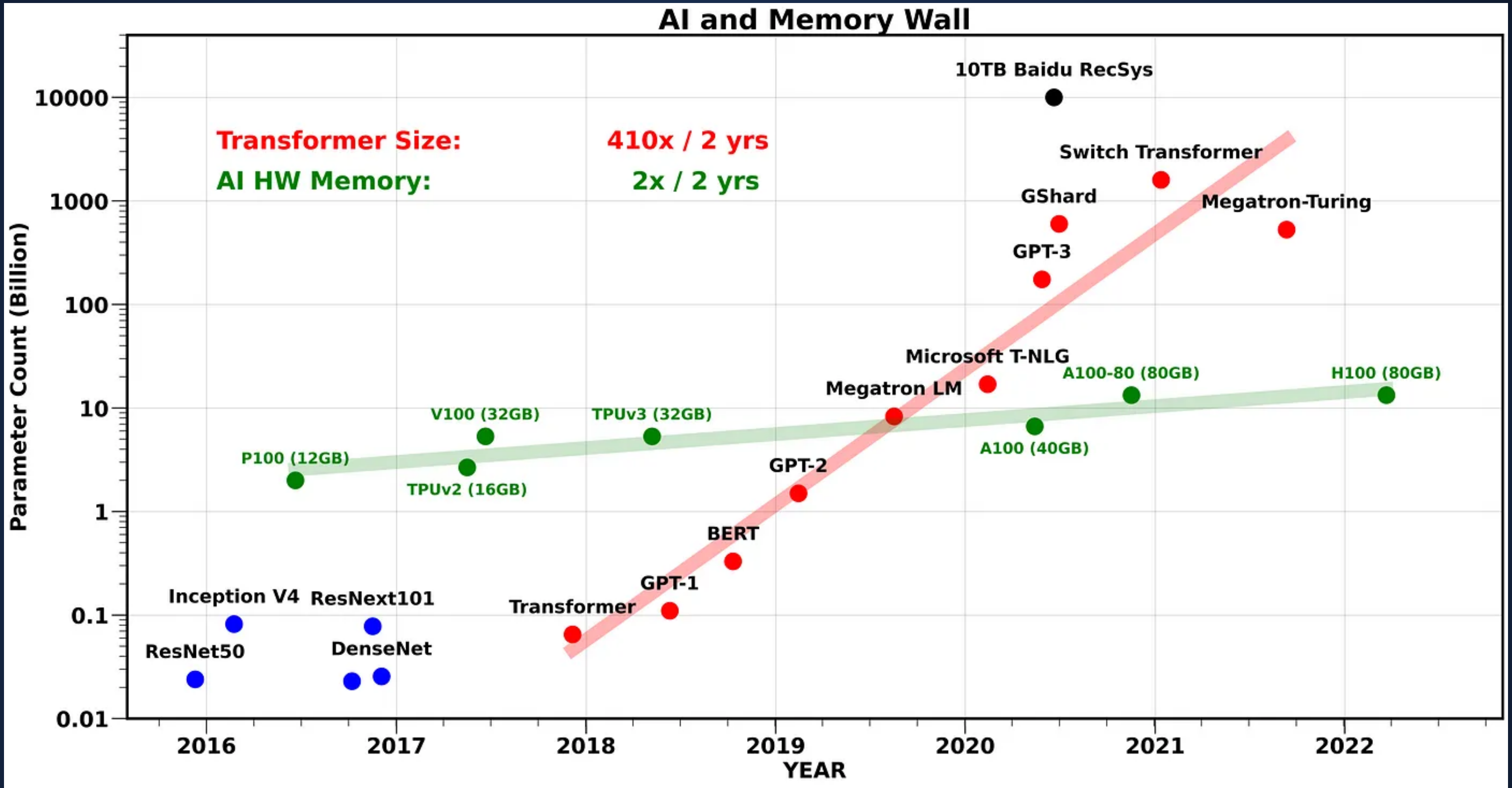


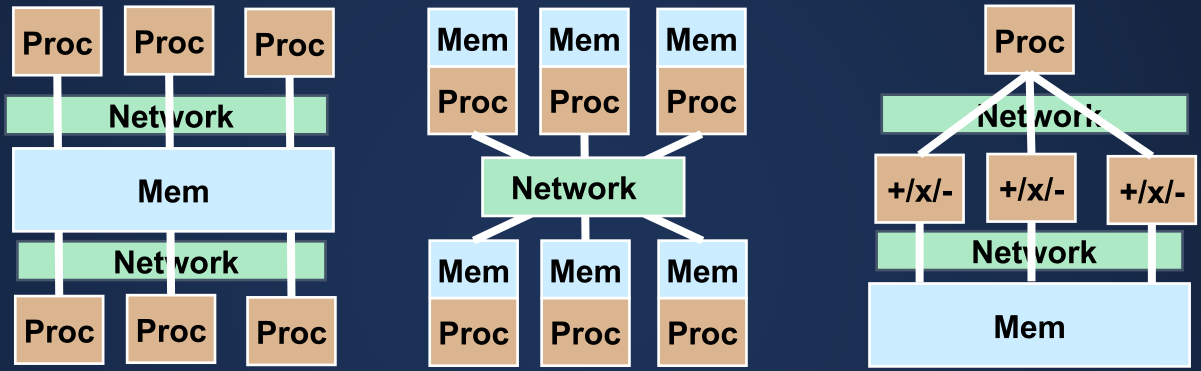
Figure source: Amir Gholami
https://medium.com/riselab/ai-and-memory-wall-2cb4265cb0b8

If you were plowing a field, which would you rather use?

Two strong oxen or 1024 chickens?

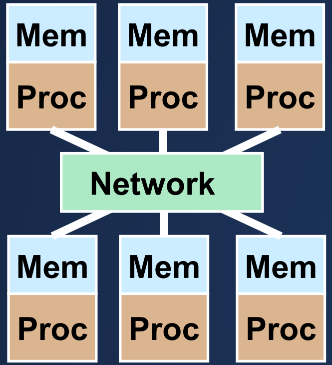
- Seymour Cray

What is a Parallel Computer?



Shared Memory (SMP) or Multicore	**High Performance Computing (HPC) or Distributed Memory**	**Single Instruction Multiple Data (SIMD)**

What is a Parallel Computer?



High Performance Computing (HPC) or Distributed Memory

A **distributed memory multiprocessor** has processors with their own memories connected by a high speed network

Also called a **cluster**

A **high performance computing (HPC)** system contains 100s or 1000s of such processors (nodes)

- Why is high-performance computing often synonymous with parallel computing?
- Why do we care so much about interconnect and communication?

Performance = parallelism

Efficiency = locality

- Bill Dally (NVIDIA and Stanford)

Some of the World’s Fastest Computers

The Top500 List

Units of Measure for HPC

- High Performance Computing (HPC) units are:
  - Flop: floating point operation, usually double precision unless noted
  - Flop/s: floating point operations per second
  - Bytes: size of data (a double precision floating point number is 8 bytes)
- Typical sizes are millions, billions, trillions…

Kilo	Kflop/s = 10^3 flop/sec	Kbyte = $10^3 \sim 2^{10}$ = 1024 bytes (KiB)
Mega	Mflop/s = 10^6 flop/sec	Mbyte = $10^6 \sim 2^{20}$ bytes (MiB)
Giga	Gflop/s = 10^9 flop/sec	Gbyte = $10^9 \sim 2^{30}$ bytes (GiB)
Tera	Tflop/s = 10^{12} flop/sec	Tbyte = $10^{12} \sim 2^{40}$ bytes (TiB)
Peta	Pflop/s = 10^{15} flop/sec	Pbyte = $10^{15} \sim 2^{50}$ bytes (PiB)
Exa	Eflop/s = 10^{18} flop/sec	Ebyte = $10^{18} \sim 2^{60}$ bytes (EiB)
Zetta	Zflop/s = 10^{21} flop/sec	Zbyte = $10^{21} \sim 2^{70}$ bytes (ZiB)
Yotta	Yflop/s = 10^{24} flop/sec	Ybyte = $10^{24} \sim 2^{80}$ bytes (YiB)

We are here

- Current fastest (public) machines are petaflop systems
  - Up-to-date list at www.top500.org

The TOP500 Project

- 500 most powerful computers in the world
- Updated twice a year:
  - ISC' xy in June in Germany
  - SCxy in November in the U.S.
- All information available from the TOP500 web site at: www.top500.org

Yardstick: Floating Point Operations per Second (FLOP/s) Rmax of Linpack

- Solve Ax=b, Matrix A is dense with random entries
- Dominated by dense matrix-matrix multiply

TOP500® SUPERCOMPUTER SITES

#	NOVEMBER 2021	Manufacturer	Computer	Country	Cores	Rmax [Pflops]	Power [MW]
1	RIKEN Center for Computational Science	Fujitsu	Fugaku Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D	Japan	7,630,848	442.0	29.9
2	Oak Ridge National Laboratory	IBM	Summit IBM Power System, P9 22C 3.07GHz, Mellanox EDR, NVIDIA GV100	USA	2,414,592	148.6	10.1
3	Lawrence Livermore National Laboratory	IBM	Sierra IBM Power System, P9 22C 3.1GHz, Mellanox EDR, NVIDIA GV100	USA	1,572,480	94.6	7.4
4	National Supercomputing Center in Wuxi	NRCPC	Sunway TaihuLight NRCPC Sunway SW26010, 260C 1.45GHz	China	10,649,600	93.0	15.4
5	Lawrence Berkeley National Laboratory (NERSC)	HPE	Perlmutter HPE Cray EX235n, AMD EPYC 7763 64C, 2.45GHz, NVIDIA A100, Slingshot-10	USA	761,856	70.8	2.59
6	NVIDIA Corporation	NVIDIA	Selene DGX A100 SuperPOD, AMD 64C 2.25GHz, NVIDIA A100, Mellanox HDR	USA	555,520	63.5	2.65
7	National University of Defense Technology	NUDT	Tianhe-2A ANUDT TH-IVB-FEP, Xeon 12C 2.2GHz, Matrix-2000	China	4,981,760	61.4	18.5
8	Forschungszentrum Jülich (FZJ)	Atos	JUWELS Booster Module BullSequana XH2000, AMD EPYC 24C 2.8GHz, NVIDIA A100, Mell. HDR	Germany	449,280	44.1	1.76
9	Eni S.p.A	Dell EMC	HPC5 PowerEdge C4140, Xeon 24C 2.1GHz, NVIDIA T. V100, Mellanox HDR	Italy	669,760	35.5	2.25
10	Azure East US 2	MS Azure	Voyager-EUS2 - ND96amsr_A100_v4, AMD EPYC 7V12 48C 2.45GHz, NVIDIA A100, Mellanox HDR	USA	253,440	30.0	

#	JUNE 2022	Manufacturer	Computer	Country	Cores	Rmax [Pflops]	Power [MW]
1	Oak Ridge National Laboratory	HPE	**Frontier** HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-10	USA	8,730,112	1,102	21.1
2	RIKEN Center for Computational Science	Fujitsu	**Fugaku** Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D	Japan	7,630,848	442.0	29.9
3	EuroHPC / CSC	HPE	**LUMI** HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-10	Finland	1,268,736	151.9	2.9
4	Oak Ridge National Laboratory	IBM	**Summit** IBM Power System, P9 22C 3.07GHz, Mellanox EDR, NVIDIA GV100	USA	2,414,592	148.6	10.1
5	Lawrence Livermore National Laboratory	IBM	**Sierra** IBM Power System, P9 22C 3.1GHz, Mellanox EDR, NVIDIA GV100	USA	1,572,480	94.6	7.4
6	National Supercomputing Center in Wuxi	NRCPC	**Sunway TaihuLight** NRCPC Sunway SW26010, 260C 1.45GHz	China	10,649,600	93.0	15.4
7	NERSC - Lawrence Berkeley National Laboratory	HPE	**Perlmutter** HPE Cray EX235n, AMD EPYC 64C 2.45GHz, NVIDIA A100, Slingshot-10	USA	761,856	70.9	2.6
8	NVIDIA Corporation	NVIDIA	**Selene** DGX A100 SuperPOD, AMD 64C 2.25GHz, NVIDIA A100, Mellanox HDR	USA	555,520	63.5	2.7
9	National University of Defense Technology	NUDT	**Tianhe-2A** ANUDT TH-IVB-FEP, Xeon 12C 2.2GHz, Matrix-2000	China	4,981,760	61.4	18.5
10	GENCI-CINES	HPE	**Adastra** HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-10	France	319,072	46.1	0.9

