

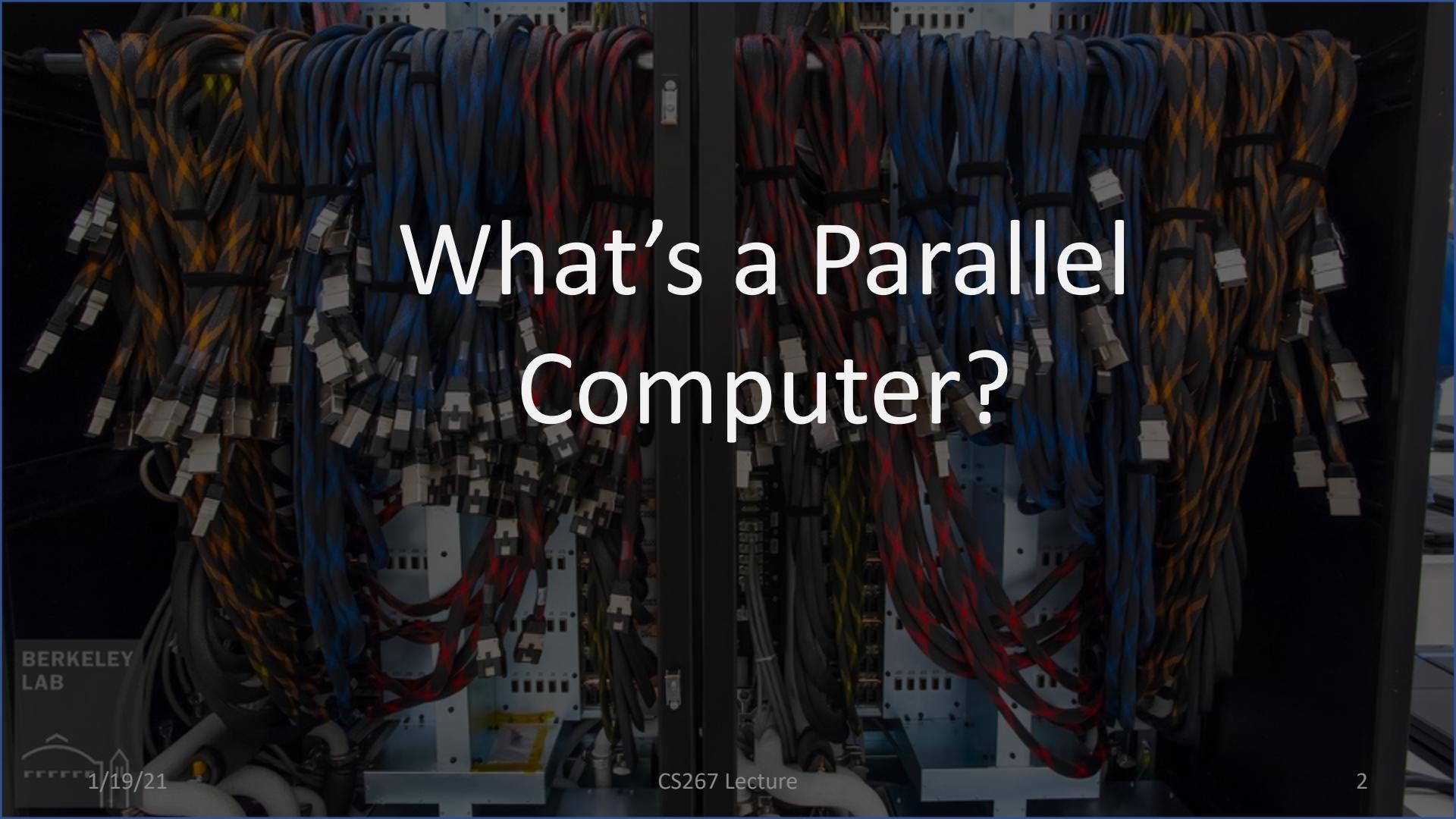
Applications of Parallel Computers

CS267/E233

<https://sites.google.com/lbl.gov/cs267-spr2021>



Survey: <https://forms.gle/XNKNXhhH4mtibMtR8>



What's a Parallel Computer?

BERKELEY
LAB



1/19/21

CS267 Lecture

2

It's all about the need for speed



Parallel Computing: Faster Solutions

Using multiple processors in parallel to solve problems more quickly than with a single processor

Compute the prime factors of 1 billion numbers:



If we had 1 million processors...

Sum (reduction) in parallel

- Add n values



Serial: $O(n)$

Parallel: $O(\log n)$

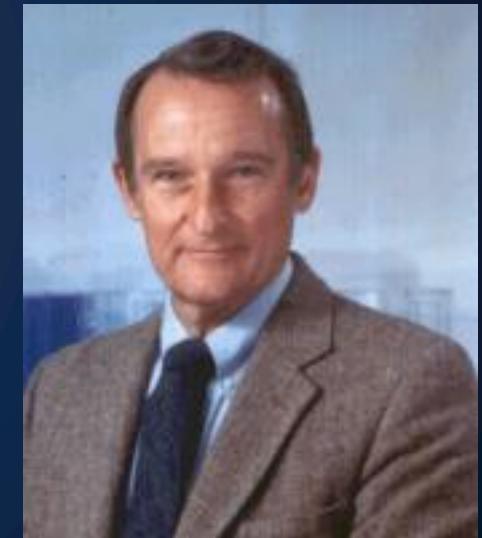
Uses n processors!

- Takes advantage of associativity in +

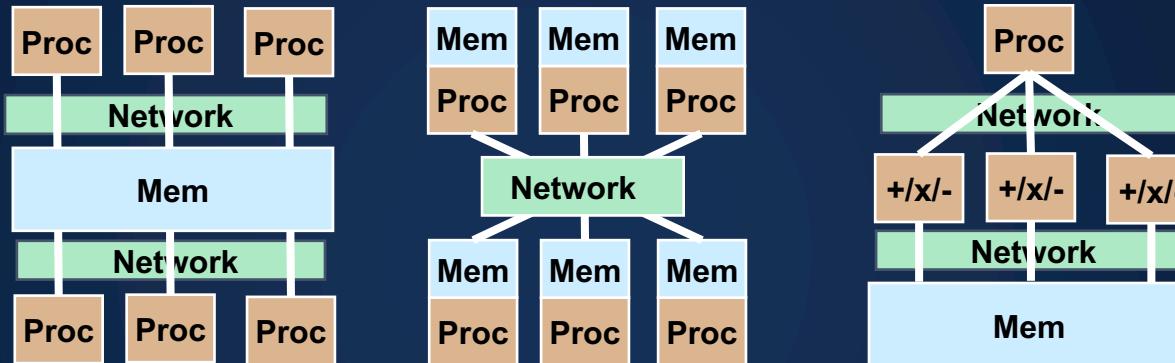
If you were plowing a field, which would you rather use?

Two strong oxen or 1024 chickens?

- Seymour Cray



What is a Parallel Computer?

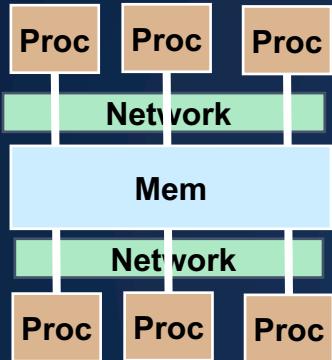


Shared Memory (SMP) or
Multicore

High Performance
Computing (HPC) or
Distributed Memory

Single Instruction Multiple
Data (SIMD)

What is a Parallel Computer?



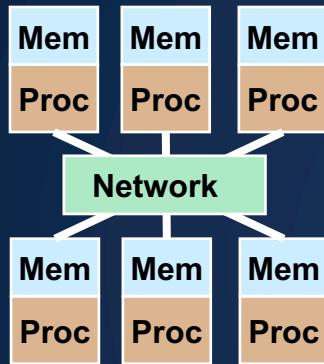
A **shared memory multiprocessor** (SMP*) by connecting multiple processors to a single memory system

A **multicore processor** contains multiple processors (cores) on a single chip

Shared Memory (SMP) or
Multicore

* Technically, SMP stands for “Symmetric Multi-Processor”

What is a Parallel Computer?



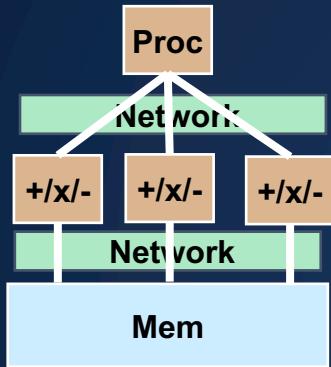
A **distributed memory multiprocessor** has processors with their own memories connected by a high speed network

Also called a **cluster**

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

High Performance Computing (HPC) or Distributed Memory

What is a Parallel Computer?

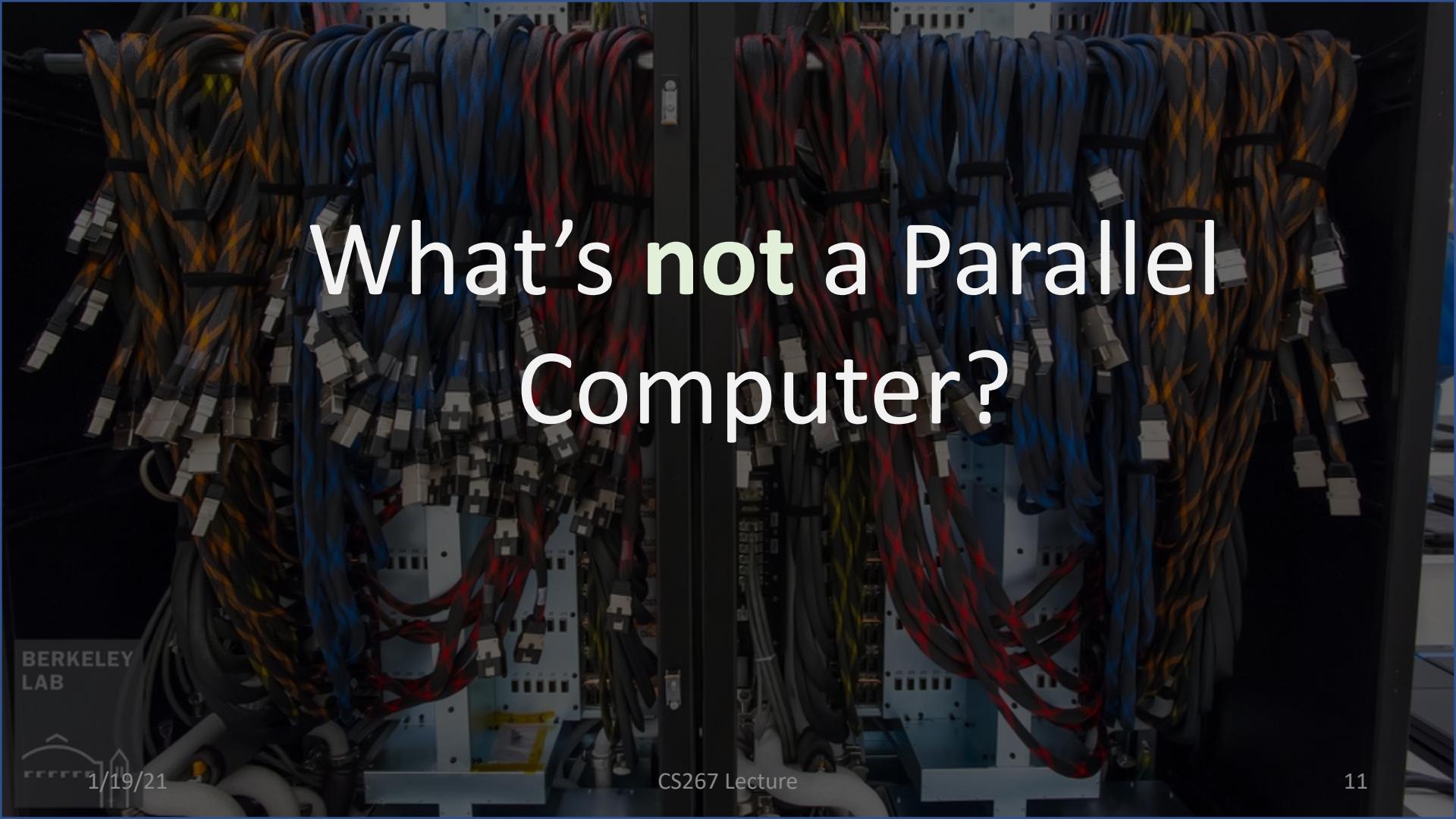


A **Single Processor Multiple Data (SIMD)** computer has multiple processors (or functional units) that perform the same operation on multiple data elements at once

Most single processors have **SIMD units** with ~2-8 way parallelism

Single Instruction Multiple Data (SIMD)

Graphics processing units (**GPUs**) use this as well



What's not a Parallel Computer?

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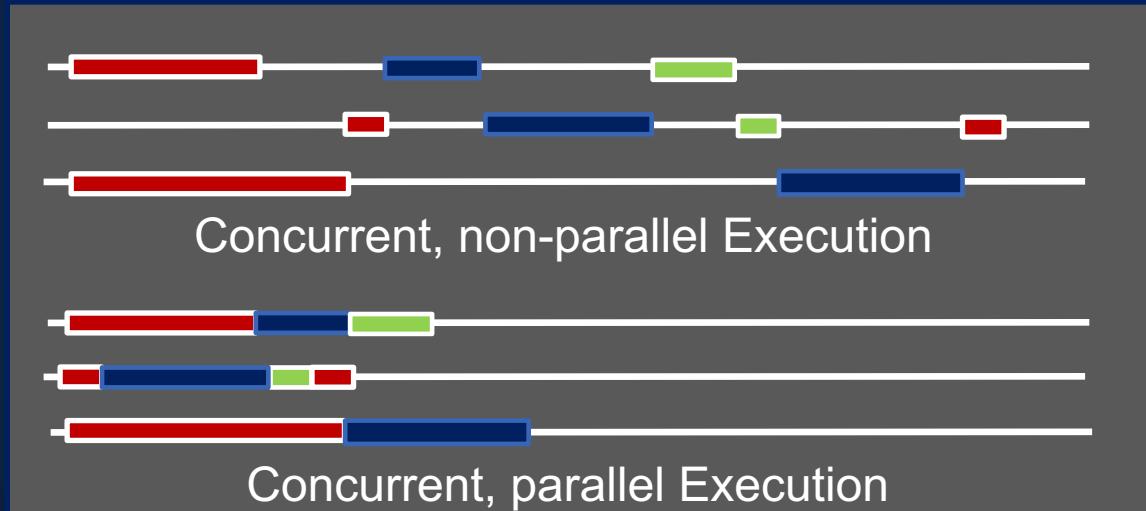
1/19/21

CS267 Lecture

11

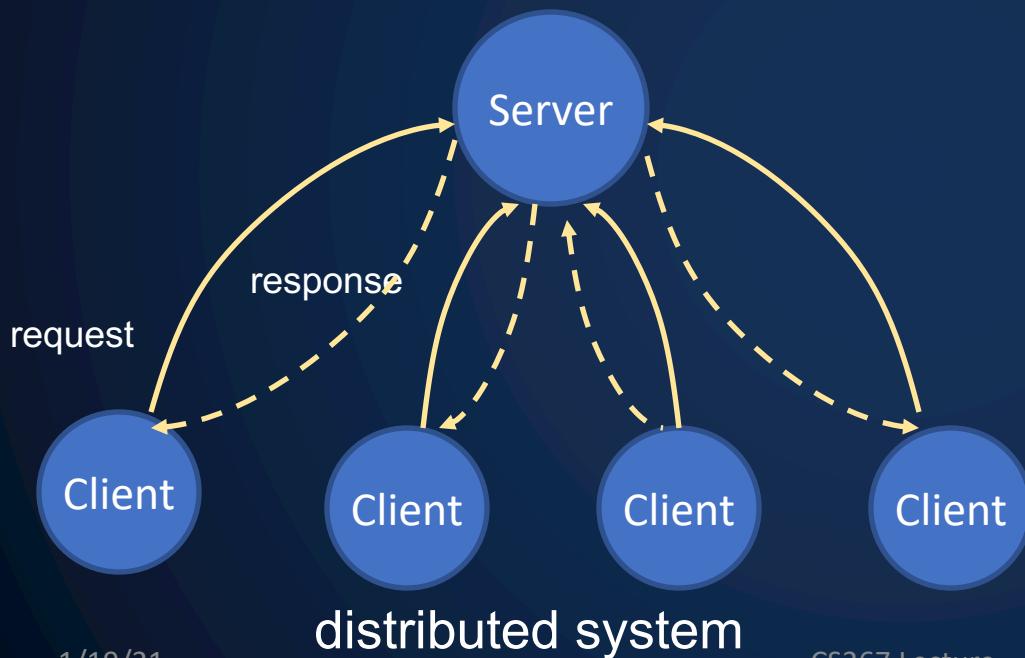
Concurrency vs. Parallelism

- Concurrency: multiple tasks are *logically* active at one time.
- Parallelism: multiple tasks are *actually* active at one time.



