

Beyond Exascale Computing

Kathy Yelick

**Vice Chancellor for Research
and Robert S. Pepper Professor of
Electrical Engineering and Computer Sciences
U.C. Berkeley**

**Senior Faculty Scientist
Computing Sciences
Lawrence Berkeley National Laboratory**

National Academies Study

Kathy Yelick (Chair)

John Bell

Bill Carlson

Fred Chong

Dona Crawford

Jack Dongarra

Mark Dean

Ian Foster

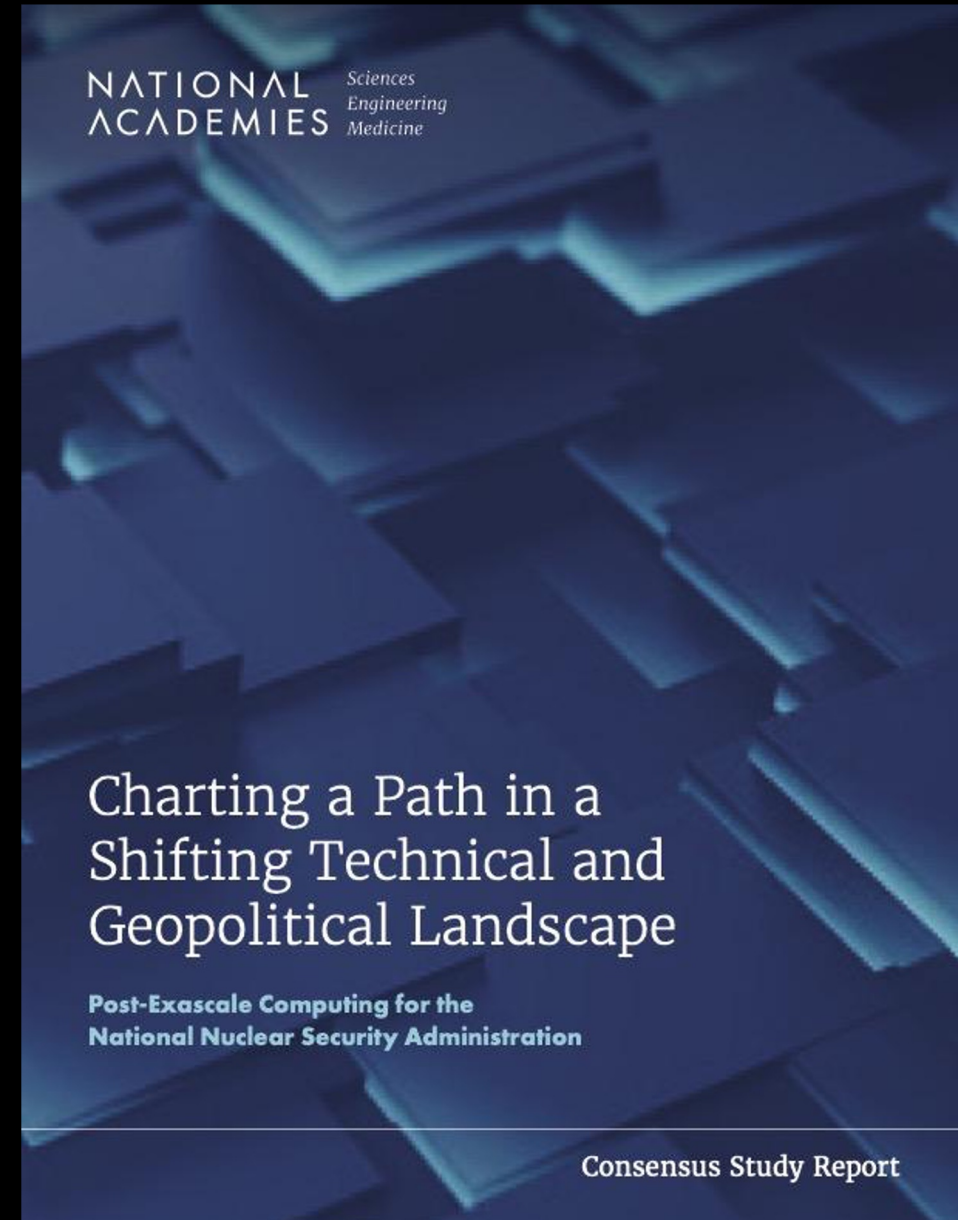
Charlie McMillan

Dan Meiron

Daniel Reed

Karen Willcox

(report at www.cstb.org)