#	NOVEMBER 2022	Manufacturer	Computer	Country	Cores	Rmax [Pflops]	Power [MW]
1	Oak Ridge National Laboratory	HPE	**Frontier** HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-11	USA	8,730,112	1,102	21.1
2	RIKEN Center for Computational Science	Fujitsu	**Fugaku** Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D	Japan	7,630,848	442.0	29.9
3	EuroHPC / CSC	HPE	**LUMI** HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-11	Finland	2,069,760	309.1	6.0
4	EuroHPC / CINECA	Atos	**Leonardo** Atos BullSequana XH2000, Xeon 32C 2.6GHz, NVIDIA A100, HDR Infiniband	Italy	1,463,616	174.7	5.6
5	Oak Ridge National Laboratory	IBM	**Summit** IBM Power System, P9 22C 3.07GHz, Mellanox EDR, NVIDIA GV100	USA	2,414,592	148.6	10.1
6	Lawrence Livermore National Laboratory	IBM	**Sierra** IBM Power System, P9 22C 3.1GHz, Mellanox EDR, NVIDIA GV100	USA	1,572,480	94.6	7.4
7	National Supercomputing Center in Wuxi	NRCPC	**Sunway TaihuLight** NRCPC Sunway SW26010, 260C 1.45GHz	China	10,649,600	93.0	15.4
8	NERSC - Lawrence Berkeley National Laboratory	HPE	**Perlmutter** HPE Cray EX235n, AMD EPYC 64C 2.45GHz, NVIDIA A100, Slingshot-10	USA	761,856	70.9	2.6
9	NVIDIA Corporation	NVIDIA	**Selene** DGX A100 SuperPOD, AMD 64C 2.25GHz, NVIDIA A100, Mellanox HDR	USA	555,520	63.5	2.7
10	National University of Defense Technology	NUDT	**Tianhe-2A** ANUDT TH-IVB-FEP, Xeon 12C 2.2GHz, Matrix-2000	China	4,981,760	61.4	18.5

TOP500 NOVEMBER 2023		Manufacturer	Computer	Country	Cores	Rmax [Pflops]	Power [MW]
1	Oak Ridge National Laboratory	HPE	**Frontier** HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-11	USA	8,730,112	1,102	21.1
2	Argonne National Laboratory	HPE	**Aurora*** HPE Cray EX Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11	USA	4,742,808	585.3	24.6
3	Microsoft Azure	Microsoft	**Eagle** Microsoft NDv5 Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR	USA	1,123,200	561.2	
4	RIKEN Center for Computational Science	Fujitsu	**Fugaku** Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D	Japan	7,630,848	442.0	29.9
5	EuroHPC / CSC	HPE	**LUMI** HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-11	Finland	2,069,760	309.1	6.0
6	EuroHPC / CINECA	Atos	**Leonardo** Atos BullSequana XH2000, Xeon 32C 2.6GHz, NVIDIA A100, HDR Infiniband	Italy	1,463,616	174.7	5.6
7	Oak Ridge National Laboratory	IBM	**Summit** IBM Power System, P9 22C 3.07GHz, Mellanox EDR, NVIDIA GV100	USA	2,414,592	148.6	10.1
8	EuroHPC/BSC	EVIDEN	**MareNostrum 5 ACC** BullSequana XH3000, Xeon Platinum 8460Y+ 40C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR200	Spain	680,960	138.20	2.5
9	NVIDIA Corporation	NVIDIA	**Eos NVIDIA DGX SuperPOD** NVIDIA DGX H100, Xeon Platinum 8480C 56C 3.8GHz, NVIDIA H100, Infiniband NDR400	USA	485,888	121.40	
10	Lawrence Livermore National Laboratory	IBM	**Sierra** IBM Power System, P9 22C 3.1GHz, Mellanox EDR, NVIDIA GV100	USA	1,572,480	94.6	7.4

NOVEMBER 2024		Manufacturer	Computer	Country	Cores	Rmax [Pflops]	Power [MW]
1	Lawrence Livermore National Laboratory	HPE	El Capitan HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8Ghz, AMD Instinct MI300A, Slingshot-11,	USA	11,039,616	1,742	29.5
2	Oak Ridge National Laboratory	HPE	Frontier HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-11	USA	9,066,176	1,353	24.6
3	Argonne National Laboratory	HPE	Aurora HPE Cray EX Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11	USA	9,264,128	1,012	38.7
4	Microsoft Azure	Microsoft	Eagle Microsoft NDv5 Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR	USA	2,073,600	561.2	
5	Eni S.p.A.	HPE	HPC6 HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-11	Italy	2,069,760	309.1	6.0
6	RIKEN Center for Computational Science	Fujitsu	Fugaku Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D	Japan	7,630,848	442.0	29.9
7	Swiss National Supercomputing Centre (CSCS)	HEP	Alps HPE Cray EX254n NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Slingshot-11	Switzer land	2,121,600	434.90	7.1
8	EuroHPC / CSC	HPE	LUMI HPE Cray EX235a, AMD EPYC 64C 2.0GHz, Instinct MI250X, Slingshot-11	Finland	2,752,704	379.7	7.1
9	EuroHPC / CINECA	Atos	Leonardo Atos BullSequana XH2000, Xeon 32C 2.6GHz, NVIDIA A100, HDR Infiniband	Italy	1,824,768	241.2	7.5
10	Lawrence Livermore National Laboratory	HPE	Toulumne HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8Ghz, AMD Instinct MI300A, Slingshot-11	USA	1,161,216	208.10	3.4

El Capitan (#1) System Overview

Lawrence Livermore National Laboratory

System Performance

- Peak performance of 2.79 double precision exaFLOPS Measured Top500 performance (Rmax) was 1.742 exaFLOPS

Each node has

- 4 chips of AMD Instinct MI300A GPUs
- Each chip co-packages 4th Gen AMD EPYC CPU with 24 cores
- 4X128 GB of HBM3 memory, shared by both the CPU and GPU dies

The system includes

- 11,136 nodes
- Slingshot interconnect

Fugaku (#6) System Overview

RIKEN Center for Computational Science (R-CCS)

System Performance

- Peak performance of 442 petaflops (per TOP500 Rmax),
- 2.0 EFLOPS on a different mixed-precision benchmark
- The fastest system on the HPCG benchmark with 16 Teraflop/s

Each node has

- Fujitsu A64FX CPU (48+4 cores) per node
- HBM2 32 GiB

The system includes

- 158,976 nodes
- Custom Tofu Interconnect D
- 1.6 TB NVMe SSD/16 nodes (L1)
- 150 PB Lustre Filesystem (L2)
- Cloud storage (L3)

R-CCS

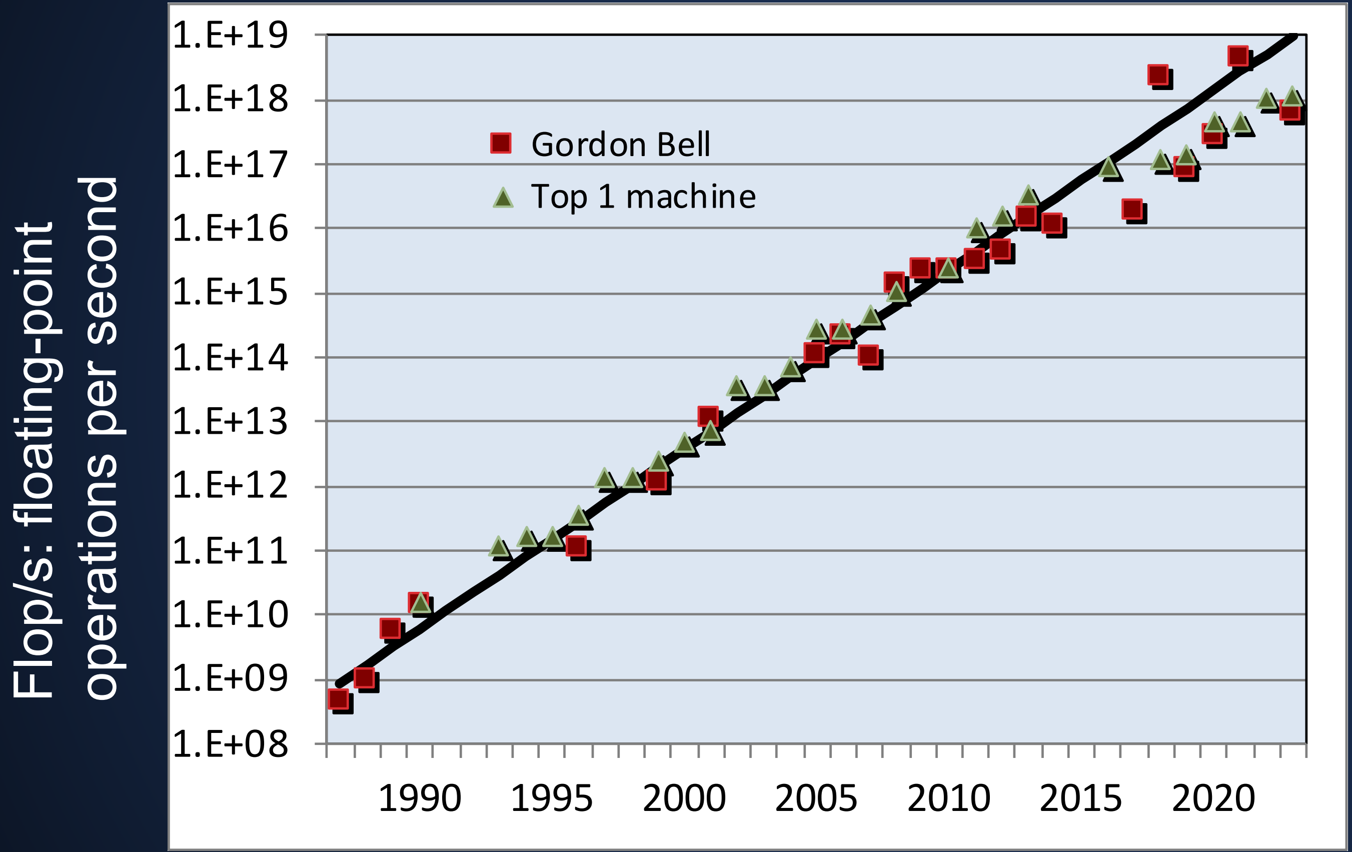
Perlmutter at NERSC (#1 in Berkeley)

GPU part	**Peak:** 63.8 PFlop/s **GPUs:** 2 NVIDIA A100	**Proc:** 1 AMD Epyc 7763 **Nodes:** 1792 **Memory:** 256 GB per node	**NICs/node:** 4 Slingshot 11 **MemBW:** 1.55 TB/s per GPU **GPU memory:** 40 GB HBM
CPU part	**Peak:** 7.7PFlop/s	**Proc:** 2 AMD Epyc 7763 **Nodes:** 3072 **Memory:** 512 GB per node	**NICs/node:** 1 Slingshot 11 **MemBW:** 204.8 GB/s per CPU

Gordon Bell Prizes: Science at Scale

Established in 1987 with a cash award of $10,000 (since 2011), funded by Gordon Bell, a pioneer in HPC.
For innovation in applying *HPC to applications in science, engineering, and data analytics*.