Parallel Computer vs. Distributed System

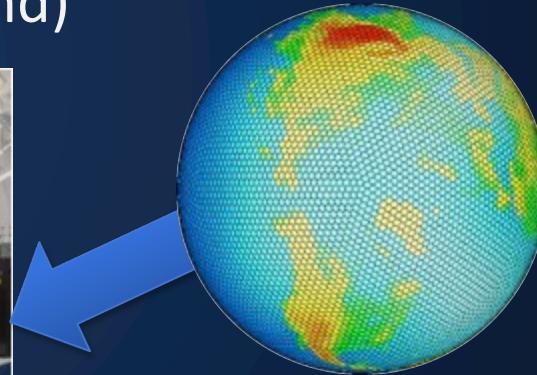
- A distributed system is *inherently* distributed, i.e., serving clients at different locations



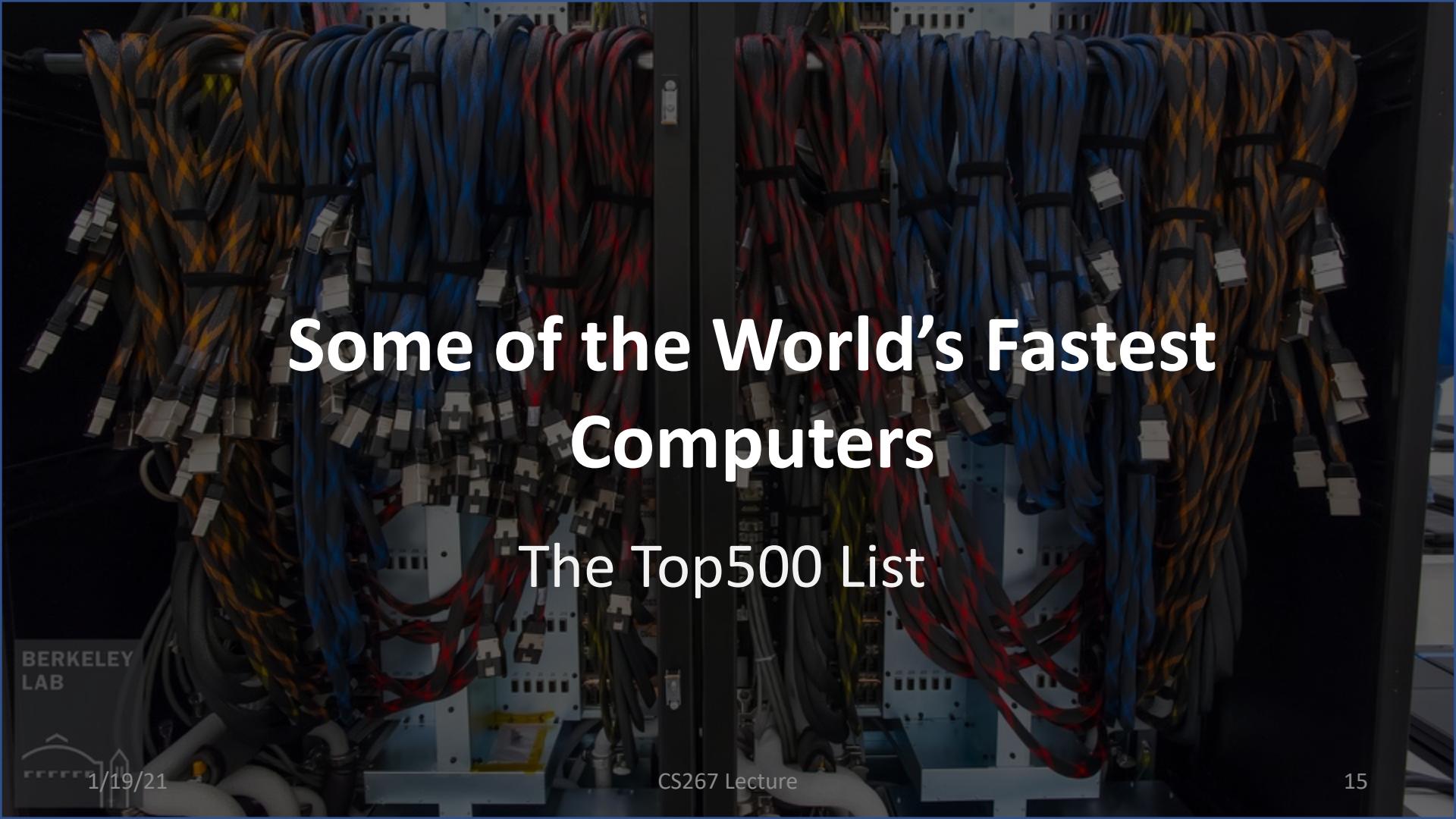
A parallel computer may use ***distributed memory*** (multiple processors with their own memory) for more performance

The Fastest Computers (for Science) Have Been Parallel for a Long Time

- Fastest Computers in the world: top500.org
- LBNL's Cori Computer has over 680,000 cores and ~30 Petaflops (10^{15} math operations / second)



*Supercomputing is
done by parallel
programming*



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

Goal

- 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



#	TOP 500 SUPERCOMPUTER SITES	Site	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	NVIDIA Corporation	NVIDIA	Selene DGX A100 SuperPOD, AMD 64C 2.25GHz, NVIDIA A100, Mellanox HDR	USA	555,520	63.5	2.65	
6	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	
7	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	
8	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	
9	Texas Advanced Computing Center / Univ. of Texas	Dell	Frontera Dell C6420, Xeon Platinum 8280 28C 2.7GHz, Mellanox HDR	USA	448,448	23.5		
10	1/19/23 Saudi Aramco	HPE	Dammam-7 Cray CS-Storm, Xeon G. 20C 2.5GHz, NVIDIA T. V100, IB HDR 100	Saudi Arabia	672,520	22.48		

Summit (#1 in US) System Overview



System Performance

- Peak performance of 200 petaflops for modeling & simulation
- Peak of 3.3 ExaOps for data analytics and artificial intelligence

Each node has

- 2 IBM POWER9 processors
- 6 NVIDIA Tesla V100 GPUs
- 608 GB of fast memory
- 1.6 TB of NVMe memory

The system includes

- 4608 nodes
- Dual-rail Mellanox EDR InfiniBand network
- 250 PB IBM Spectrum Scale file system transferring data at 2.5 TB/s



Fugaku (#1 Worldwide) System Overview

System Performance

- Peak performance of 442 petaflops (per TOP500 Rmax),
- 2.0 EFLOPS on a different mixed-precision benchmark

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)



Cori at NERSC (#1 in Berkeley, CA)

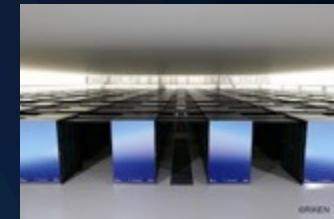
Phase 1	Peak: 2.8 PFlop/s Proc: 3800 Haswell (ph 1) Cores: 2.3 GHz, 16/proc Proc Peak: 0.6 TFlop/s	Memory: 0.3 PB Storage: shared	
Phase 2	Peak: 28PFlop/s LinPack: 14 Pflops/s Power: 4 MW	Processor: 9300 KNL Cores: 1.4 GHz, 68/proc Node Peak: 3 TFlop/s	Memory: 1.31 PB MemBW: 1 PB/s HBM,DDR Storage: 28 PB



Performance History and Projection

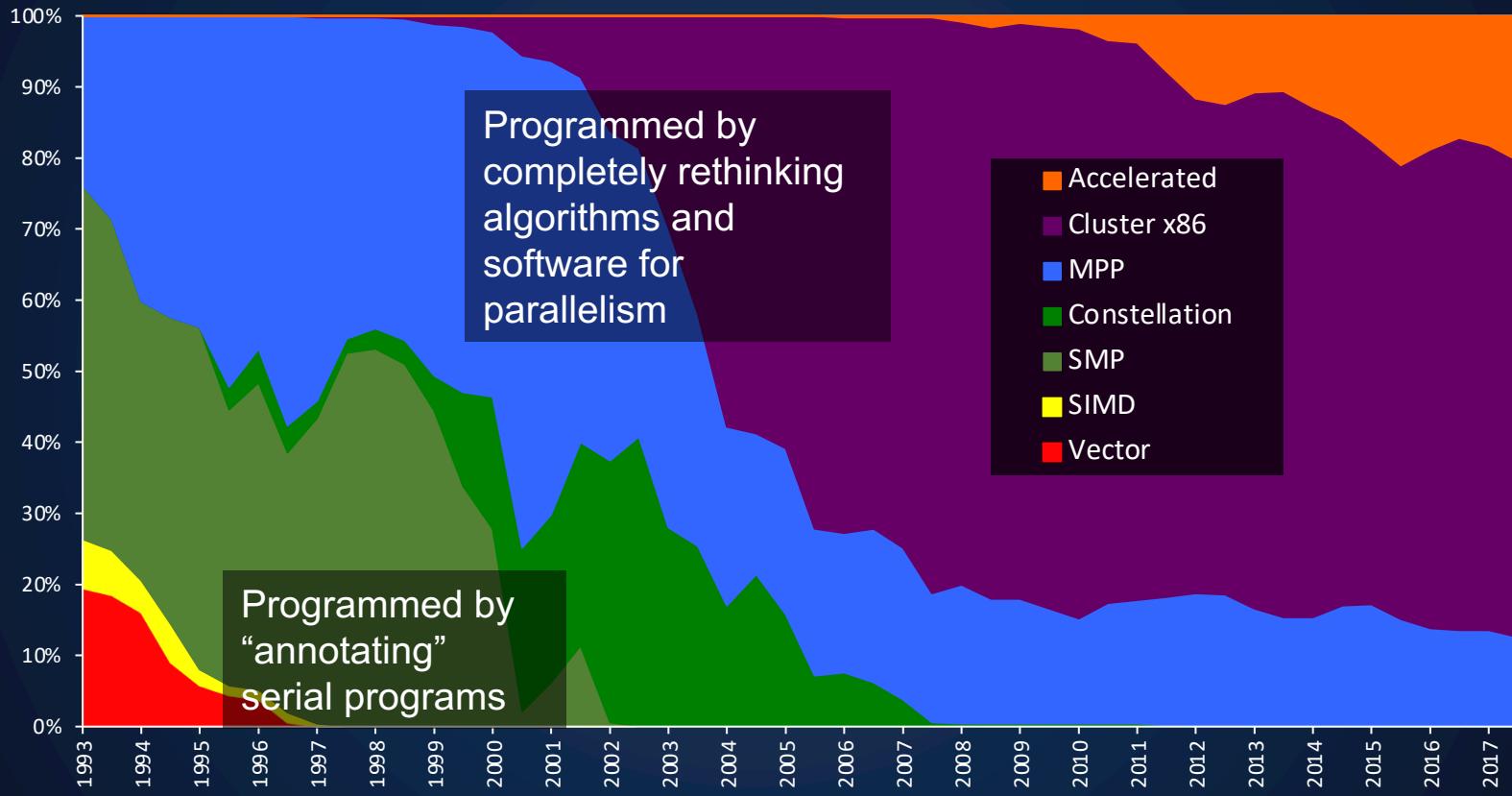


Other Algorithms / Arithmetic

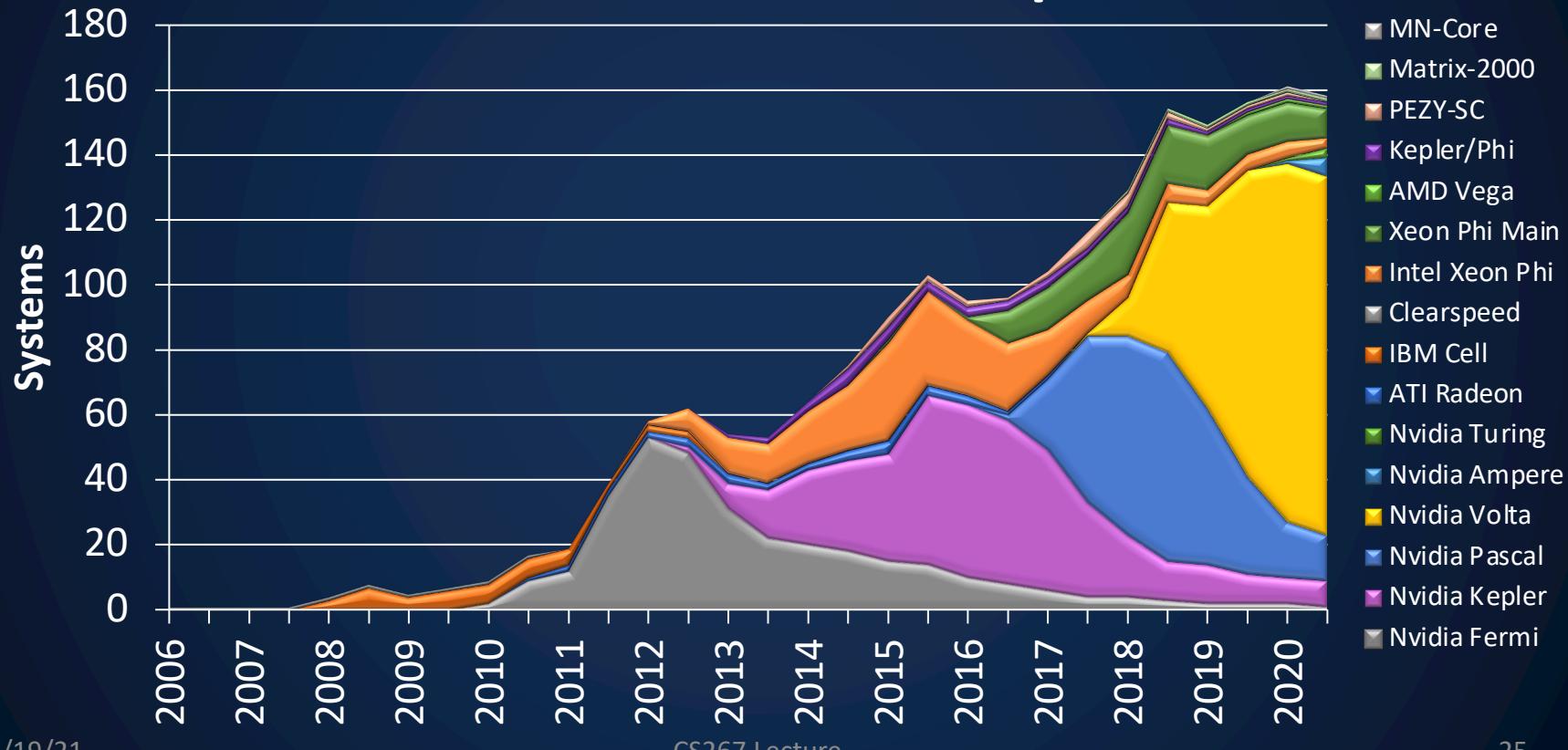


- Mixed precision iterative refinement approach solved a matrix of order 16,957,440 on Fugaku.
 - Composed of nodes made up of Fujitsu's ARM A64fx Processor
 - The run used 158,976 nodes of Fugaku, 7,630,848 cores
 - Used a random matrix with large diagonal elements to insure convergence.
- Mixed precision HPL achieved 2.004 Eflop/s
 - 4.5 X over DP precision HPL (442 PFLOPS).
 - 67 Gflops/Watt
- Same accuracy compared to full 64 bit precision

From Vector Supercomputers to Massively Parallel Accelerator Systems



Accelerators in the Top500



Average System Age

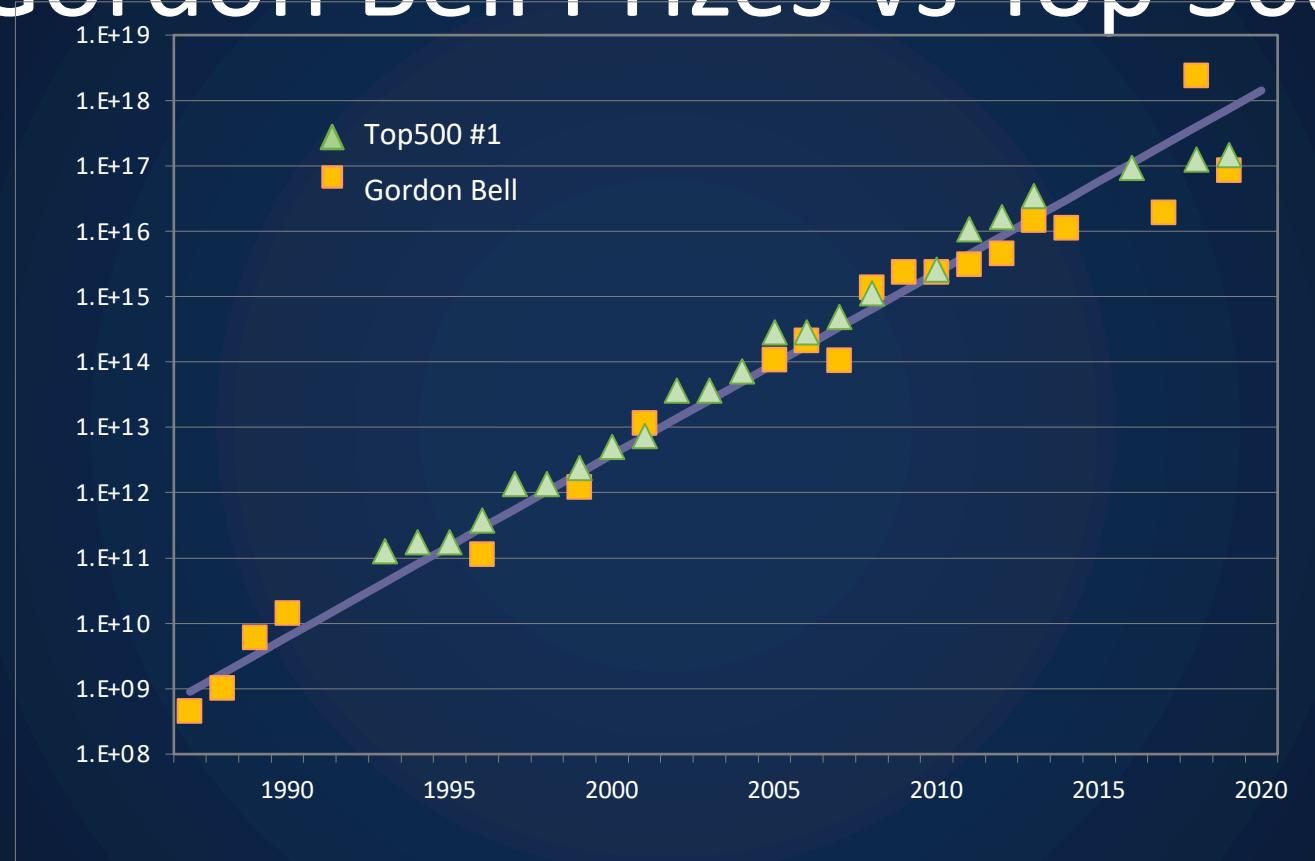


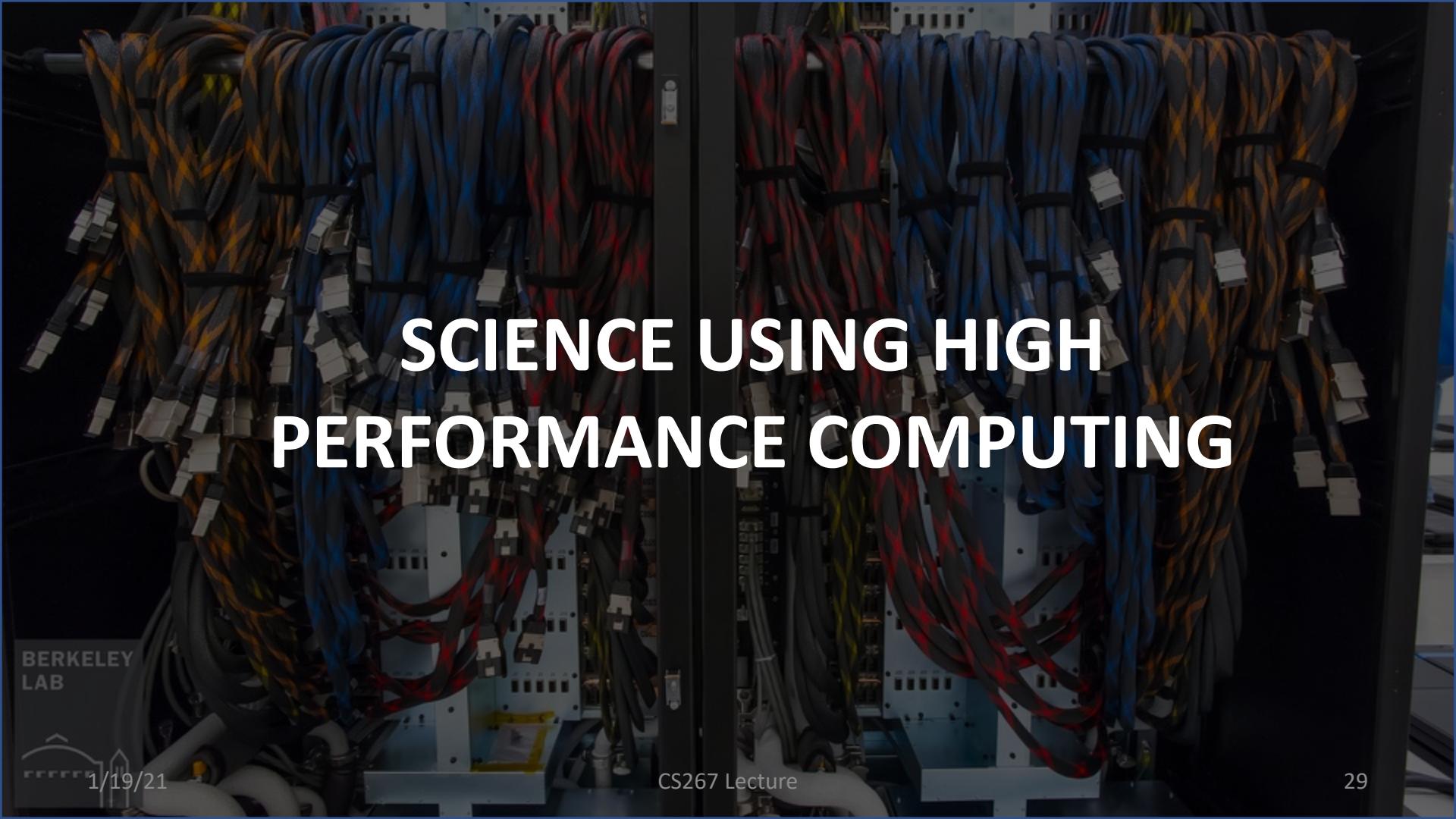
Gordon Bell Prizes: Science at Scale



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 500



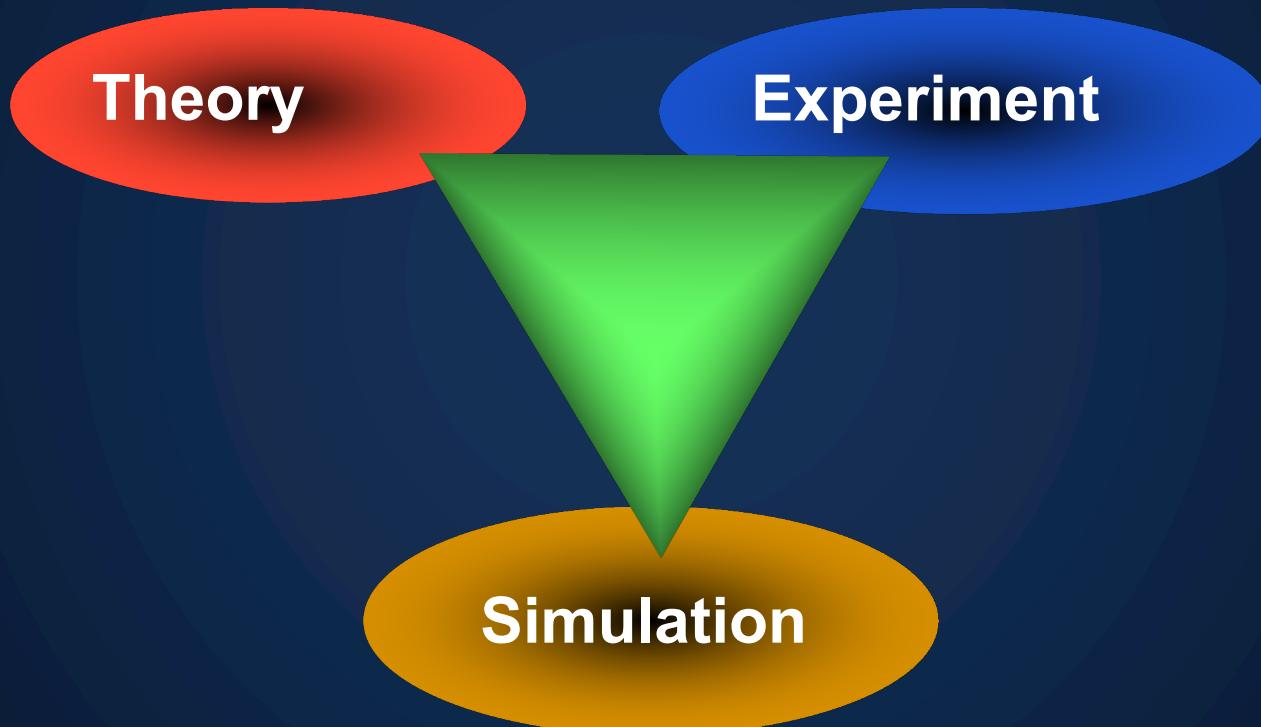


SCIENCE USING HIGH PERFORMANCE COMPUTING

BERKELEY
LAB



Simulation: The Third Pillar of Science



Simulation in Science and Engineering

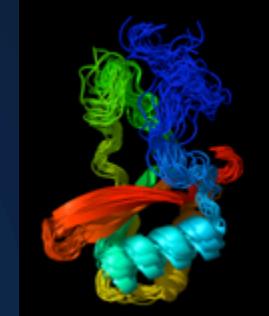
High performance simulation used to understand things that are:

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

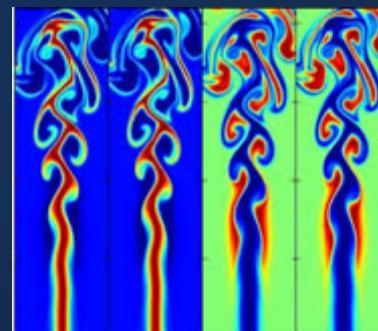
for experiments



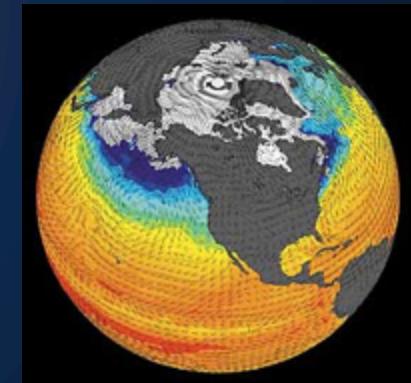
Understanding the universe



Proteins and diseases

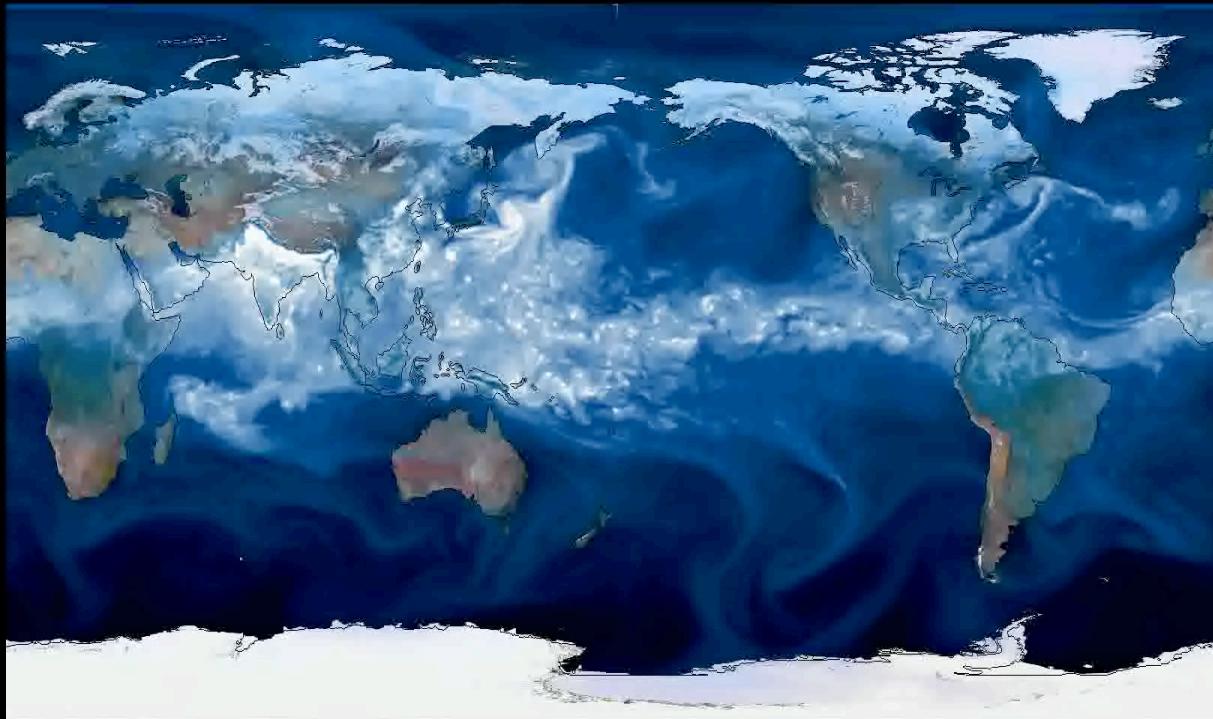


Energy-efficient jet engines



Climate change

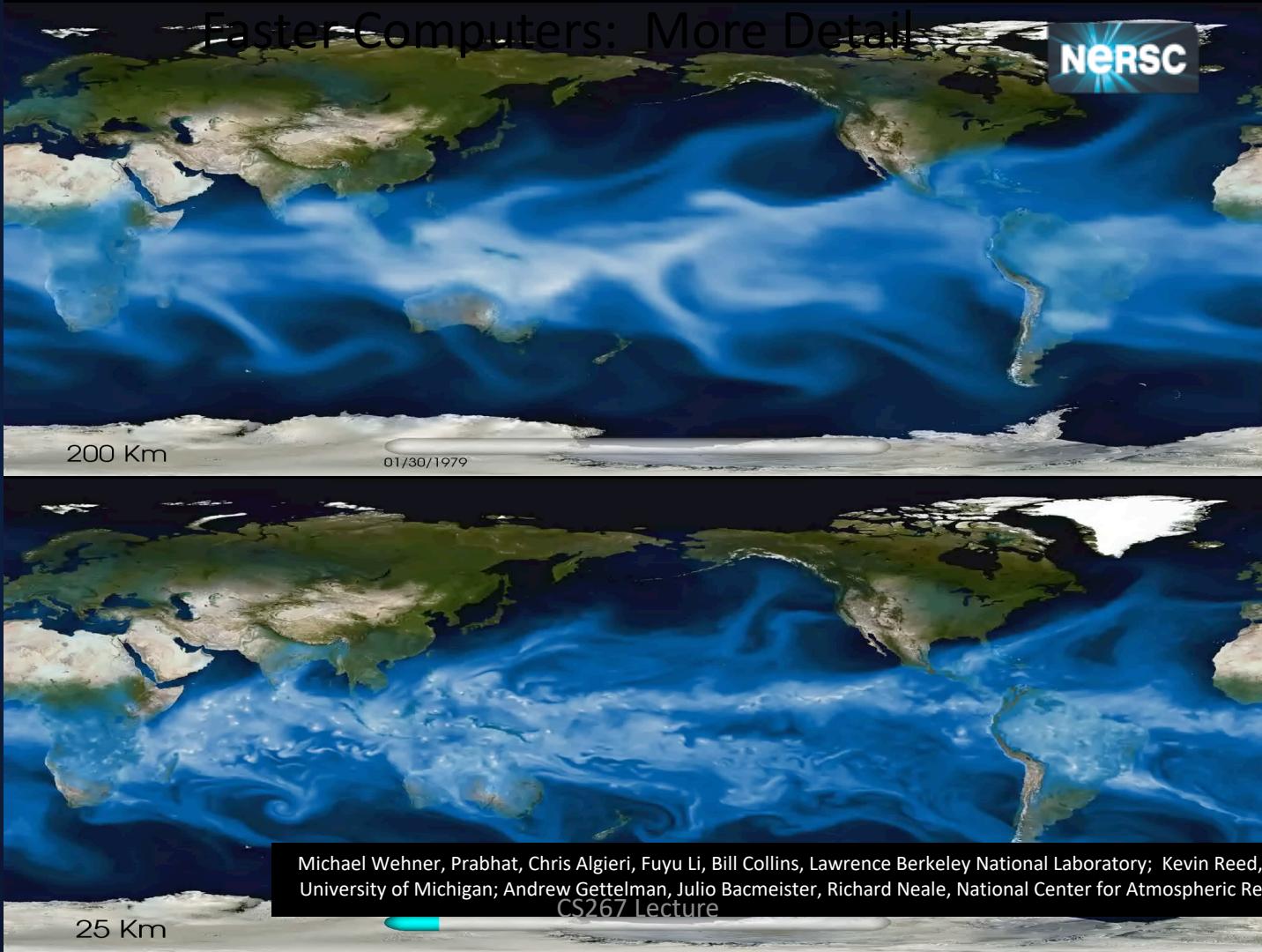
Simulations Show the Effects of Climate Change in Hurricanes



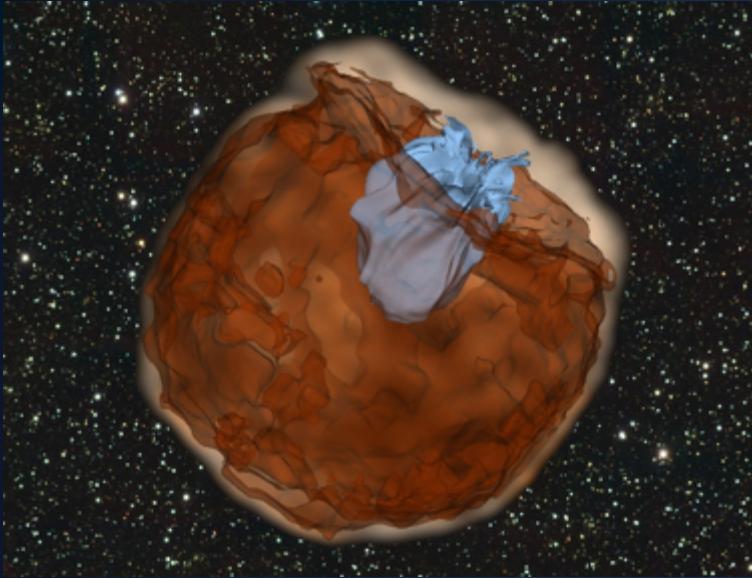
Michael Wehner and Prabhat, Berkeley Lab