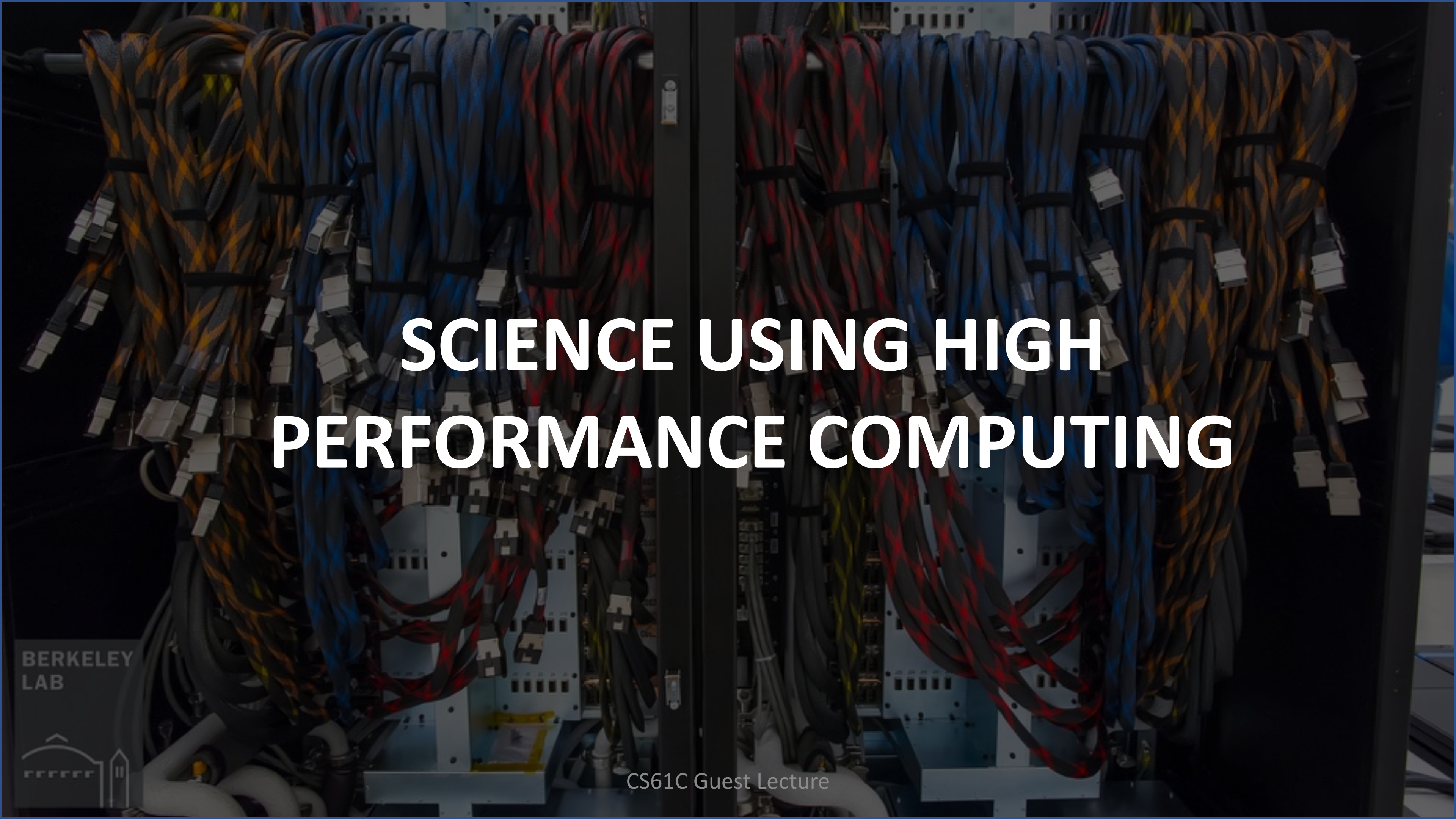
Gordon Bell Prizes vs Top 1



Lines above the Top #1:

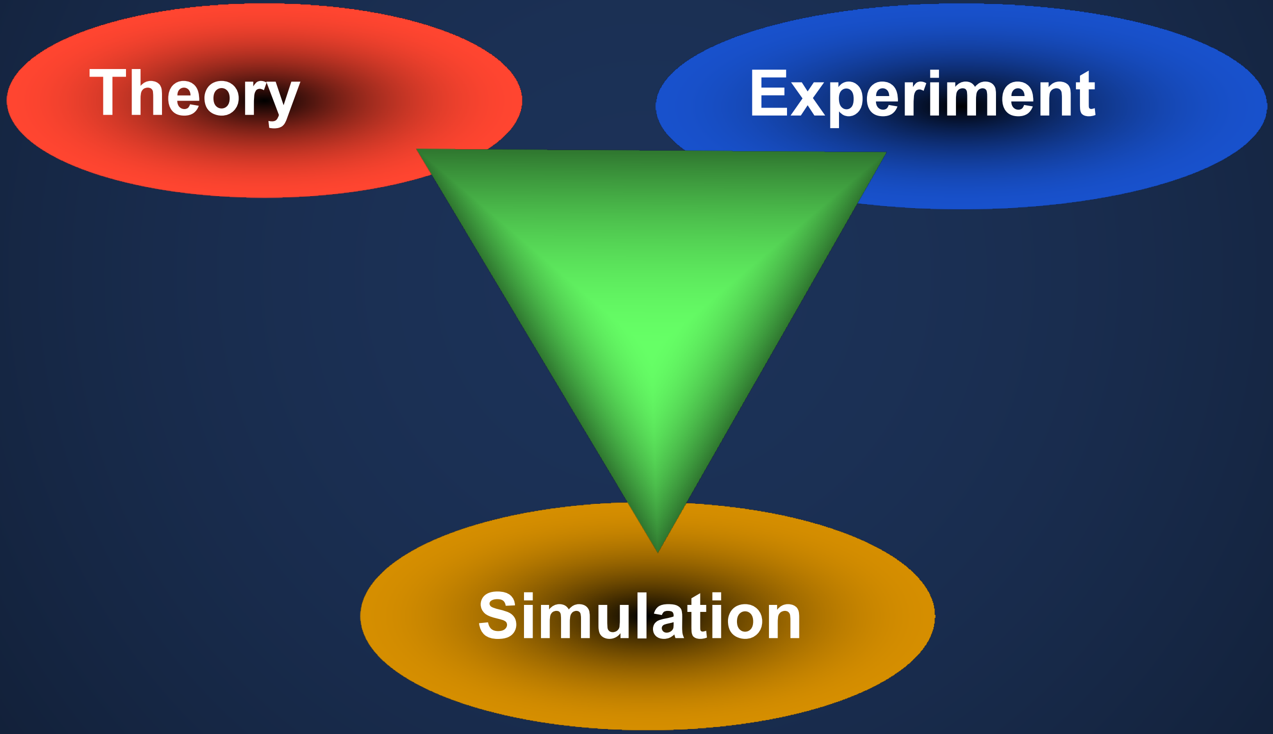
- AI flops
- Mixed half/single precision

SCIENCE USING HIGH PERFORMANCE COMPUTING



BERKELEY LAB

Simulation: The Third Pillar of Science



Simulation in Science and Engineering

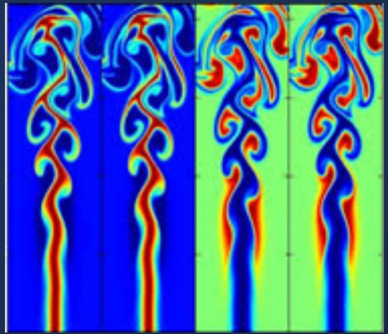
High performance simulation used to understand things that are:

- too big
- too small
- too fast
- too slow
- too expensive or
- too dangerous

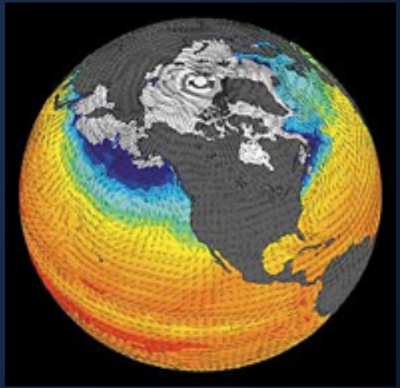
for experiments

Understanding the universe

Proteins and diseases



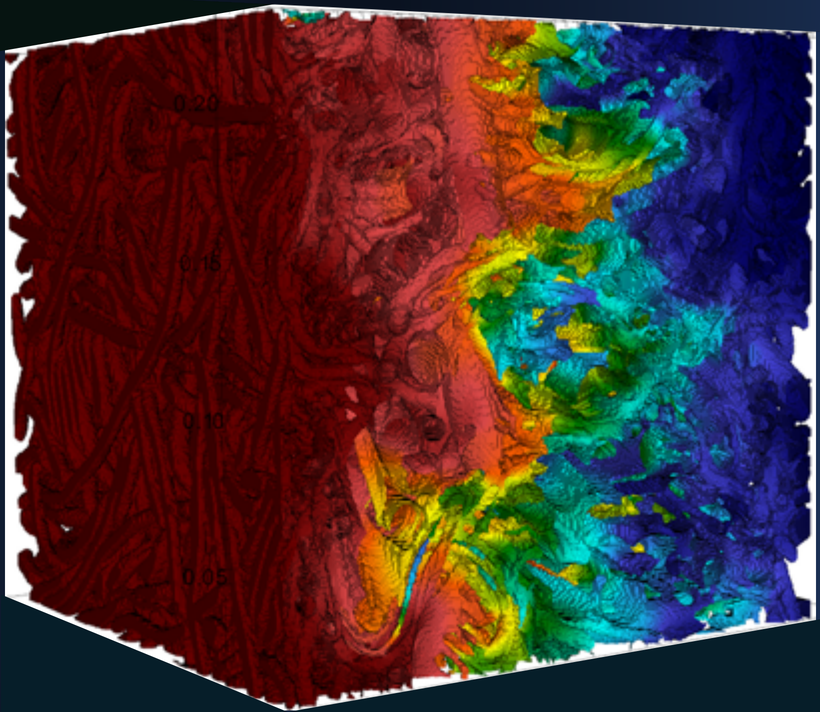
Energy-efficient jet engines



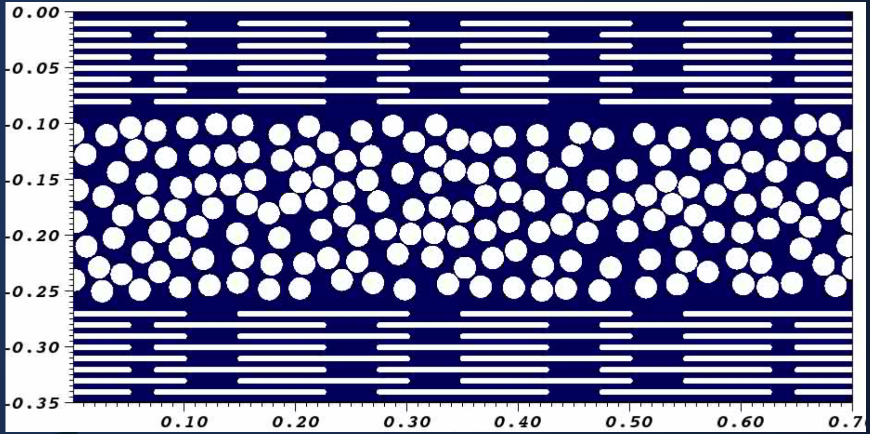
Climate change

HPC for Energy Efficiency in Industry

Paper industry is 4th Largest Energy Consumer in US

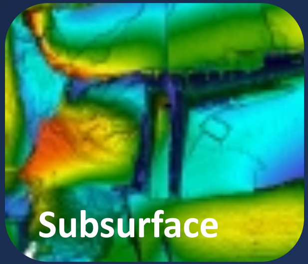


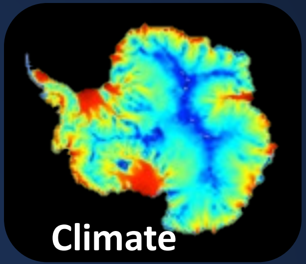
Chombo-Pulp: Apply adaptive embedded boundary solver to resolve flow around pulp fibers and in felt pore space