Faster Computers: More Detail

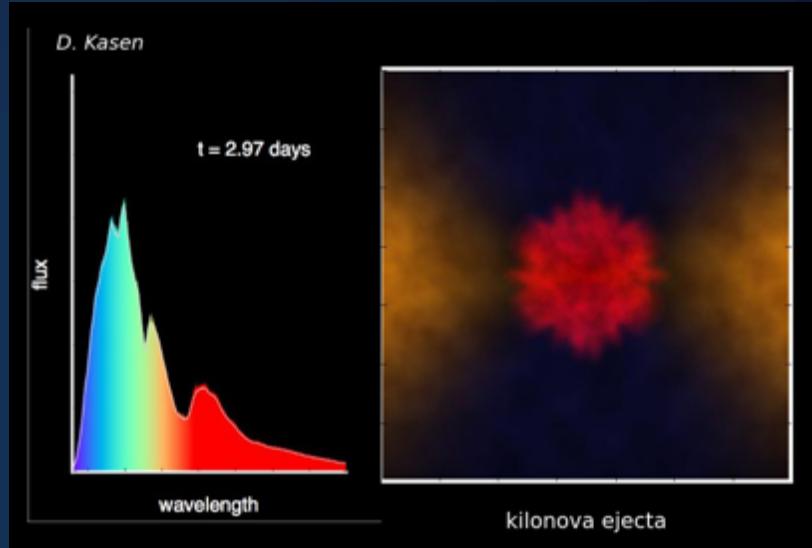
NERSC



HPC for Astrophysics



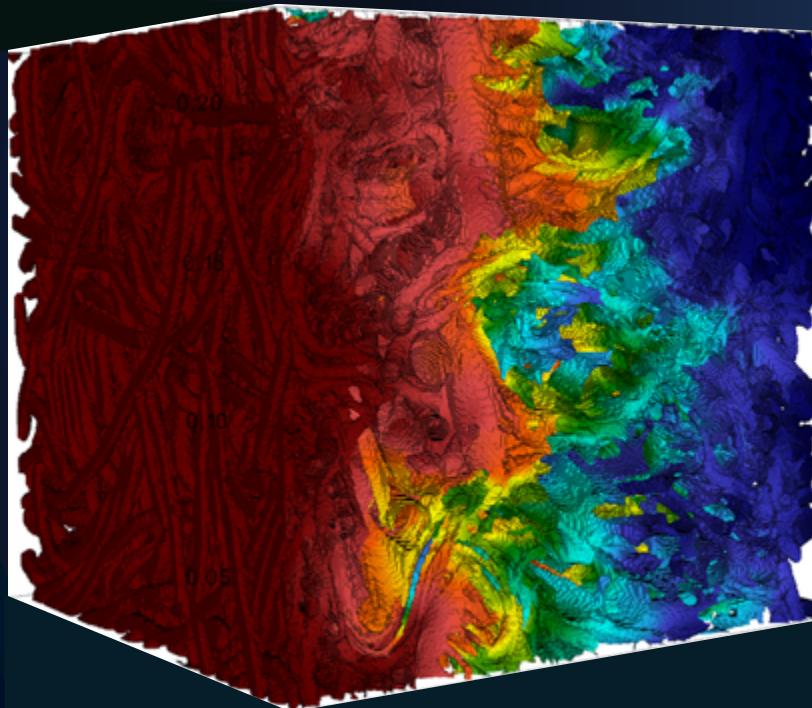
Expanding debris from a supernova explosion (red) running over and shredding a nearby star (blue)



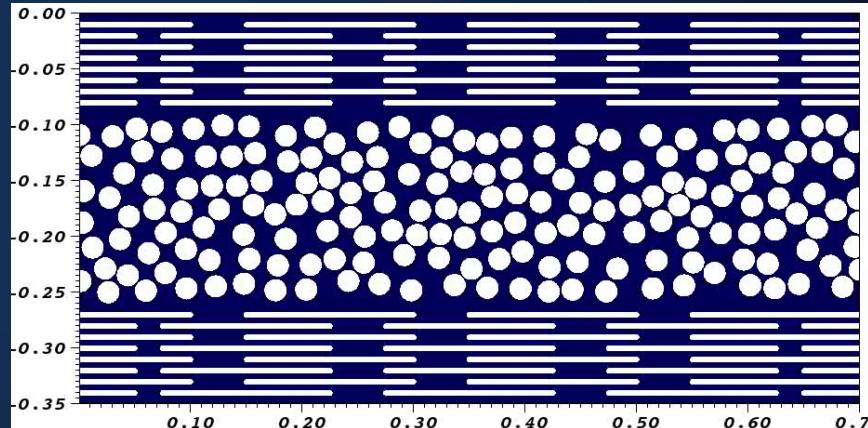
Ligo and Virgo observations match earlier simulations of gravitational waves from neutron star merger. Simulations predict ~200 earth masses of gold; ~500 of platinum

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

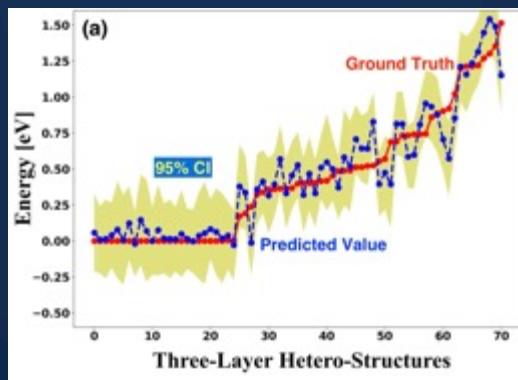
High Throughput HPC for Materials Design

Design of Materials for Batteries, Solar Panels and More



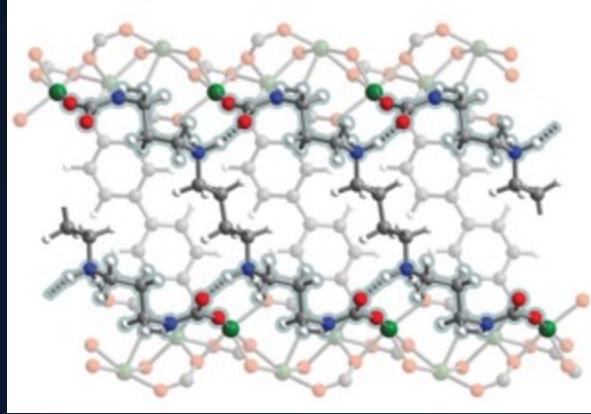
NANOPOROUS MATERIALS	530,243
INORGANIC COMPOUNDS	131,613
BAND STRUCTURES	76,194
MOLECULES	49,705

Data



- Use of Bayesian optimization for layered materials
- [Bassman et al, npj Computational Materials 2018]

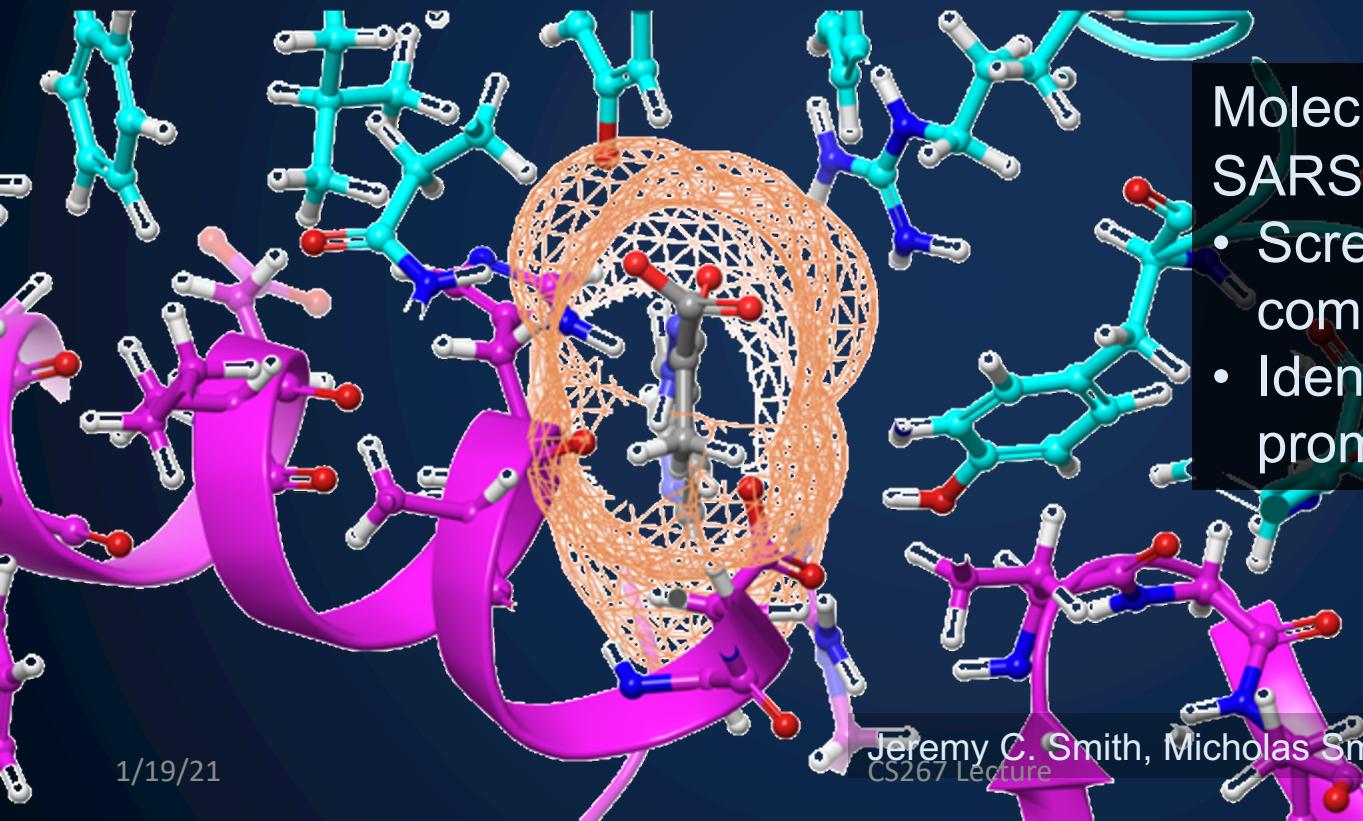
HPC for Carbon Capture



Metal Organic Frameworks (MOFs) to capture carbon in natural gas plants.

- ▶ Removes >90% of CO₂ from flue, 6X more than current (amine) technology.
- ▶ Steam to regenerate the MOF to reuse
- ▶ Exploring MOF design space with Density Functional Theory (DFT)

Screening known drugs for COVID-19



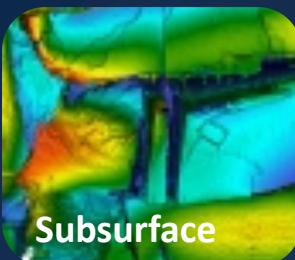
Molecular docking to
SARS-CoV-2 spike protein

- Screened 8,000 compounds
- Identified 77 of the most promising

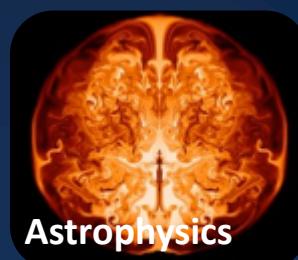
“Exascale” Applications at Berkeley Lab (LBNL)



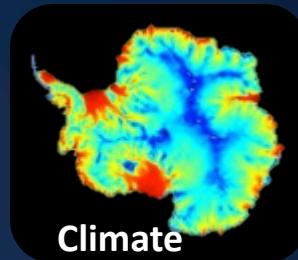
Accelerators



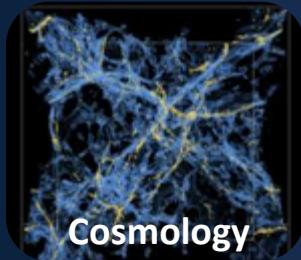
Subsurface



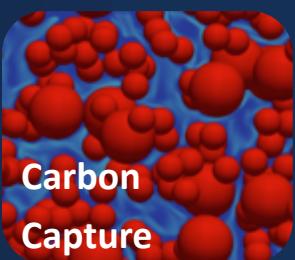
Astrophysics



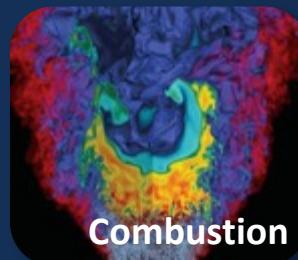
Climate



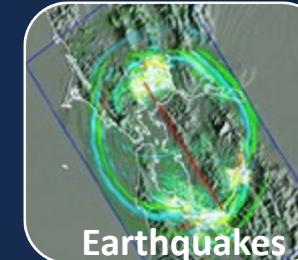
Cosmology



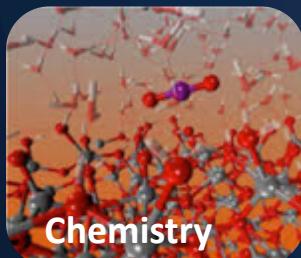
Carbon
Capture



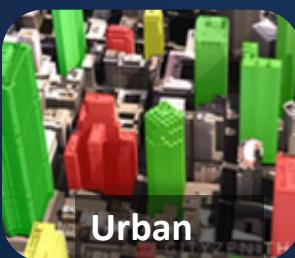
Combustion



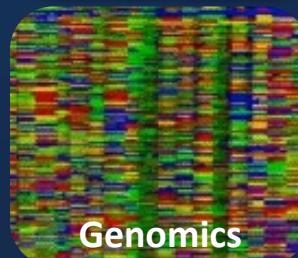
Earthquakes



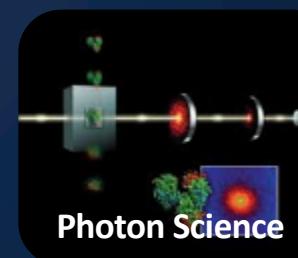
Chemistry



Urban

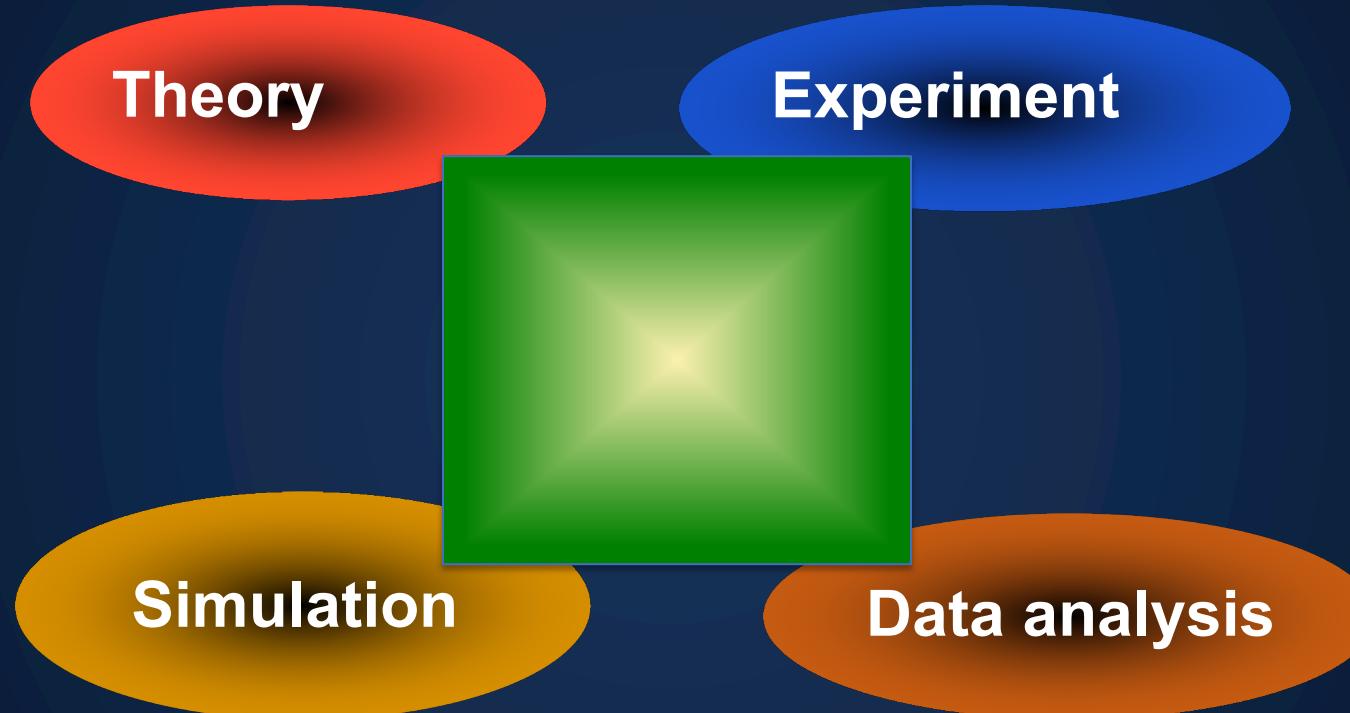


Genomics



Photon Science

The Fourth Paradigm of Science



Data analytics in science and engineering

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

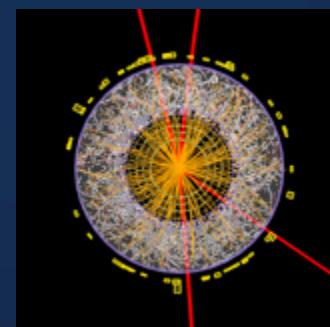
- too big
- too complex
- too fast (streaming)
- too noisy
- too heterogeneous for measurement alone



Images from telescopes



Genomes from sequencers

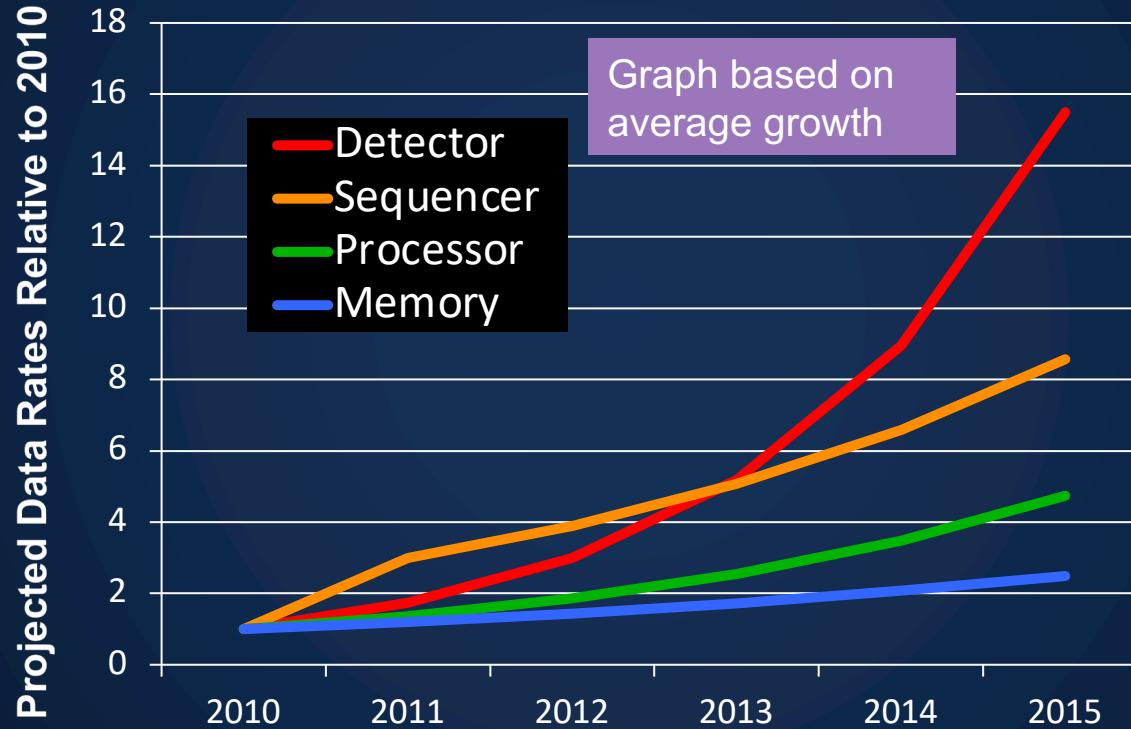


Particle from detectors



Sensor data

Data Growth is Outpacing Computing Growth



Graph based on
average growth

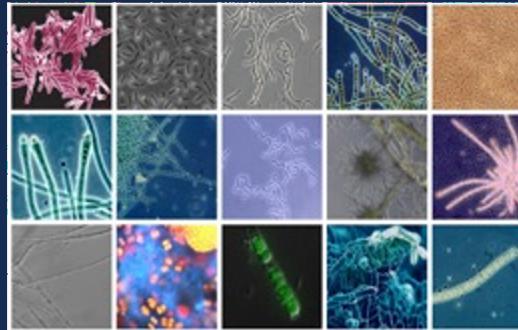
High Performance Data Analytics (HPDA) for Genomics



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



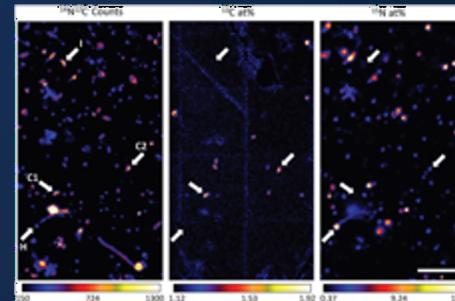
What are the seasonal fluctuations in a
wetland mangrove? (1.6 TB)



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

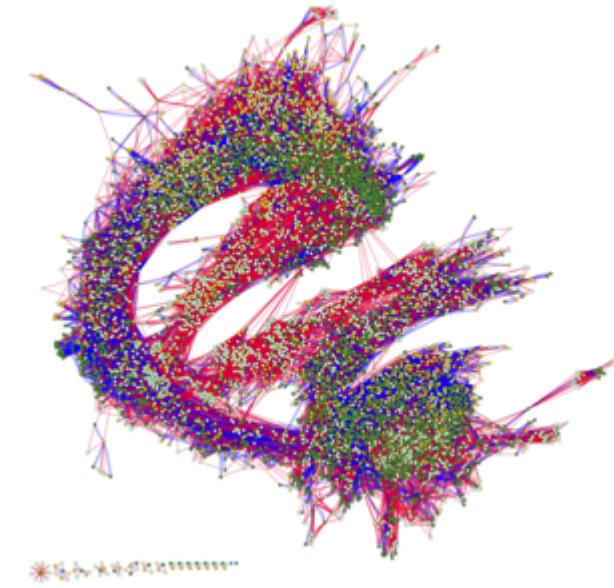


How do microbes affect disease and growth of
switchgrass for biofuels (4TB)



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

Analysis of Genomic Data



Dark green nodes: Kalanchoë genes

Yellow nodes: pineapple genes

Light green: model plant that uses a different photosynthesis strategy.

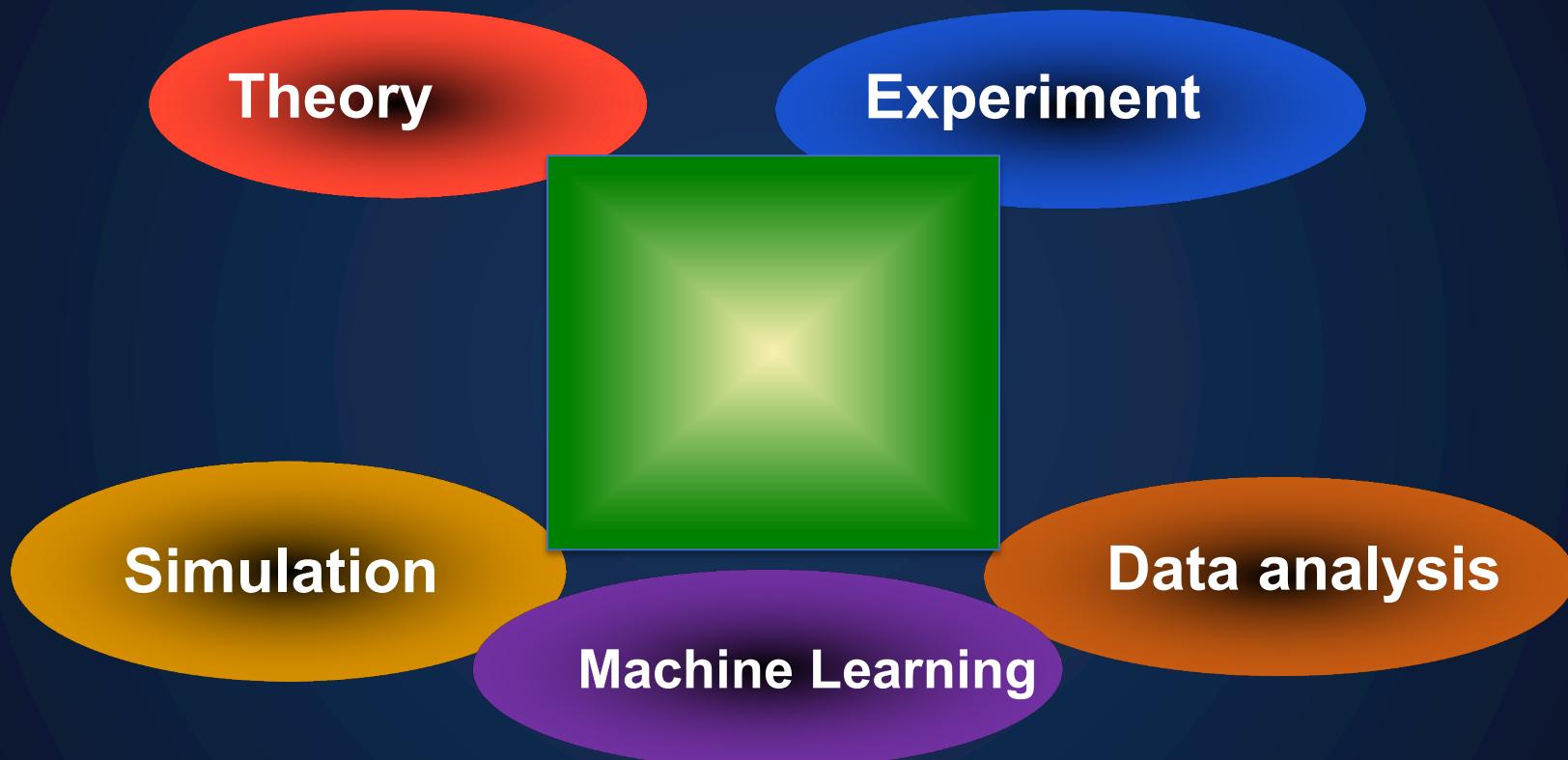
Blue edges: positive correlations

Red edges show negative correlations a

- Correlations of gene expression in plants that use different photosynthesis strategies.
- Kalanchoë and pineapple both use water-sparing photosynthesis
- 2.36 exaops / second on Summit computer
 - exaop = 10^{18} 16-bit ops
 - Gordon Bell Prize at SC18

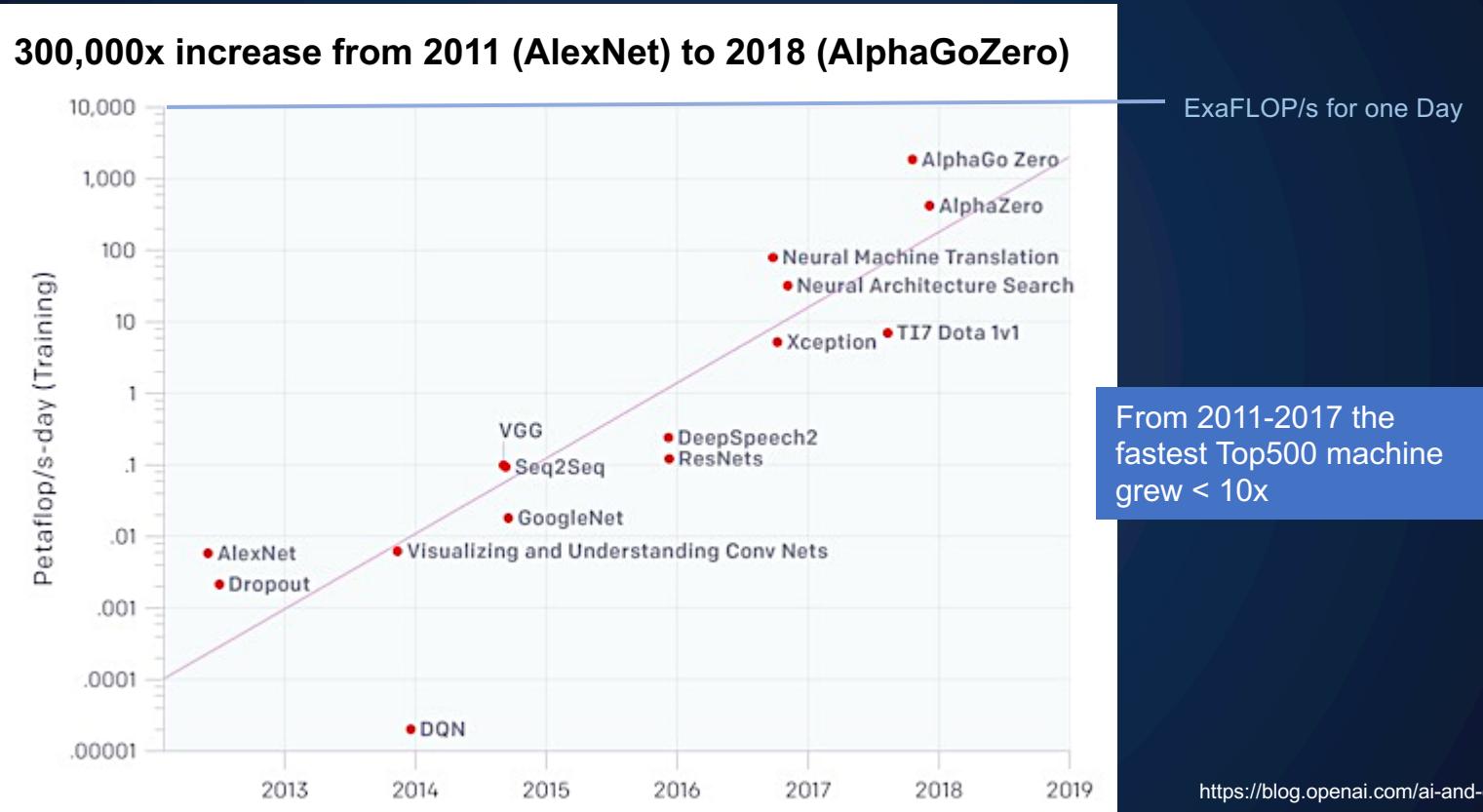
Sharlee Climer, Kjiersten Fagnan, Daniel Jacobson, Wayne Joubert, Amy Justice, David Kainer, Deborah Weighill

The Fifth Paradigm of Science ?



Machine learning demands more computing

300,000x increase from 2011 (AlexNet) to 2018 (AlphaGoZero)



Data Analytics via Supervised Learning

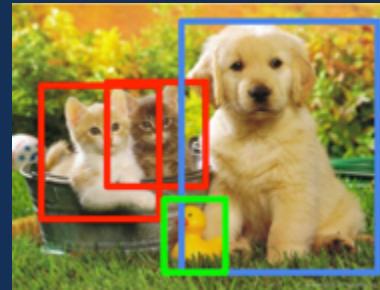
Classification



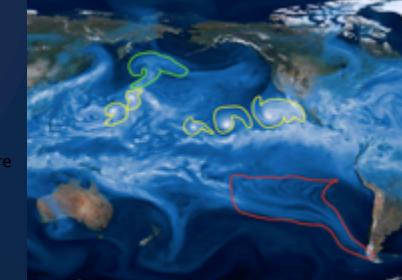
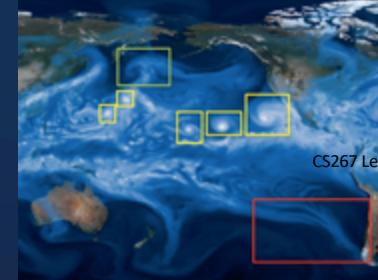
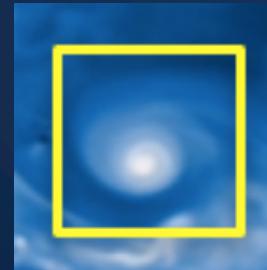
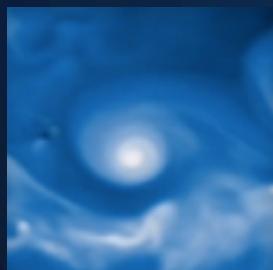
Classification
+ Localization



Object Detection



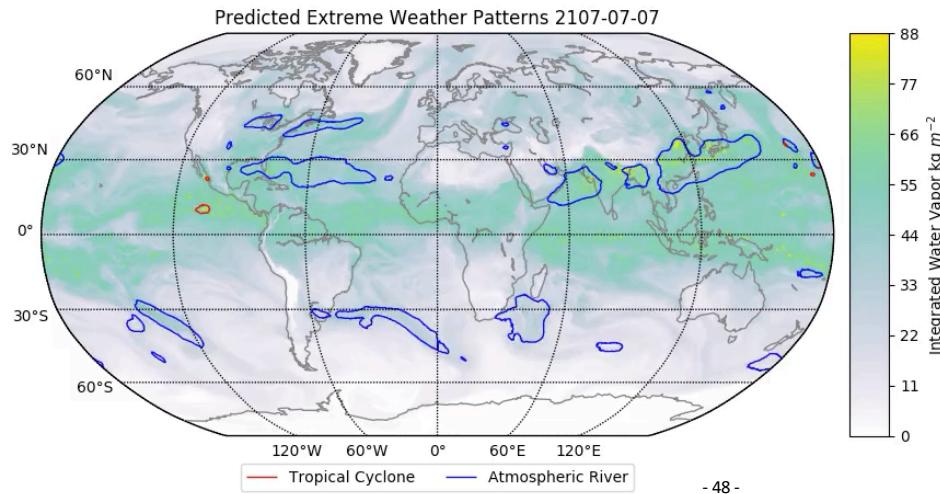
Instance
Segmentation



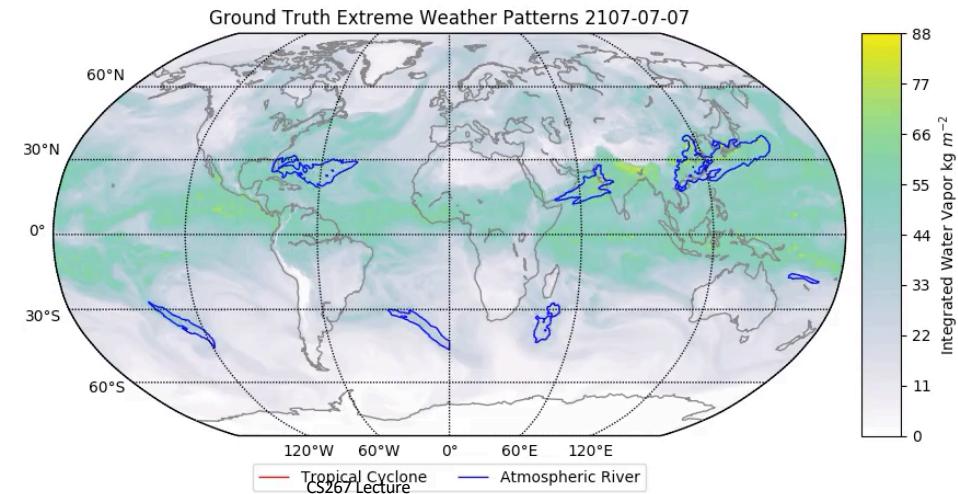
Extending image-based methods to complex, 3D, scientific data sets is non-trivial!