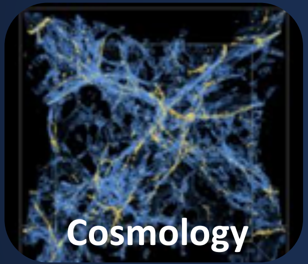


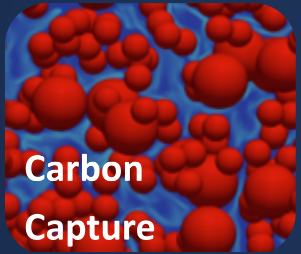
Adaptive mesh refinement and interface tracking

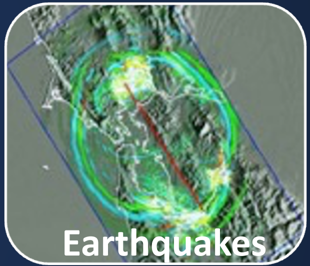
“Exascale” Applications at Berkeley Lab (LBNL)

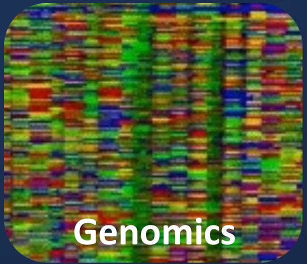


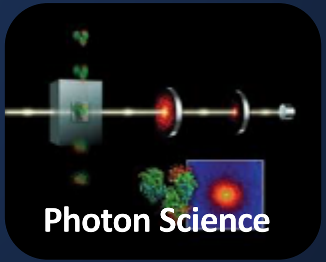




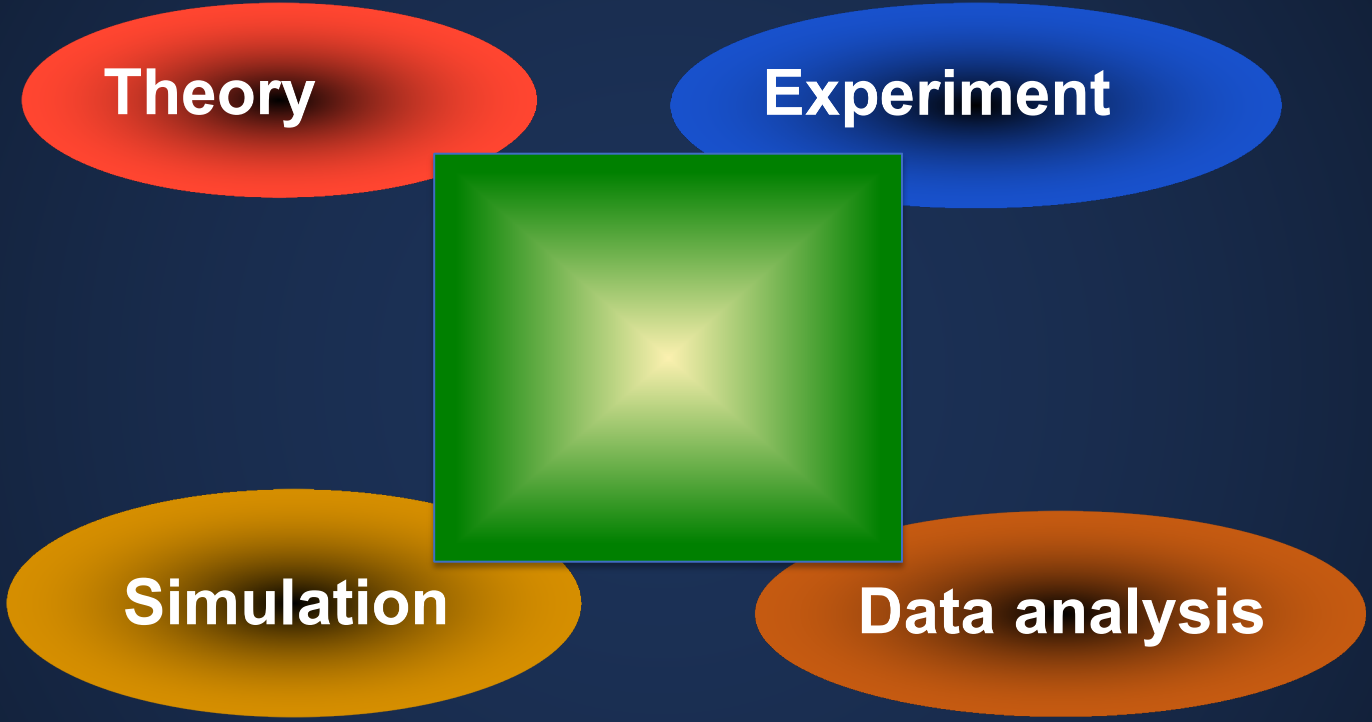








The Fourth Paradigm of Science



Data analytics in science and engineering

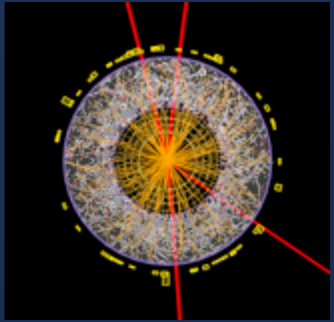
High Performance Data Analytics (HPDA) is used for data sets that are:

- too big
- too complex
- too fast (streaming)
- too noisy
- too heterogeneous

for measurement alone

Images from telescopes

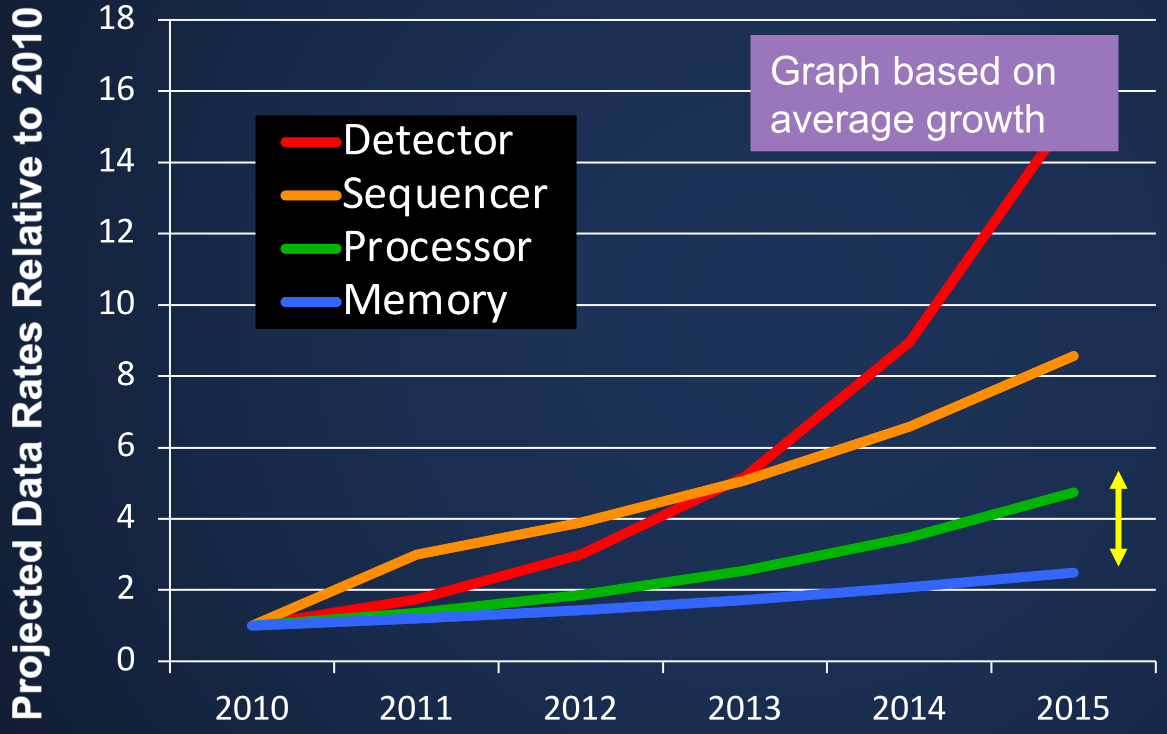
Genomes from sequencers



Particle from detectors

Sensor data

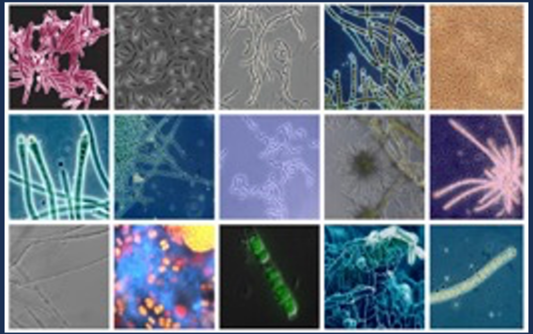
Data Growth is Outpacing Computing Growth



This gap is why we care about data movement (aka communication

High Performance Data Analytics (HPDA) for Genomics

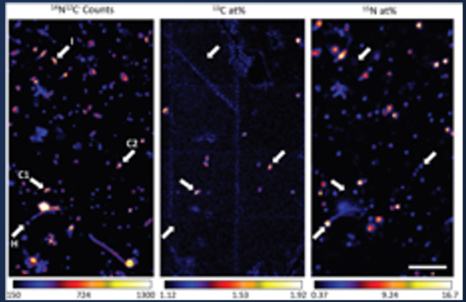
What happens to microbes after a wildfire? (1.5TB)



What are the microbial dynamics of soil carbon cycling? (3.3 TB)

How do microbes affect disease and growth of switchgrass for biofuels (4TB)

What at the seasonal fluctuations in a wetland mangrove? (1.6 TB)



Combine genomics with isotope tracing methods for improved functional understanding (8TB)

JGI-NERSC-KBase FICUS projects, MetaHipMer assembler ExaBiome project

Integrated Multifaceted Approach to Science

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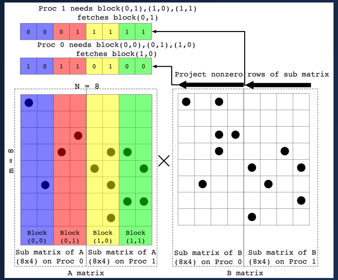
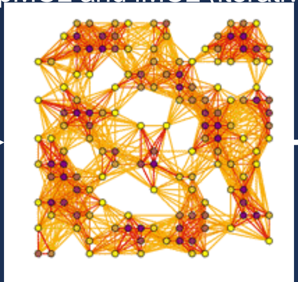
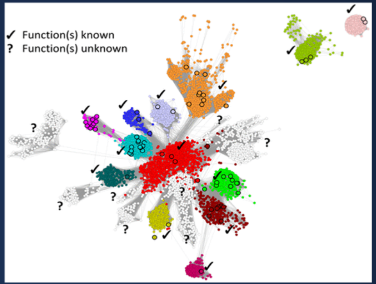