Big Data, Big Model, and Big Iron

Predicted Extreme Weather

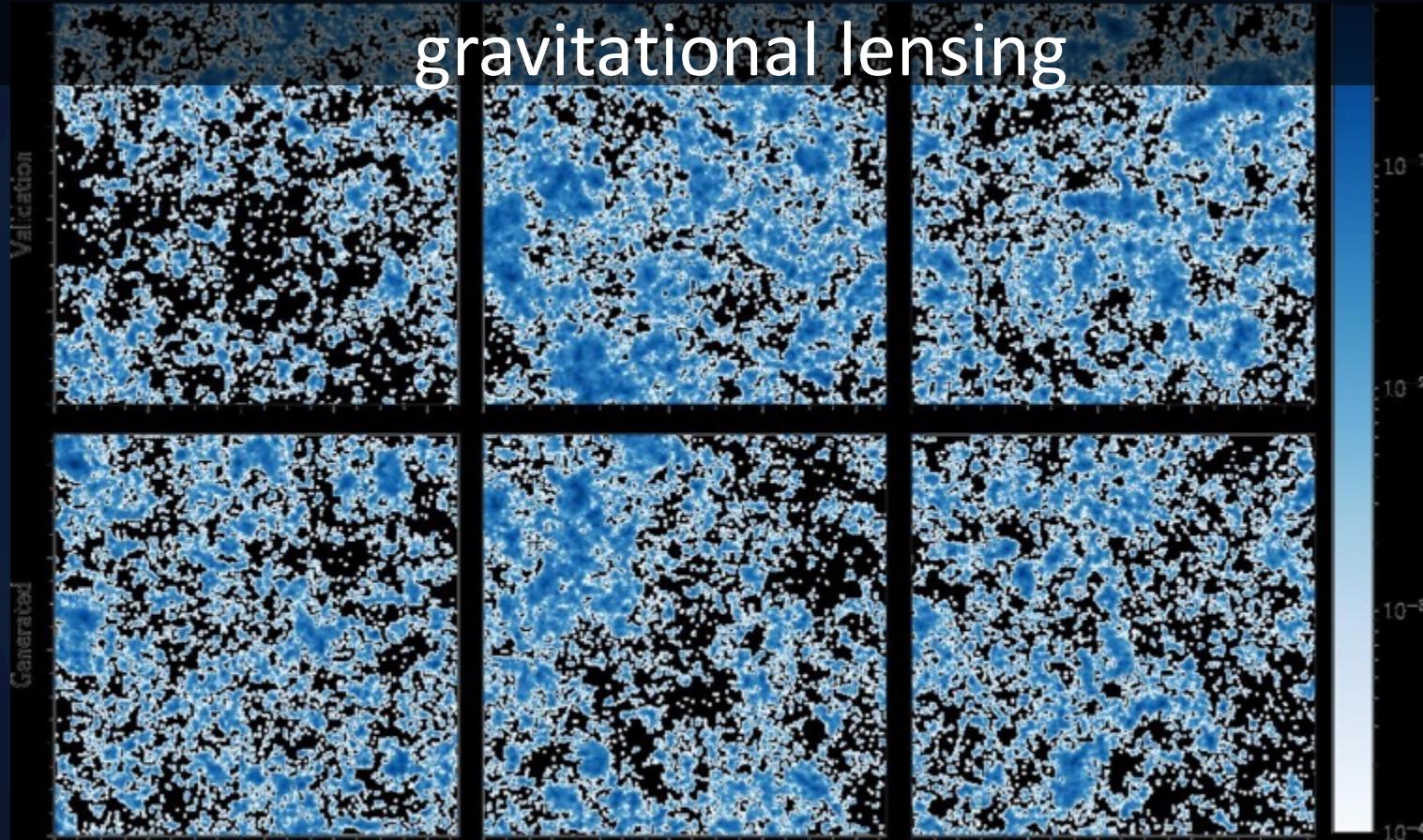


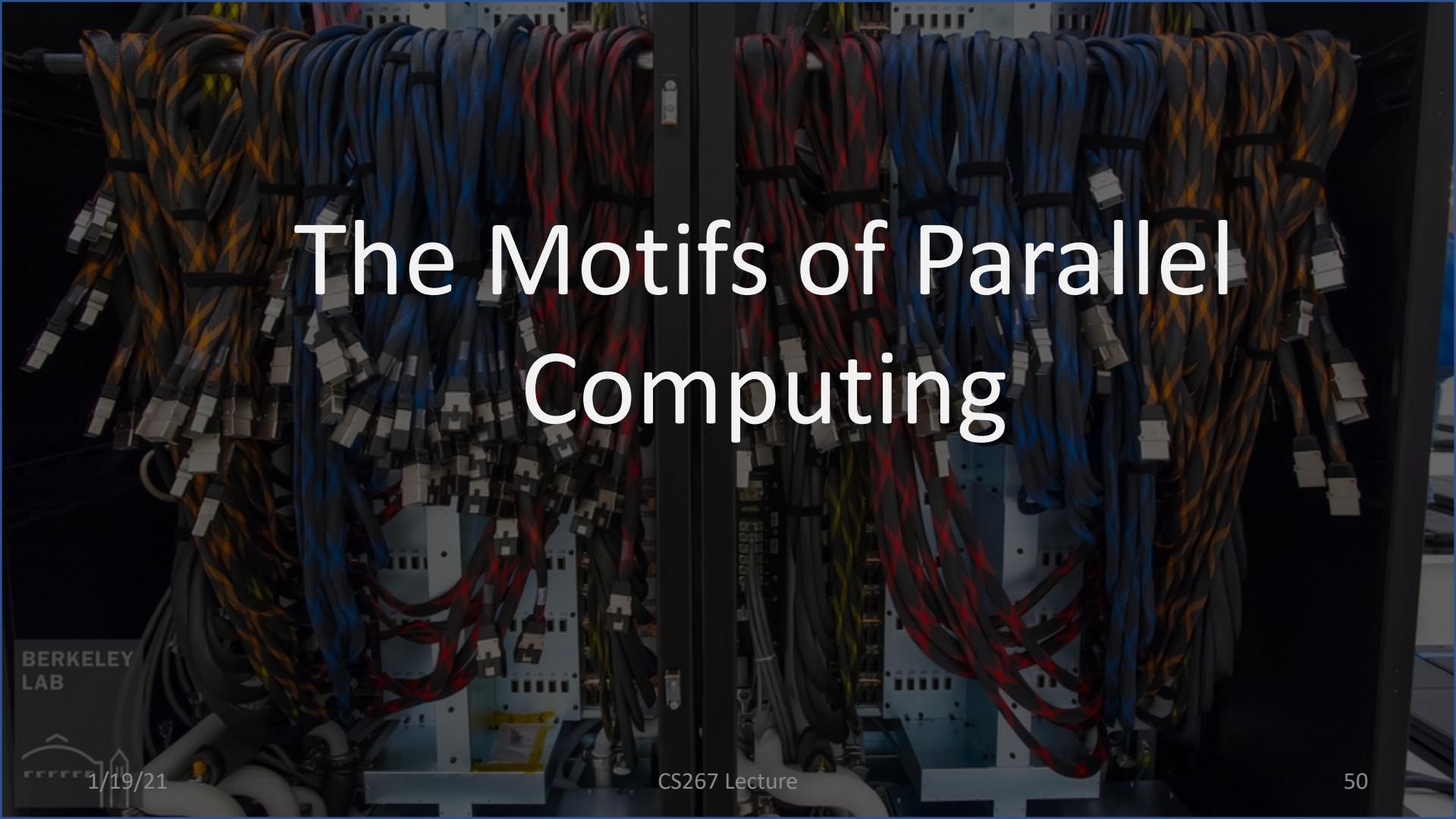
Ground Truth Extreme Weather



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

GANs to build convergence maps of weak gravitational lensing





The Motifs of Parallel Computing

BERKELEY
LAB



1/19/21

CS267 Lecture

50

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

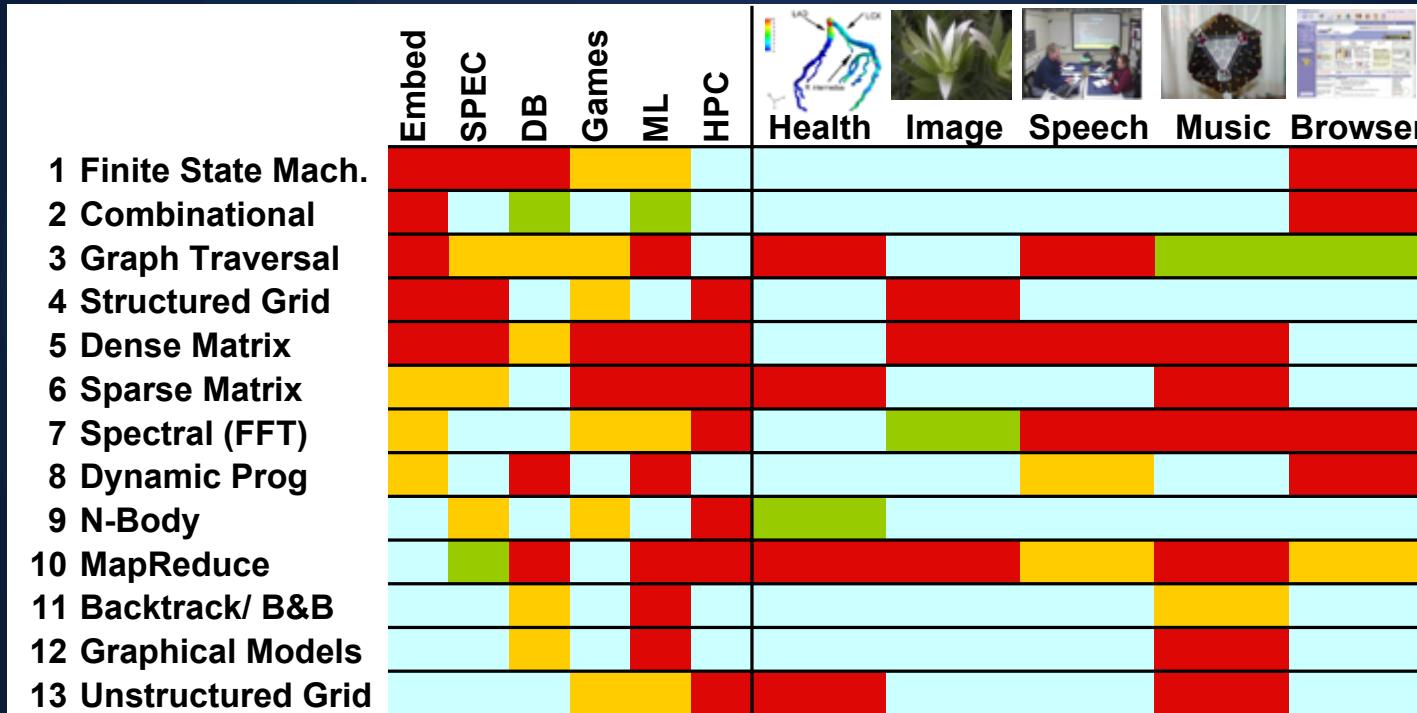


Colella's 2004 DARPA presentation "Defining Software Requirements for **Scientific** Computing"

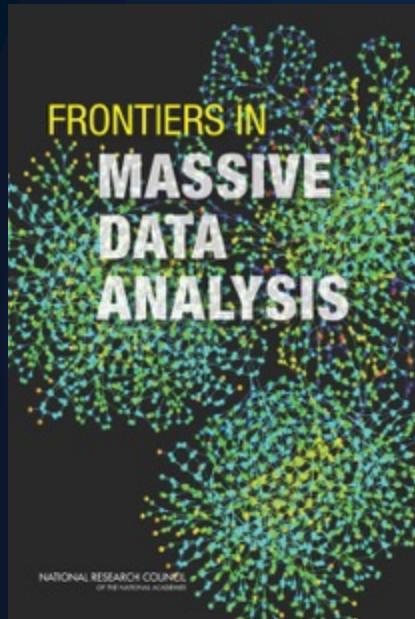
Motifs: Common Computational Methods

(Red Hot Important → Blue Cool Not Important)

What do commercial and CSE applications have in common?



Analytics vs. Simulation Motifs

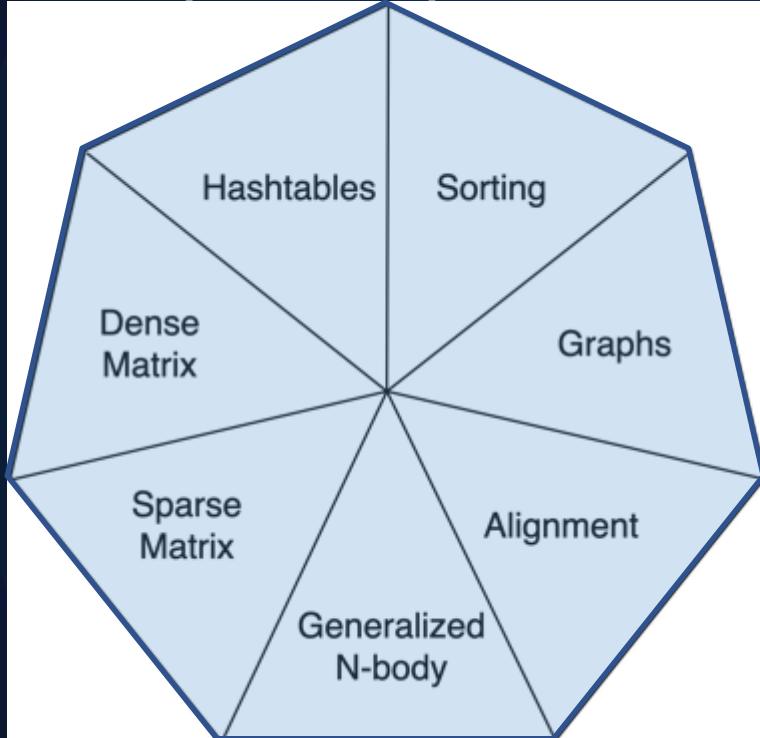


National Academies
2013

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



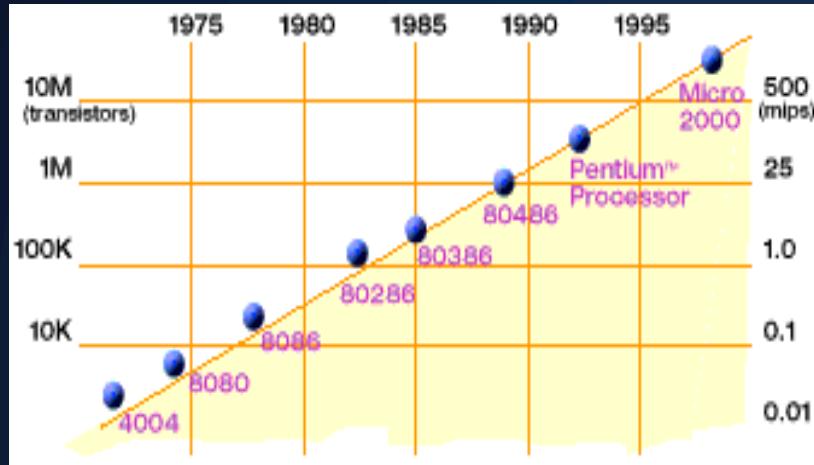
all

(since 2005)