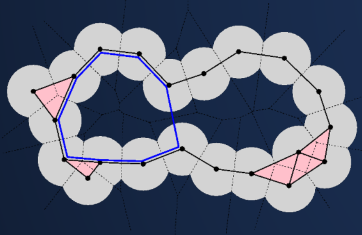
SpGEMM algorithms (workhorse of MCL variants)

Graph clustering with HipMCL and iMCL (iterative)

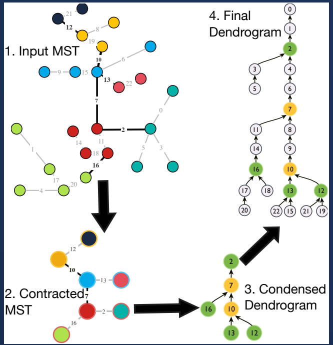




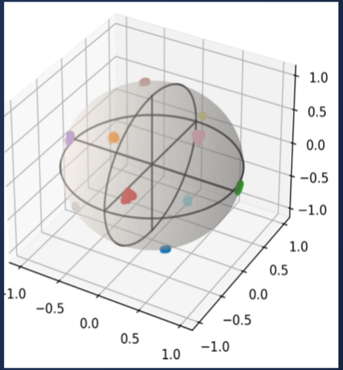
Discovery of novel protein families (enabled by HipMCL)



Persistent homology computation (basis of HDBSCAN variants)



Pandora: Parallel Dendrogram Construction Algorithm for HDBSCAN*



Metagenome binning with GenomeFace (uses HDBSCAN on embeddings)

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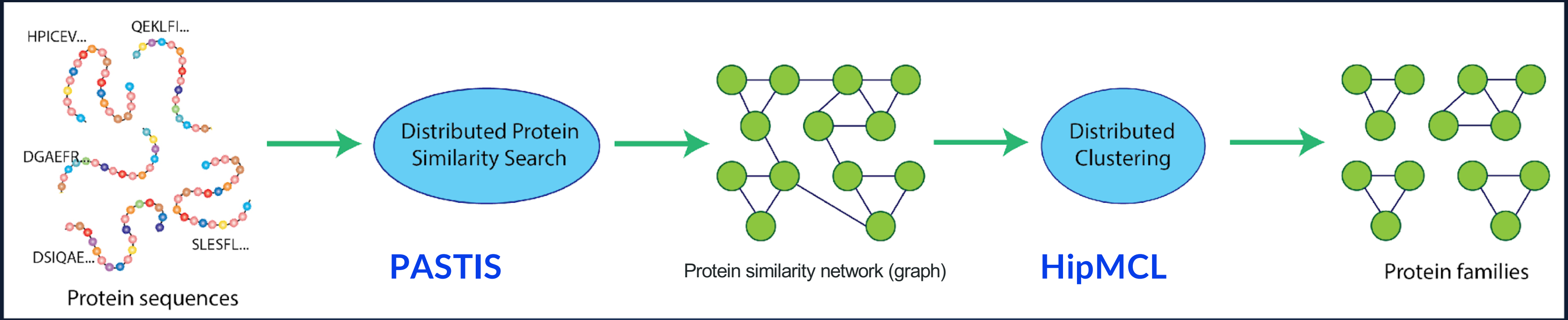
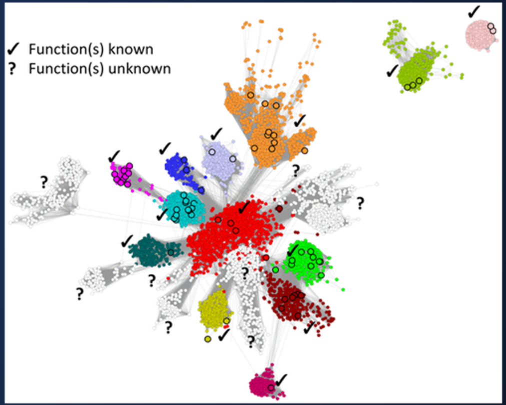
Protein Family Identification



- **Problem:** Given a large collection of proteins, identify groups of proteins that are homologous (i.e. descended from a common ancestor).
- Homologous proteins often have the same function
- Often, only sequences (and not structure) of the proteins are available, so we infer homology via sequence similarity



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Novel Protein Families in Microbial Dark Matter

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Microbial dark matter: novel proteins after removing matches to a database of over 100,000 genomes (including Archaeal, Bacteria, Viral and Eukaryotic)

Tools: PASTIS and HipMCL, both based on parallel computing techniques

Unraveling the functional dark matter through global metagenomics

Georgios A. Pavlopoulos, Fotis A. Baltoumas, Sirui Liu, Oguz Selvitopi, Antonio Pedro Camargo, Stephen Nayfach, Ariful Azad, Simon Roux, Lee Call, Natalia N. Ivanova, I. Min Chen, David Paez-Espino, Evangelos Karatzas, Novel Metagenome Protein Families Consortium, Ioannis Iliopoulos, Konstantinos Konstantinidis, James M. Tiedje, Jennifer Pett-Ridge, David Baker, Axel Visel, Christos A. Ouzounis, Sergey Ovchinnikov, Aydin Buluç & Nikos C. Kyrpides

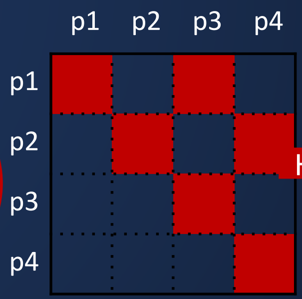
Nature **622**, 594–602 (2023) | Cite this article

Metagenomes Metatranscriptomes 26K → Proteins 8B → Unknown Proteins 1B → PASTIS → Similarity Graph of Proteins .6B

Find protein-code genes

Eliminate those that match pfam database

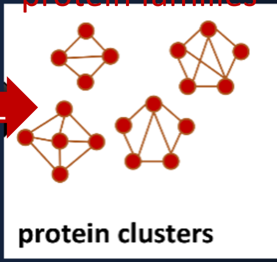
Compute similarity score on pairs



Represent as sparse matrix

HipMCL →

106,198 novel protein families



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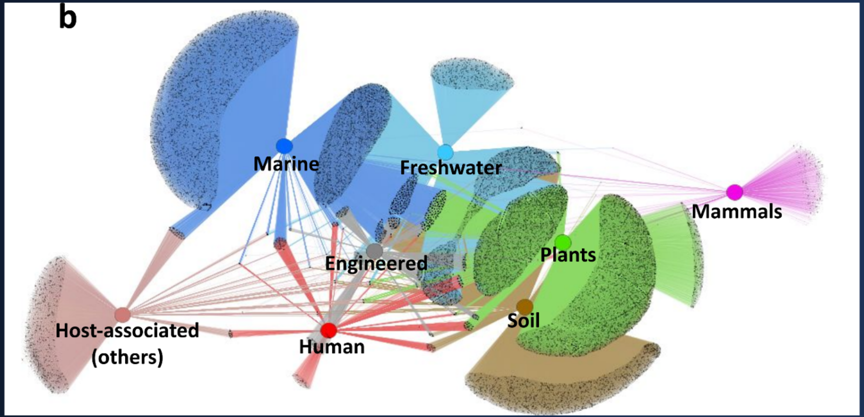
Diversity of Novel Protein Families

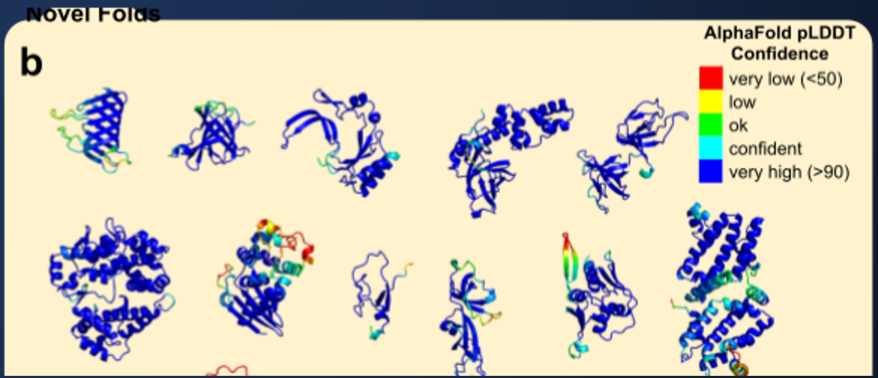
Novel protein clusters are distributed across 8 ecosystem types



Network representation of protein clusters (gray peripheral) and their associated ecosystems (colored central)

Distribution of protein structures

- 4,361 unique structures were predicted using AlphaFold
- 3,808 structures has hits in SCOPe.
- 345 has hits in Protein Data Bank (PDB).
- After further filtering, 162 structures are considered novel folds



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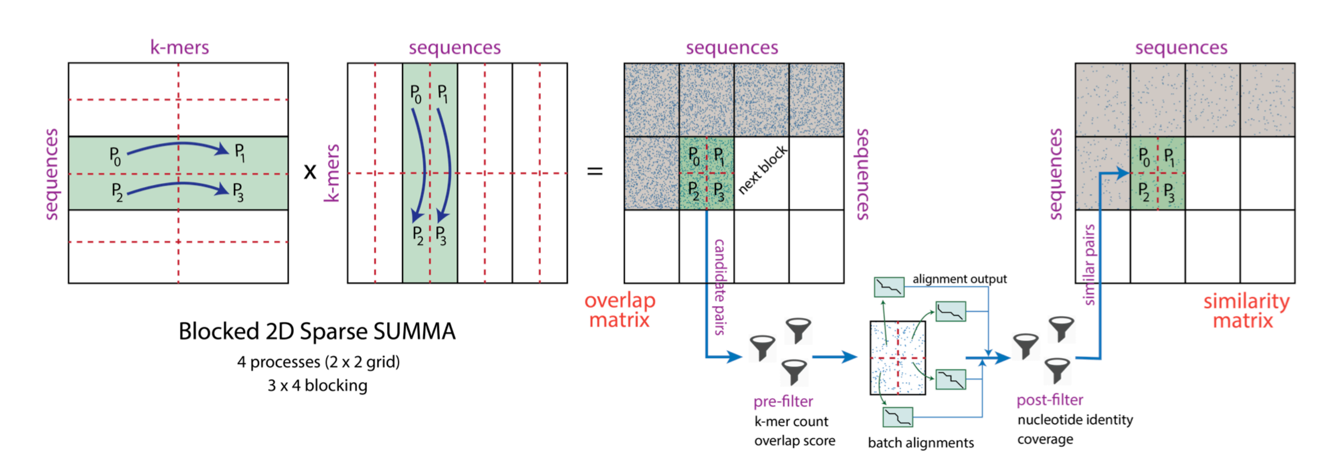
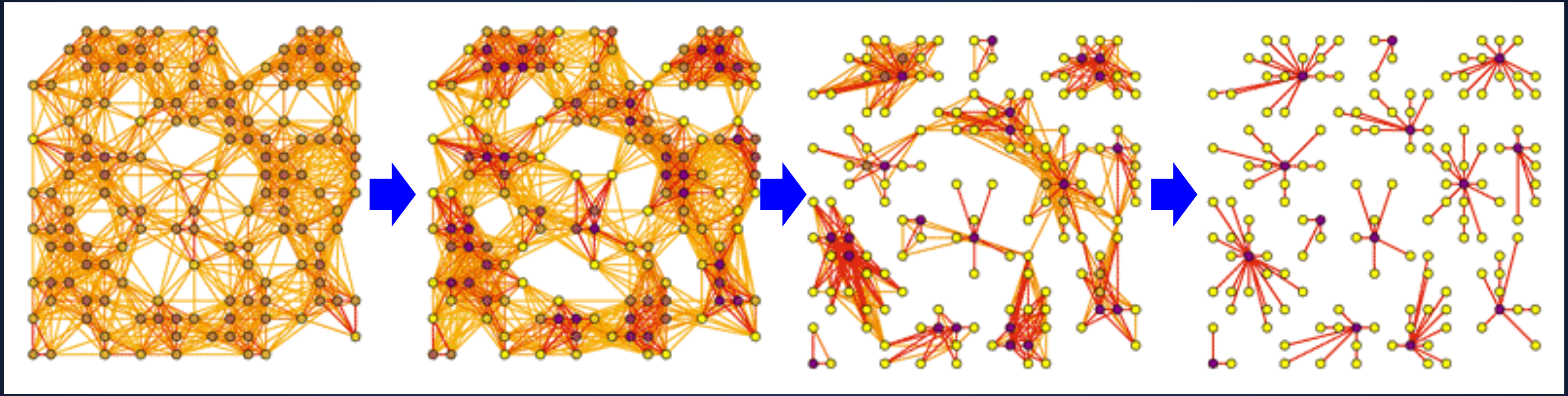
PASTIS: Many-to-many sequence alignment

Finalist for the 2022 Gordon Bell Prize

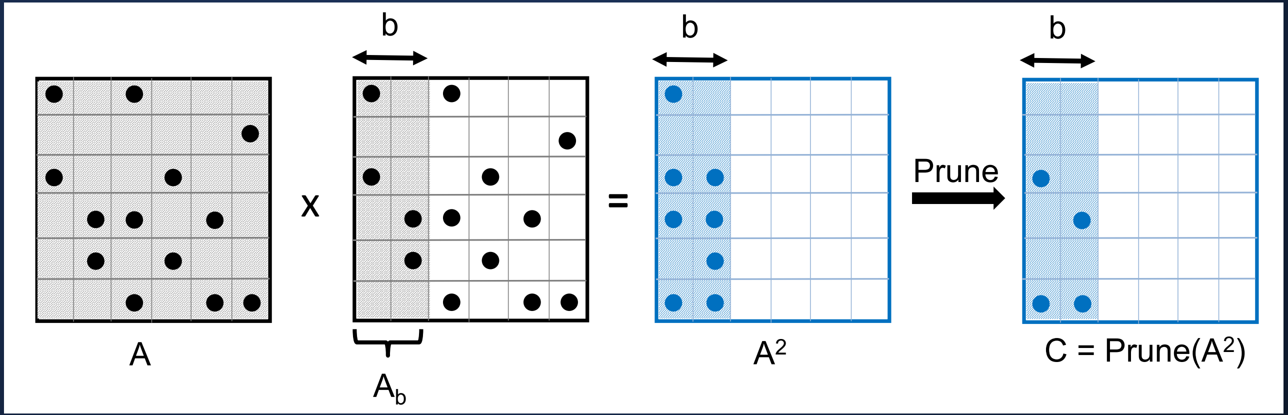


Abstract-- … We unleash the power of over 20,000 GPUs on the Summit system to perform all-vs-all protein similarity search on one of the largest publicly available datasets with 405 million proteins, in less than 3.5 hours, cutting the time-to-solution for many use cases from weeks. The variability of protein sequence lengths, as well as the sparsity of the space of pairwise comparisons, make this a challenging problem in distributed memory …

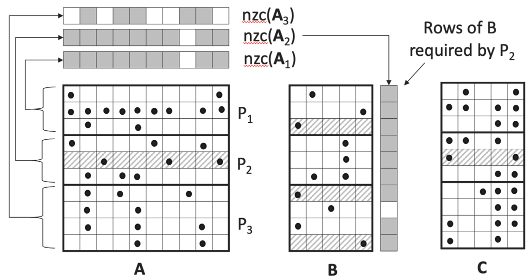
HipMCL: High-performance Markov Clustering



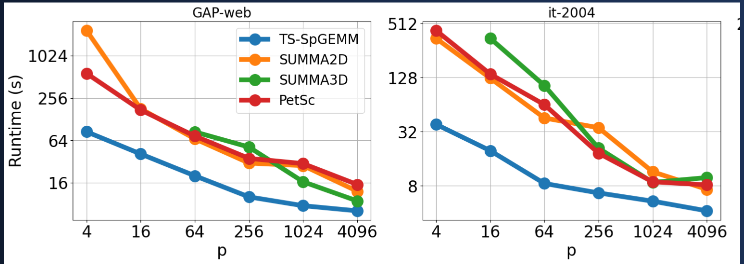
Squaring the matrix while pruning (a) small entries, (b) denser columns

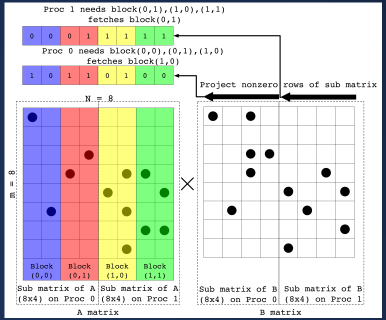


Both PASTIS and HipMCL use SpGEMM

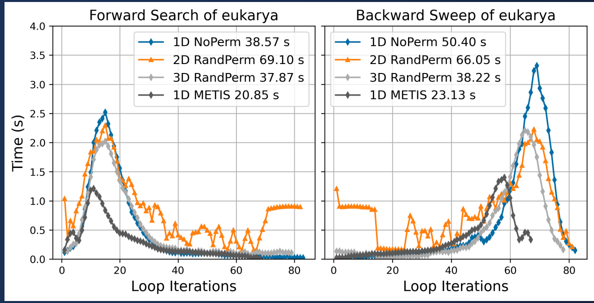


TS-SpGEMM: Tall-skinny SpGEMM for concurrent graph traversals and graph embeddings





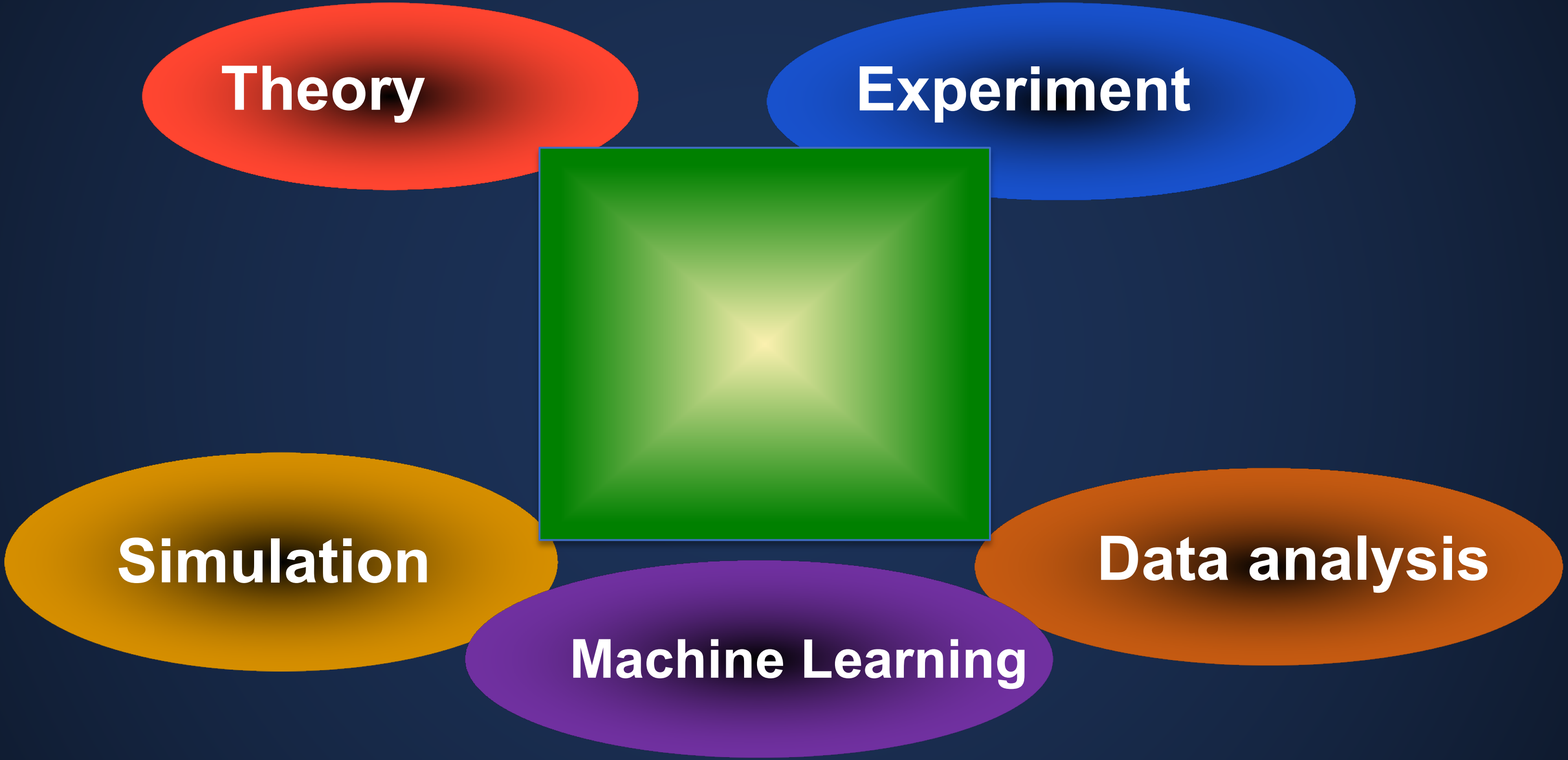
Block fetching strategy used in the 1D sparsity-aware SpGEMM algorithm



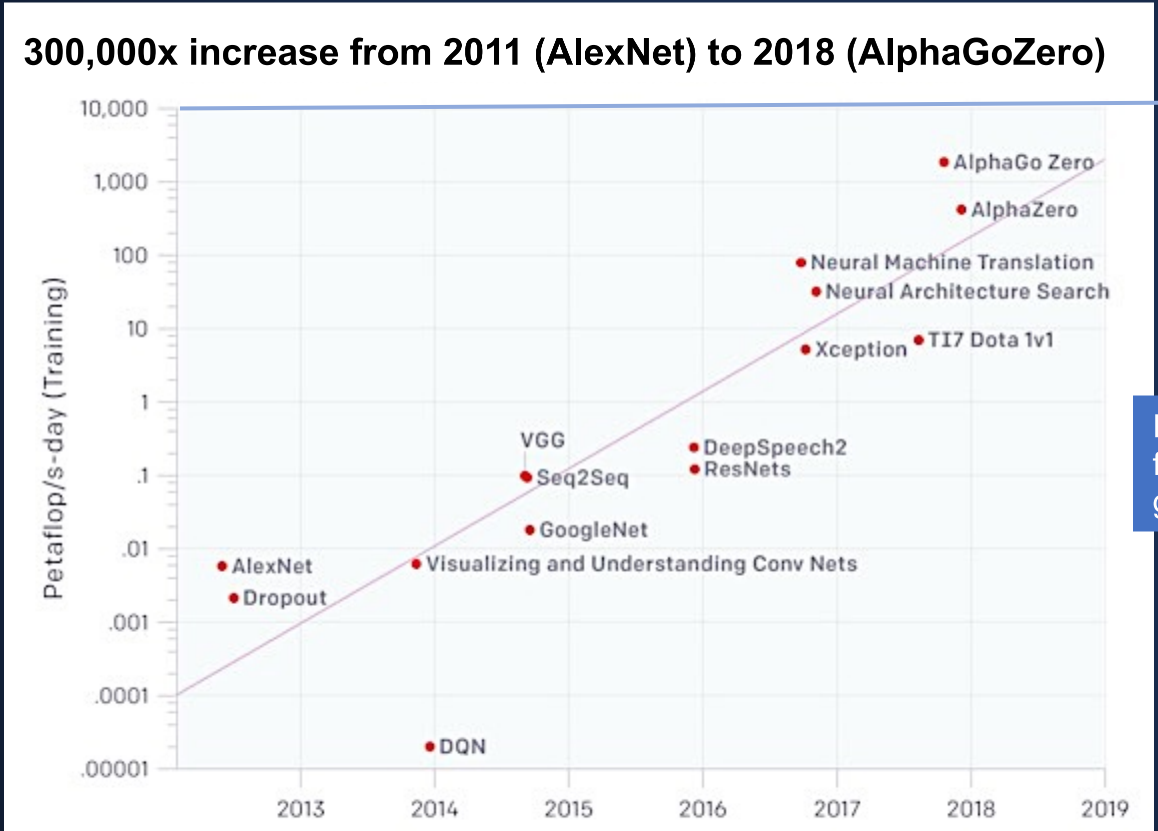
Ranawaka et al. "Distributed-Memory Parallel Algorithms for Sparse Matrix and Sparse Tall-and-Skinny Matrix Multiplication." **SC'24**

Hong and Buluc. " A sparsity-aware distributed-memory algorithm for sparse-sparse matrix multiplication." **SC'24**

The Fifth Paradigm of Science ?