Why ~~the~~ Fastest Computers are Parallel Computers

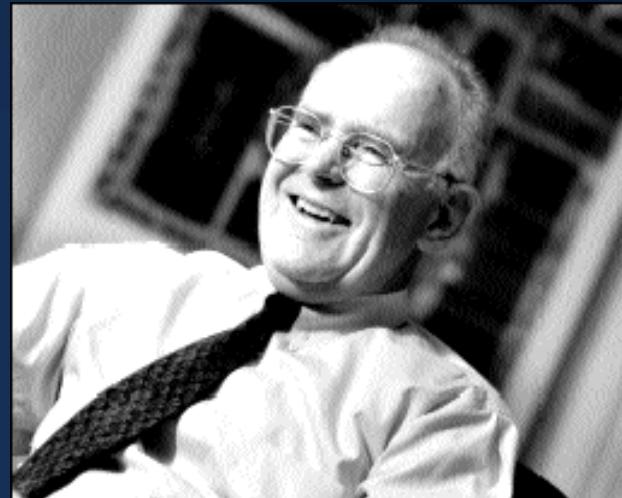
Including laptops and
handhelds

Technology Trends: Microprocessor Capacity



2X transistors/Chip Every 1.5 years
Called “Moore’s Law”

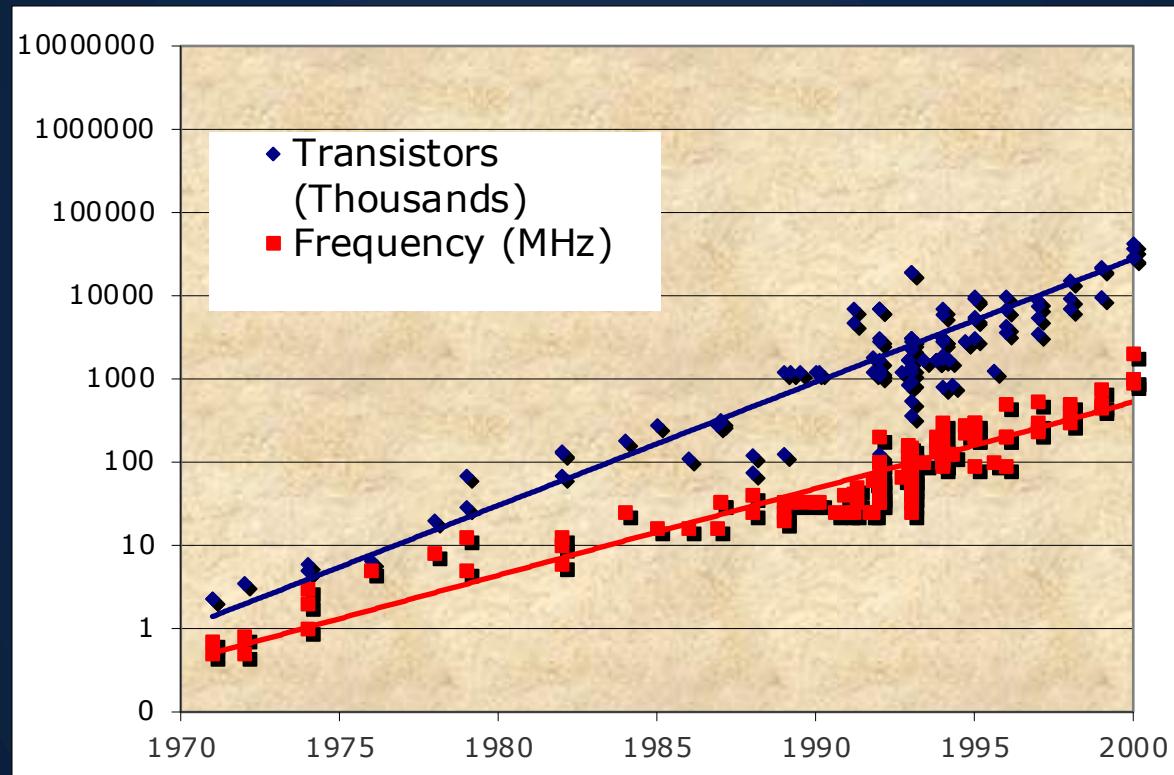
Microprocessors have become smaller, denser, and more powerful.



Gordon Moore (co-founder of Intel) predicted in 1965 that the transistor density of semiconductor chips would double roughly every 18 months.

Slide source: Jack Dongarra

Microprocessor Transistors / Clock (1970-2000)

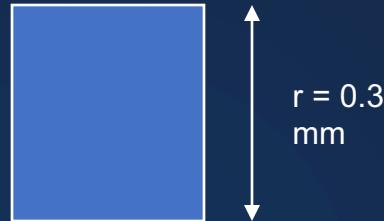


Historical Impact of Device Shrinkage

- What happens when feature size (transistor size) shrinks by a factor x ?
- Clock rate goes up by x because wires are shorter
 - actually less than x , because of power consumption
- Transistors per unit area goes up by x^2
- Die size has also increased
 - typically another factor of $\sim x$
- Raw computing power of the chip goes up by $\sim x^4$!
 - typically x^3 is devoted to either on-chip
 - parallelism: hidden parallelism such as ILP
 - locality: caches
- So some programs got x^3 times faster, without changing them

Limits: How fast can a serial computer be?

1 Tflop/s, 1
Tbyte
sequential
machine



- Consider the 1 Tflop/s (10^{12}) sequential machine:
 - Data must travel distance, r , from memory to processor.
 - To get 1 data element per cycle, this means 10^{12} times per second at the speed of light, $c = 3 \times 10^8$ m/s.
Thus $r < c/10^{12} = 0.3$ mm.
- Now put 1 Tbyte of storage in a 0.3 mm x 0.3 mm area:
 - Each bit occupies about 1 square Angstrom, or the size of a small atom.
- No choice but parallelism

But What about Heat Density

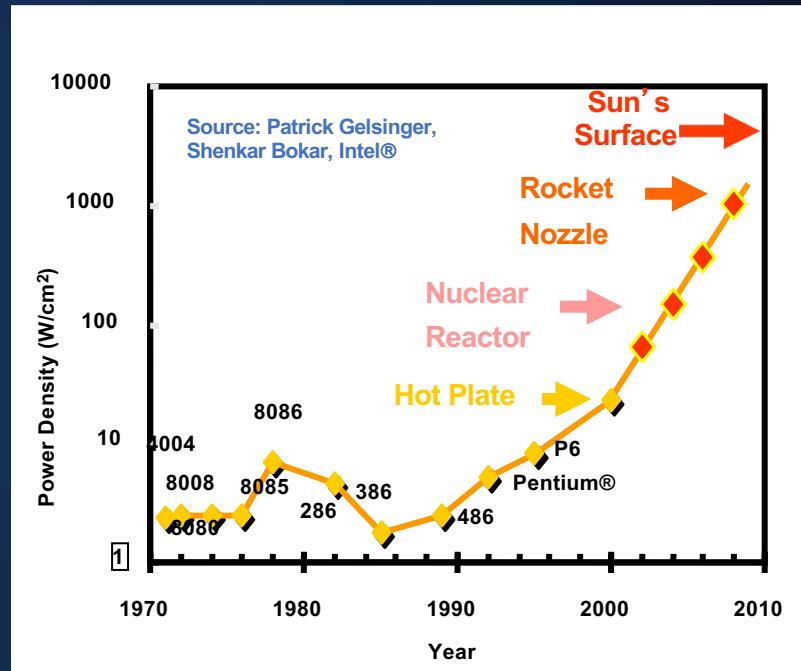


SAM SPRATT - GIZMODO

Power Density Limits Serial Performance

- *Faster processors → increase power*
 - Dynamic power is proportional to V^2fC
 - Increasing frequency (f) also increases supply voltage (V) → cubic effect
 - Increasing cores increases capacitance (C) but only linearly
 - Save power by lowering clock speed and adding parallelism
- High performance serial processors waste power
 - Speculation, dynamic dependence checking, etc. burn power
 - Implicit parallelism discovery
- More transistors, but not faster serial processors

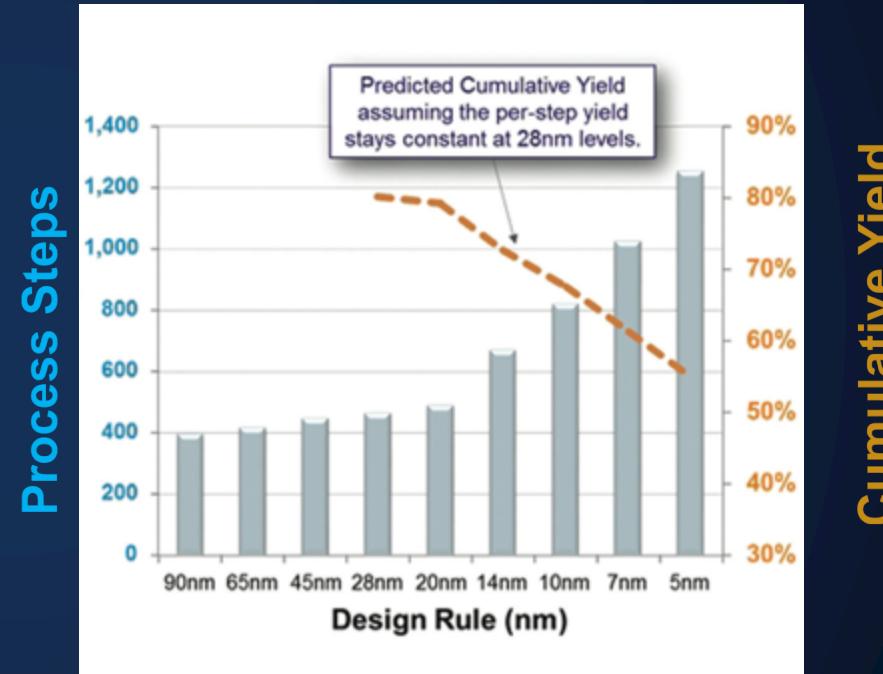
Scaling clock speed (business as usual) will not work



More drivers for parallelism: Chip yield

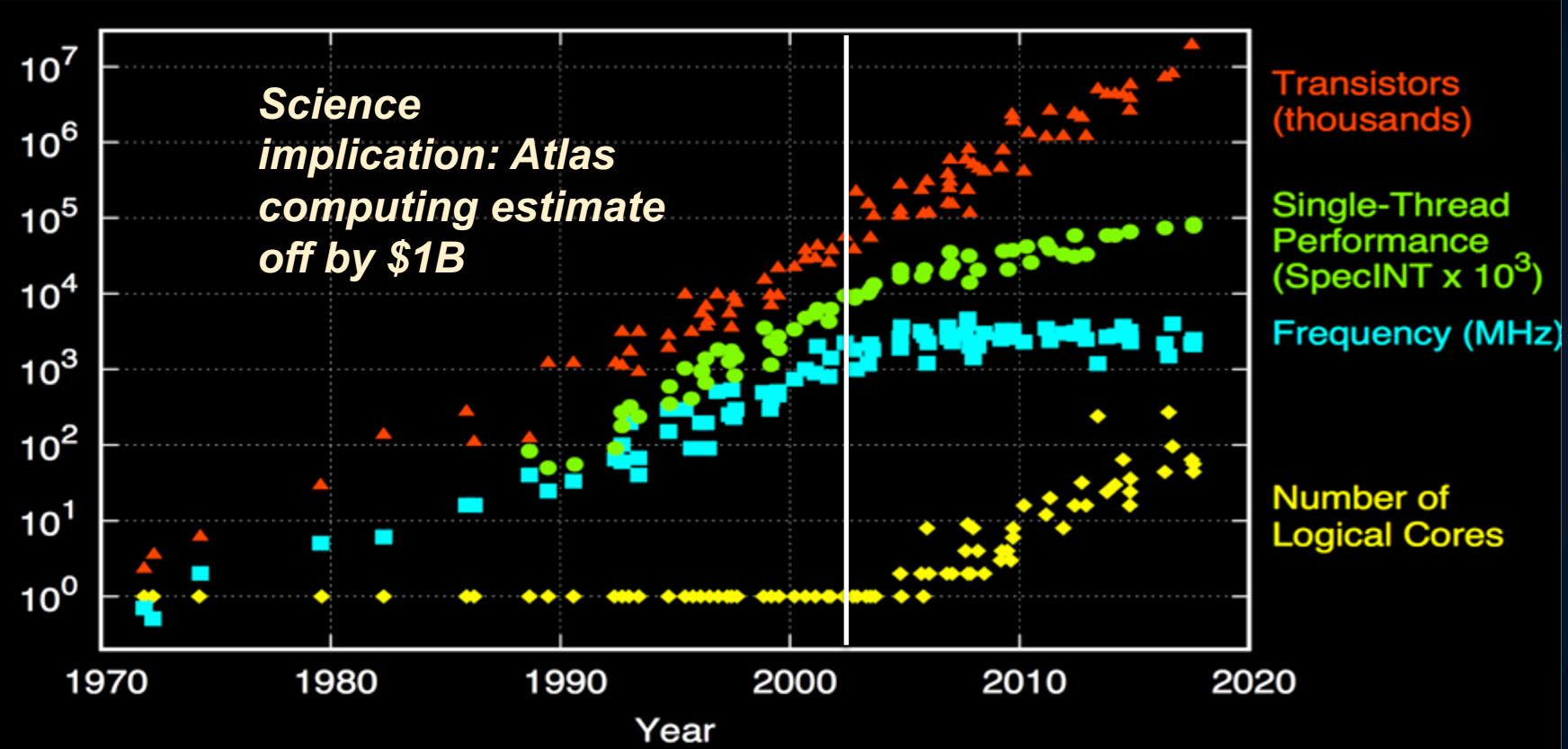
Yield

- What % of chips are usable?
- Complexity of fabrication (decreased size and number of steps) increases errors
- Parallelism helps, e.g., KNL (in Cori) sold with only 68 out of 76 “on” to improve yield



<http://electroiq.com/blog/2016/02/yield-and-cost-challenges-at-16nm-and-beyond/>

Dennard Scaling is Dead; Moore's Law Will Follow

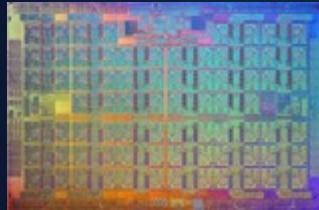


Moore's Law reinterpreted

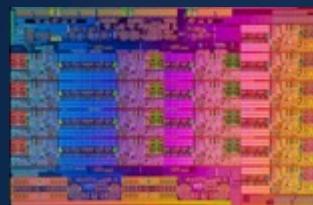
- Number of cores per chip can double every two years
- Clock speed will not increase (possibly decrease)
- Need to deal with systems with millions of concurrent threads
- Need to deal with inter-chip parallelism as well as intra-chip parallelism
- But Moore's Law is not forever... industry consortium predicts end in 2021

Parallel hardware is everywhere

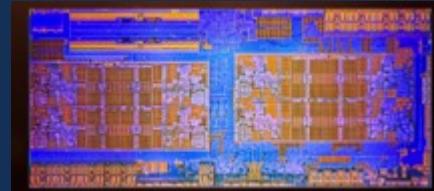
It's just about all you can find today in laptops, servers etc.



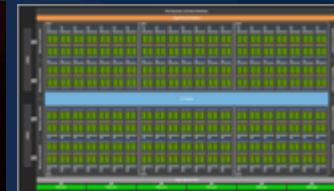
Intel® Knights
Landing (68 cores)



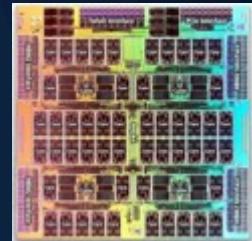
Intel® Haswell
(16 cores)



AMD Ryzden
(8 cores)

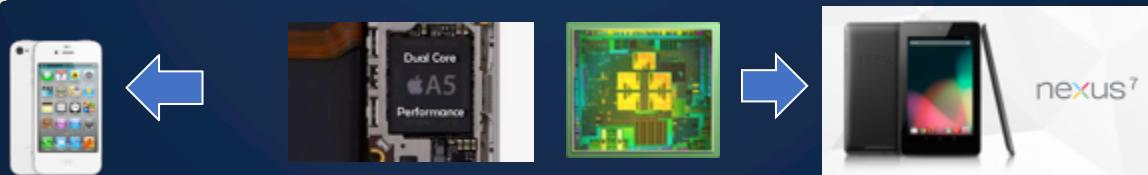


NVIDIA V100



Fujitsu ARM
(48 cores)

- Even my cell phone has a parallel processor



There's no escape!