Machine learning demands more computing



ExaFLOP/s for one Day

From 2011-2017 the fastest Top500 machine grew < 10x

https://blog.openai.com/ai-and-compute/

Machine learning demands more computing

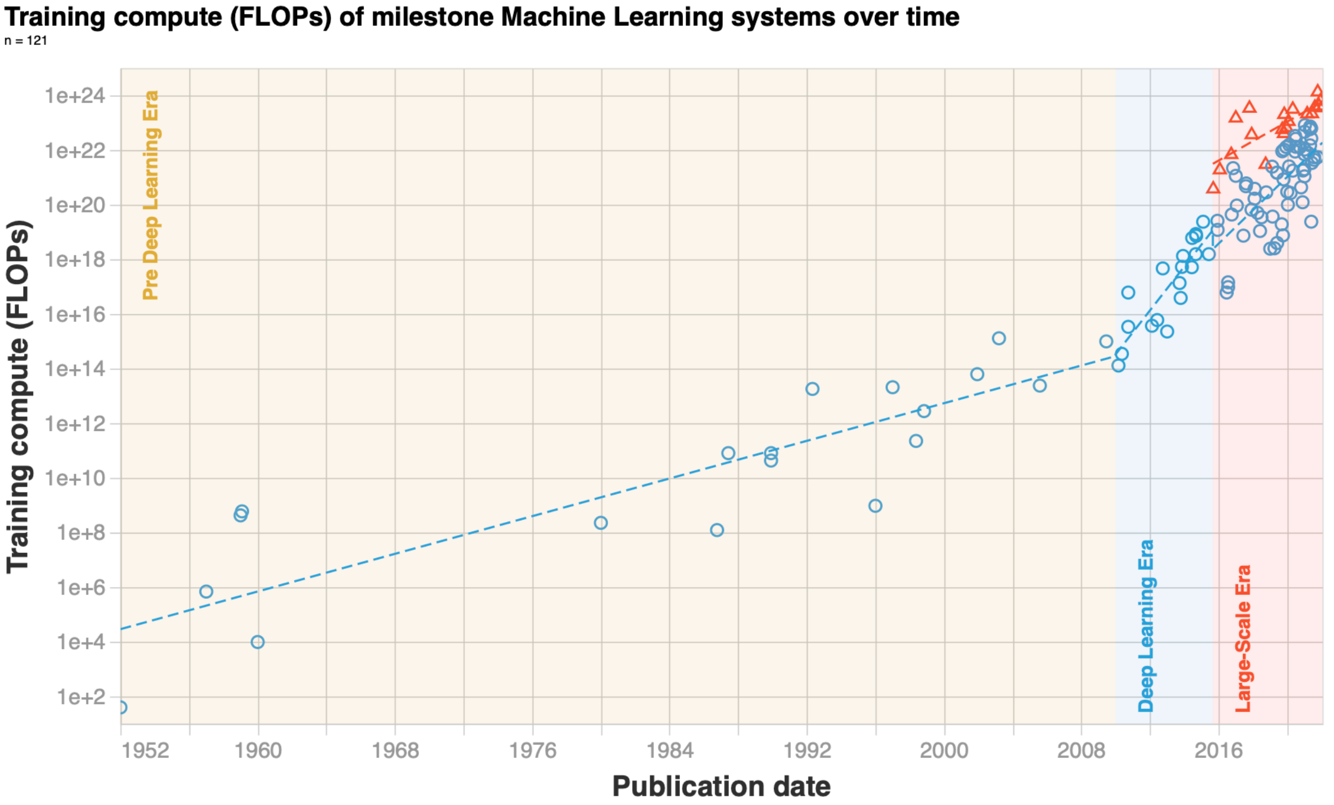


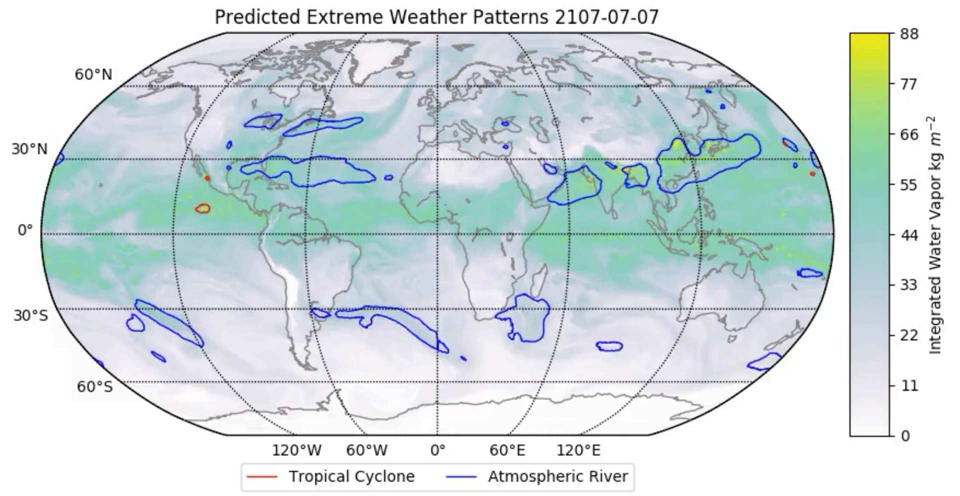
Figure 1: Trends in $n = 121$ milestone ML models between 1952 and 2022. We distinguish three eras. Notice the change of slope circa 2010, matching the advent of Deep Learning; and the emergence of a new large-scale trend in late 2015.

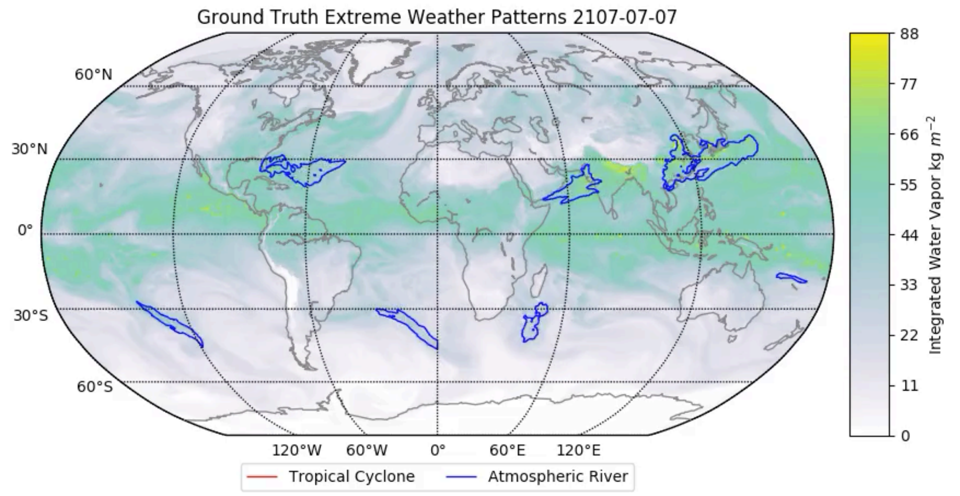
"Compute trends across three eras of machine learning", Sevilla et al., 2022

Big Data, Big Model, and Big Iron

Predicted Extreme Weather

Ground Truth Extreme Weather

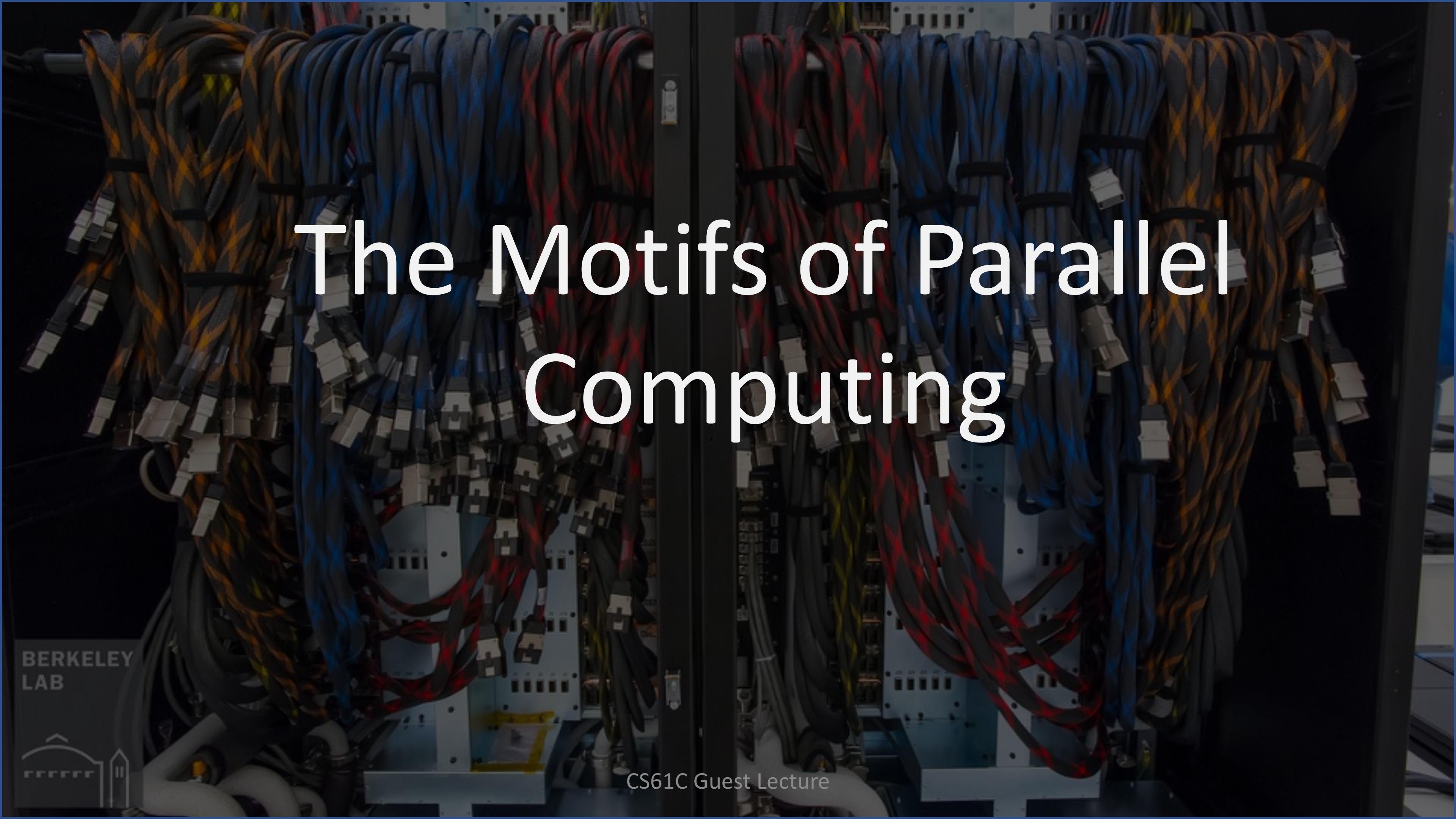




- **Deep learning results are smoother than heuristic labels**
- **Achieved over 1 EF peak on OLCF Summit: Gordon Bell Prize in 2018**

Thorsten Kurth, Sean Treichler, Joshua Romero, Mayur Mudigonda, Nathan Luehr, Everett Phillips, Ankur Mahesh, Michael Matheson, Jack Deslippe, Massimiliano Fatica, Prabhat, Michael Houston

The Motifs of Parallel Computing



How to cover all applications?

- Phil Colella's famous 7 "dwarfs" of scientific computing (simulation)

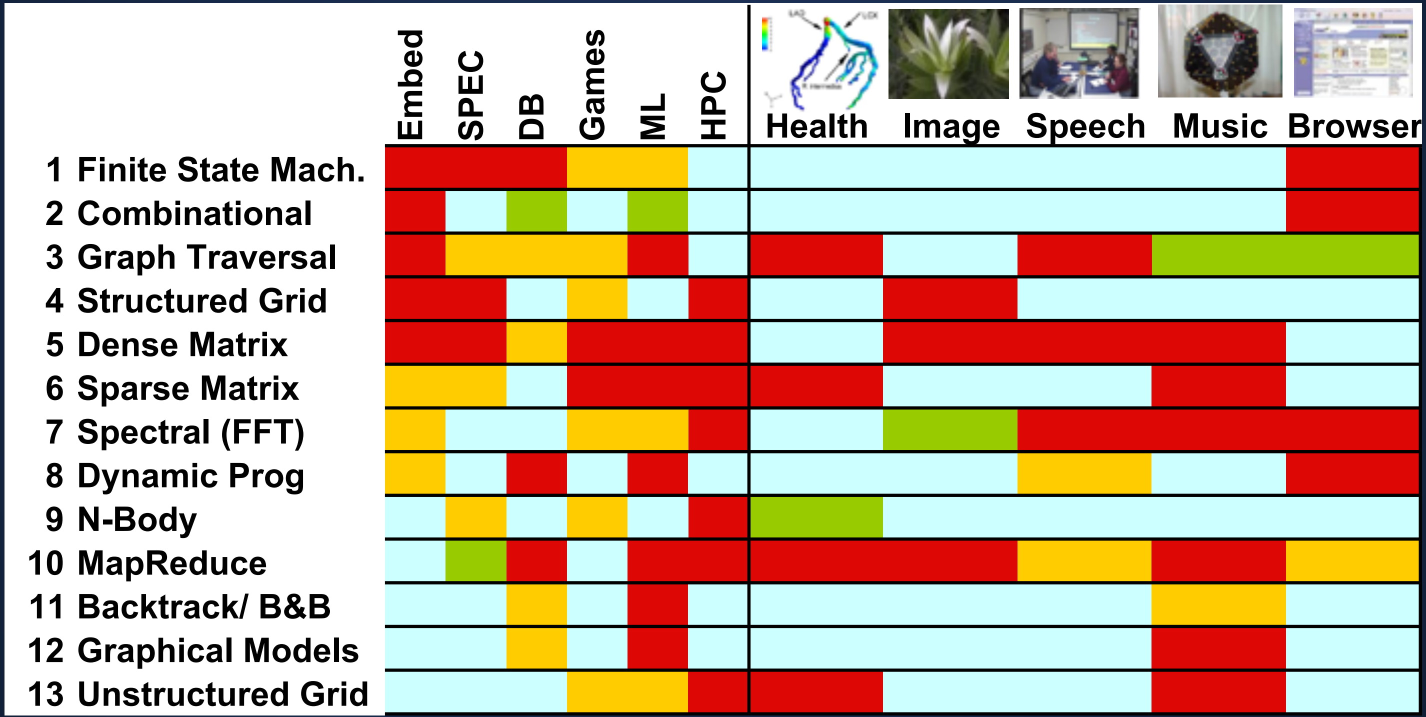
Dense Linear Algebra
Sparse Linear Algebra
Particle Methods
Structured Grids
Unstructured Grids
Spectral Methods (e.g. FFT)
Monte Carlo

Colella's 2004 DARPA presentation "Defining Software Requirements for **Scientific** Computing"

Motifs: Common Computational Methods

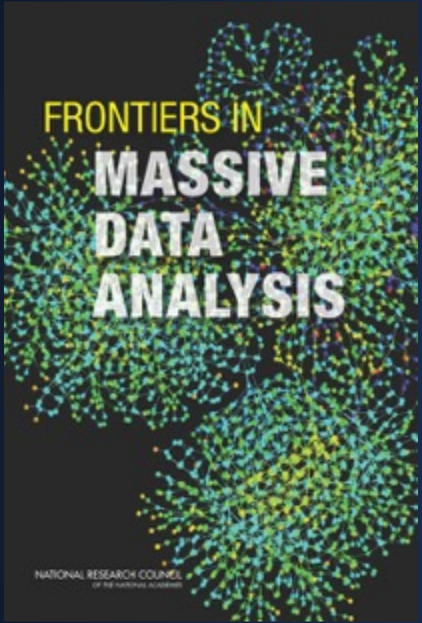
(Red Hot Important → Blue Cool Not Important)

What do commercial and CSE applications have in common?



2006 Berkeley View paper - A View of the Parallel Computing Landscape

Analytics vs. Simulation Motifs

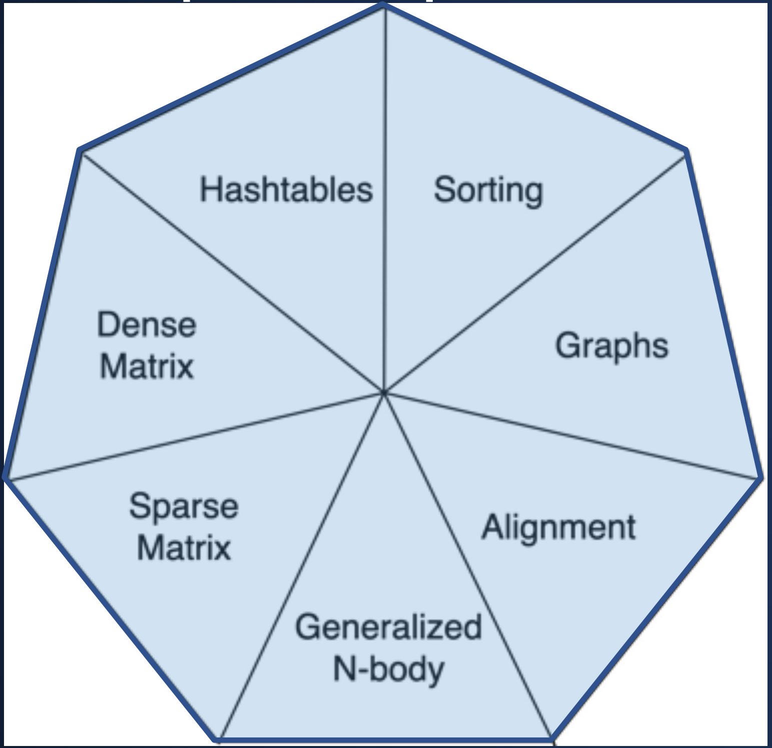


National Academies
2013

7 Giants of Data	7 Dwarfs of Simulation
Basic statistics	Monte Carlo methods
Generalized N-Body	Particle methods
Graph-theory	Unstructured meshes
Linear algebra	Dense Linear Algebra
Optimizations	Sparse Linear Algebra
Integrations	Spectral methods
Alignment	Structured Meshes

Motifs of Genomic Data Analysis

These computational patterns dominate ExaBiome



Application problems

- Overlap: Find all overlaps in a set
- Assembly: find / correct overlaps
- Distance: how good are overlaps
- Index: lookup in database

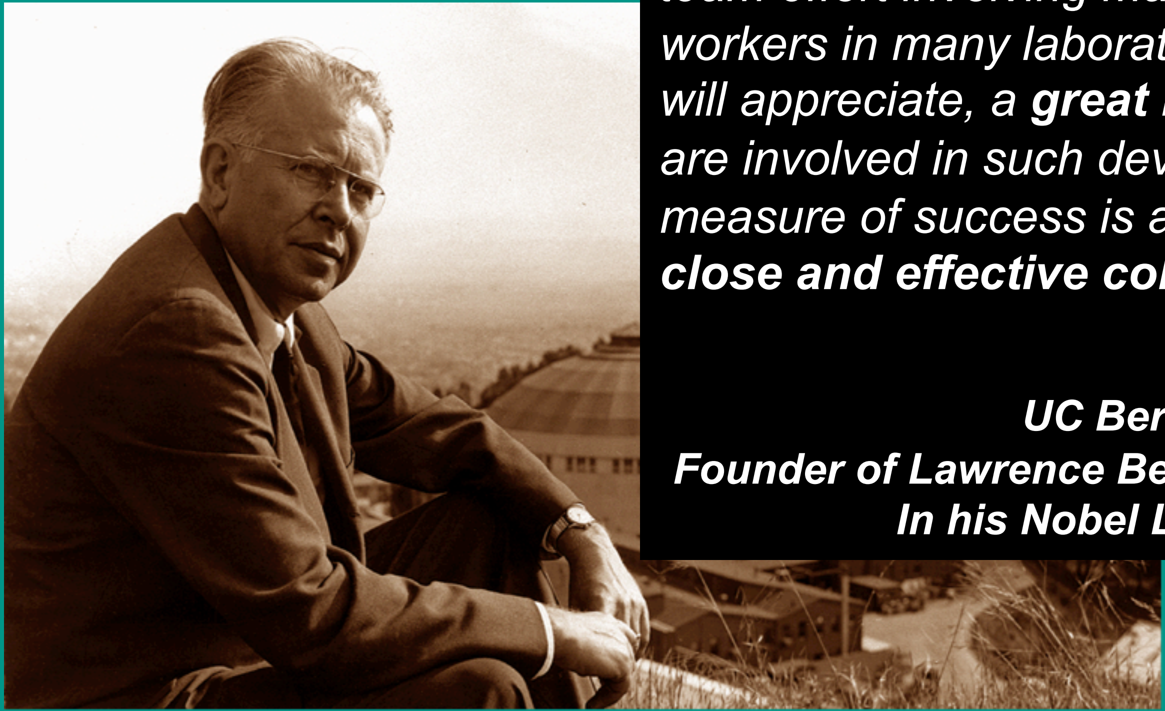
Large shared memory platforms were most common – limits science questions and approaches

Yelick, et al. "The Parallelism Motifs of Genomic Data Analysis", Philosophical Transactions A, 2020

Scientific Computing is a Team Sport

IPCC Working Groups (Intergovernment Panel and Climate Change)

Computational Science is Necessarily Collaborative



… as from the beginning the work has been a team effort involving many able and devoted co-workers in many laboratories. As I am sure you will appreciate, a ***great many diverse talents*** *are involved in such developments and whatever measure of success is achieved is dependent on* ***close and effective collaboration****.*

Ernest O. Lawrence
UC Berkeley Professor of Physics
Founder of Lawrence Berkeley National Laboratory
In his Nobel Lecture, December 11, 1951