Caution: Amdahl's Law

- Suppose only part of an application is parallel
- Amdahl's law
 - s = fraction of work done sequentially (Amdahl fraction)
 - $1-s$ is fraction parallelizable
 - P = number of processors

$$\text{Speedup}(P) = \text{Time}(1)/\text{Time}(P)$$

$$\leq 1/(s + (1-s)/P)$$

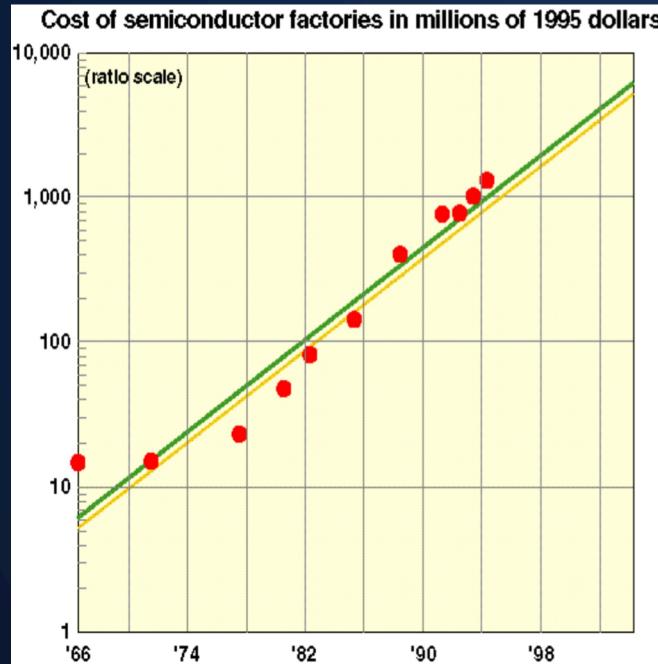
$$\leq 1/s$$

- Even if the parallel part speeds up perfectly, performance is limited by the sequential part
- E.g., $1/10^{\text{th}}$ of your code's runtime is serial \rightarrow max speedup is 10x (Cori has 65K cores)

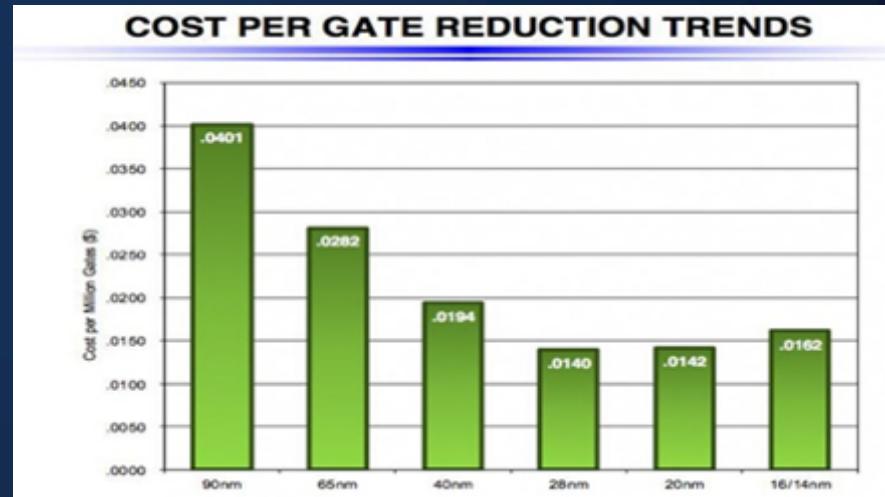
Moore's Law is Techno-Economic *approaching atomic scale, but economics is first*

Cost of fabrication facilities:

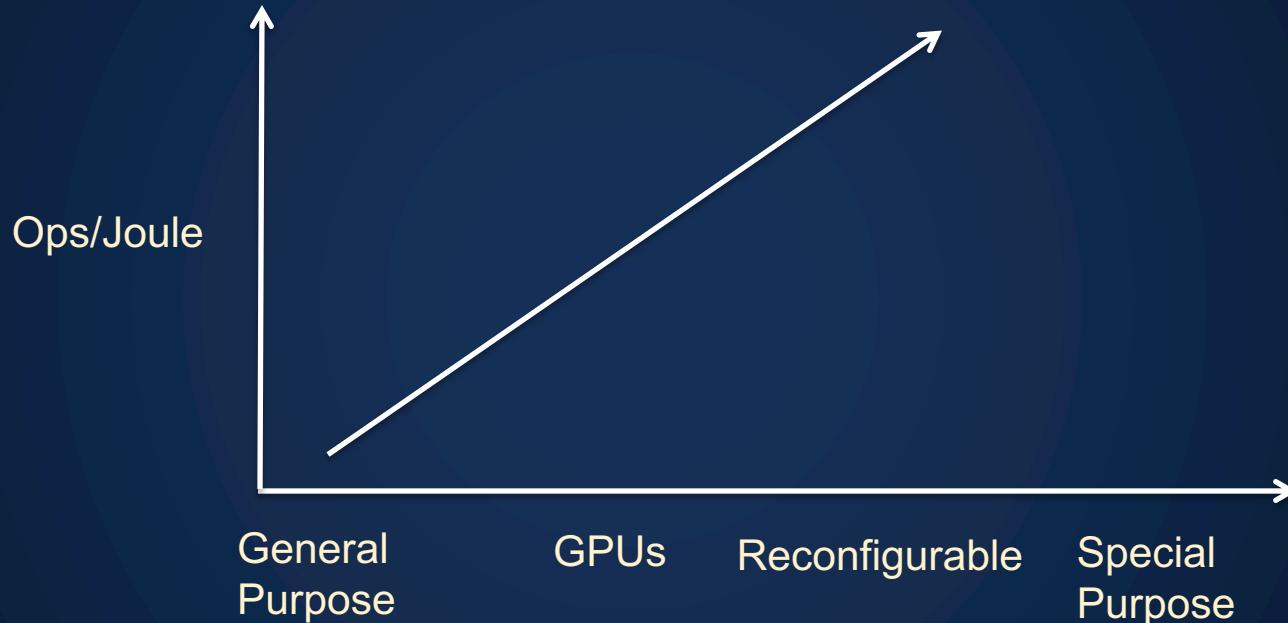
**Moore's 2nd law (Rock's law):
costs double every 4 years**



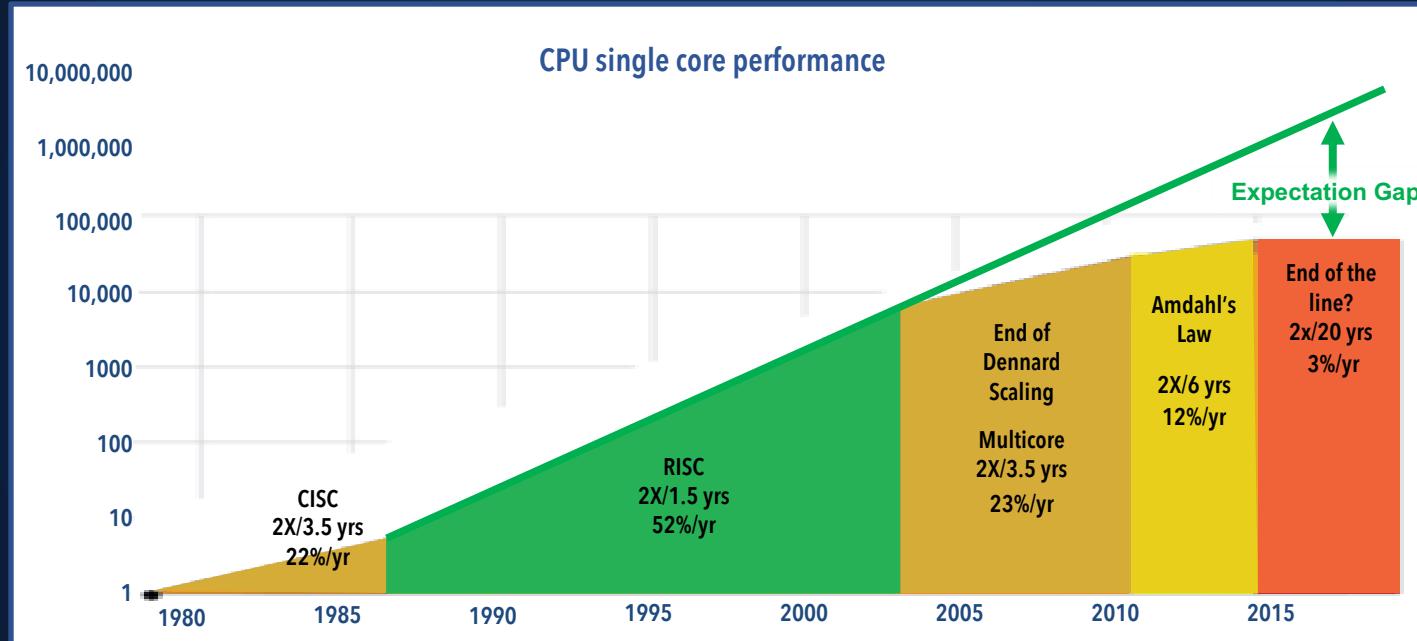
**Cost per gate not improving:
lithography and fab costs**



Specialization: End Game for Moore's Law



Traditional Scaling is Coming to an End!



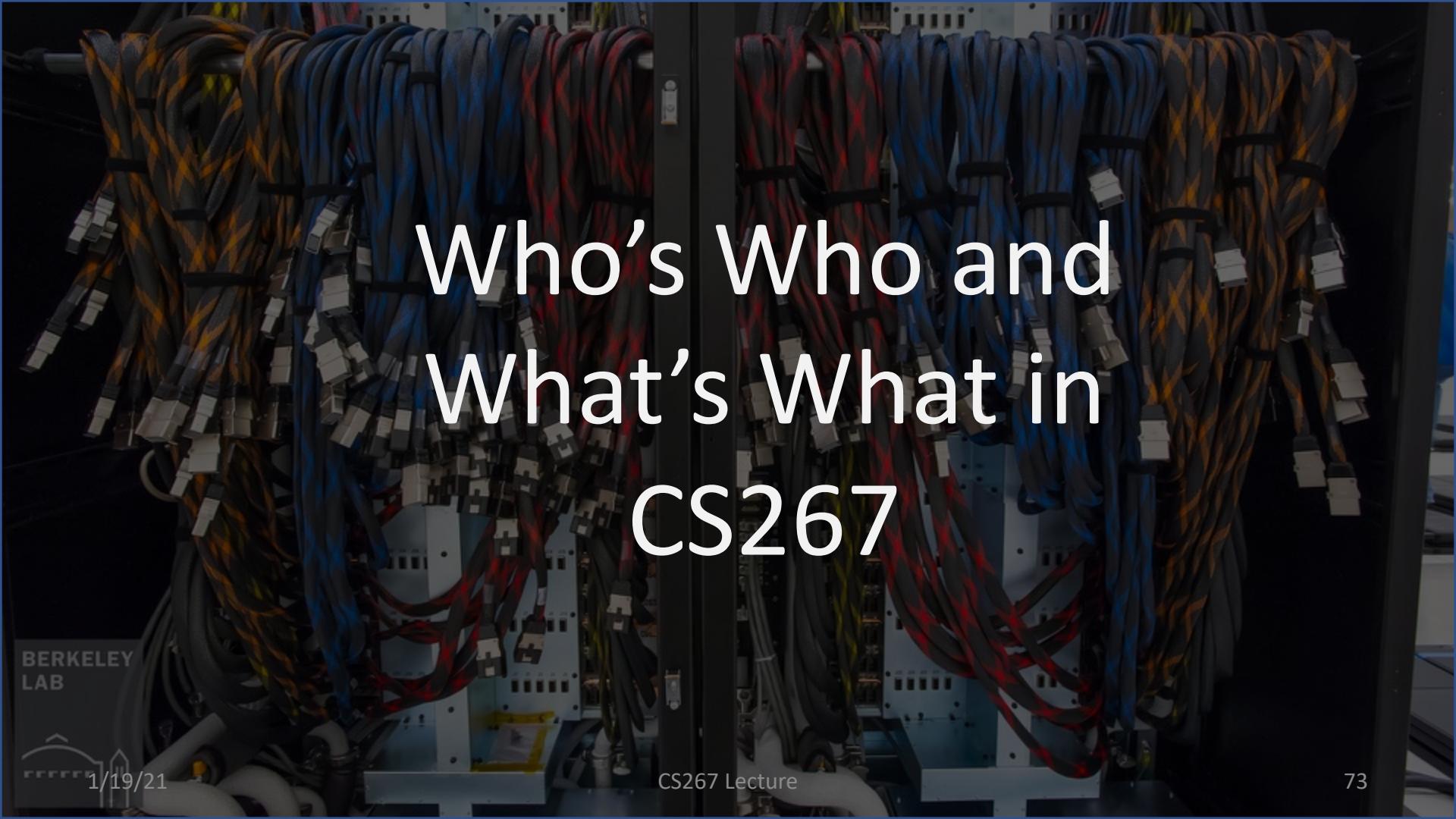
Hennessy/Patterson Turing Award presentation: Golden Age of Computer Architecture Research



Moore's Law

It's hard to think exponentially

But it's also hard to stop



Who's Who and What's What in CS267

BERKELEY
LAB



Course Staff

Instructors



Kathy Yelick



Aydın Buluç



Jim Demmel

GIs



Giulia Guidi



Melih Elibol

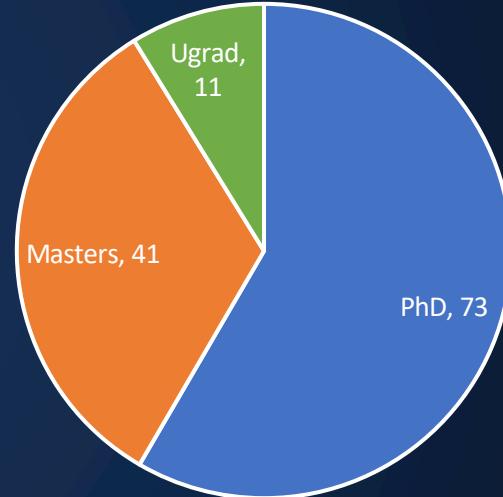
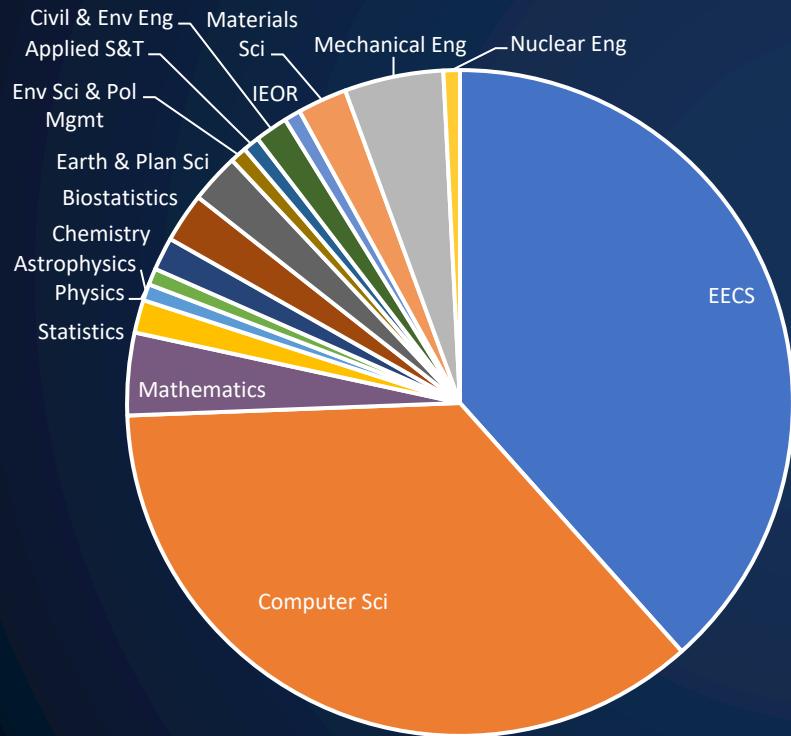


Alok Tripathy

See website for contact information and office hours. Email us at cs267@lists.eecs.berkeley.edu

CS267 Lecture

125 Students Enrolled as of 1/18



Additional ~20 undergrads awaiting enrollment codes

Universities that have offered this class

NSF XSEDE Program

- University of Kentucky
- Indiana University Southeast
- Penn State University
- New Mexico State University
- George Mason University
- Oregon State University
- Bluffton University
- Gonzaga University
- Norfolk State University
- University of Toronto
- Texas A&M University San Antonio
- Washington State University
- East Carolina University
- Morehouse College Saint Martin's University in Washington
- University of Arizona
- Adrian College in Michigan
- Clarkson University in New York
- University of Rhode Island
- University of Arkansas
- University of Cincinnati in Ohio
- University of Nevada, Las Vegas
- Fordham University in New York
- Wofford College in South Carolina
- Morgan State University in Maryland
- New Jersey Institute of Technology
- Brown University in Rhode Island
- University of Pennsylvania
- University of Toronto in Canada
- Francis Marion University in South Carolina
- University of Kentucky
- Louisiana State University
- Indiana University Southeast
- Portland State University in Oregon
- New Mexico State University
- Jarvis Christian College in Texas
- Hampden–Sydney College in Virginia
- University of Nevada, Reno
- Universidad de Puerto Rico
- Texas A&M U-Corpus Christi
- Universidad EAFIT in Columbia

Overview of the course (not in order)

- Parallel Programming Models and Machines (plus some architecture, e.g., caches)

Algorithm/machine model	Language / Library skills
Shared memory	OpenMP (pThreads)
Distributed memory	MPI
	PGAS
Data parallel	SPARK
	CUDA

- Parallelization Strategies for the “Motifs” of Scientific Computing (and Data)

Dense Linear Algebra	Monte Carlo
Sparse Linear Algebra	Spectral Methods
Particle Methods	Graphs
Structured Grids	Sorting
Unstructured Grids	Hashing

- Performance models:
 - Roofline
 - $\alpha\text{-}\beta$ (latency/bandwidth)
 - (LogP)
- Cross-cutting topics:
 - Communication avoiding
 - Load balancing
 - Hierarchical algorithms
 - Autotuning
- The Laws
 - Moore’s Law
 - Amdahl’s Law
 - Little’s Law
- Applications (in some detail)
 - Machine Learning
 - Biology
 - Cosmology

Course Logistics

- Website: <https://sites.google.com/lbl.gov/cs267-spr2021>
 - Homeworks, slides and videos from lectures, and more
- Quizzes (~1 per lecture) are due before the next lecture
- Labs will use Friday slot for optional Labs (~1 per homework)
- Homework groups will be assigned for HW1
- Piazza: <https://piazza.com/class/kjni0bj52ey3tz>
- Academic integrity