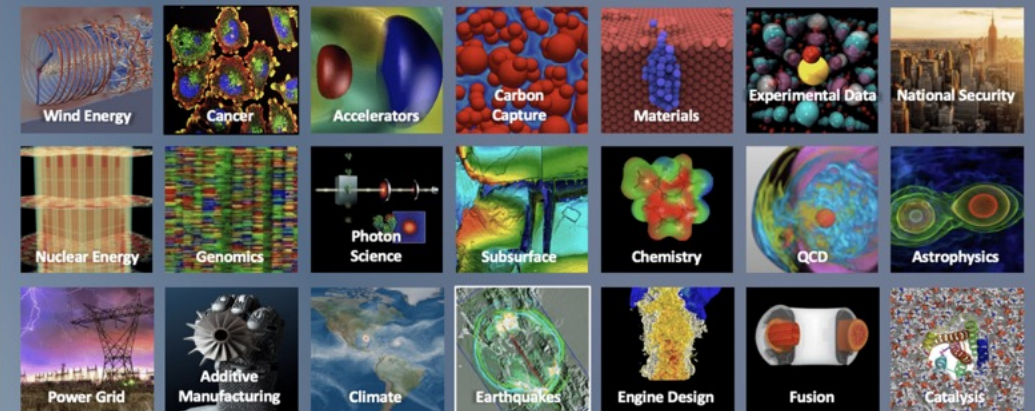
DOE ASCR Report

Jack Dongarra (Chair)
Ewa Deelman (Vice Chair)
Tony Hey
Satoshi Matsuoka
Vivek Sarkar
Greg Bell
Ian Foster
David Keyes
Dieter Kranzlmeuller
Bob Lucas
Lynne Parker
John Shalf
Dan Stanzione
Rick Stevens
Katherine Yelick

(report at www.osti.gov/)

Can the United States Maintain Its Leadership in High-Performance Computing?

A report from the ASCAC Subcommittee on American Competitiveness and Innovation to the ASCR office



Chair

Jack Dongarra, University of Tennessee, Knoxville & Oak Ridge National Laboratory

Vice Chair

Ewa Deelman, University of Southern California

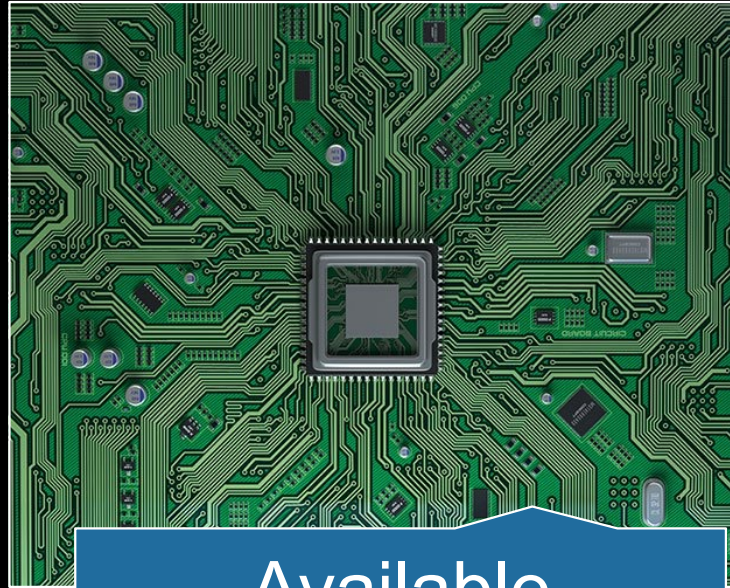
Subcommittee Members

Tony Hey, Rutherford Appleton Laboratory, Science and Technology Facilities Council, Harwell
Satoshi Matsuoka, RIKEN & Tokyo Institute of Technology
Vivek Sarkar, Georgia Institute of Technology
Greg Bell, Corelight
Ian Foster, Argonne National Laboratory & University of Chicago
David Keyes, King Abdullah University of Science and Technology
Dieter Kranzlmeuller, Leibniz Supercomputing Centre & Ludwig Maximilian University of Munich
Bob Lucas, Ansys
Lynne Parker, University of Tennessee, Knoxville
John Shalf, Lawrence Berkeley National Laboratory
Dan Stanzione, Texas Advanced Computing Center
Rick Stevens, Argonne National Laboratory & University of Chicago
Katherine Yelick, University of California, Berkeley & Lawrence Berkeley National Laboratory

Post-Exascale Computing



Computing
demand

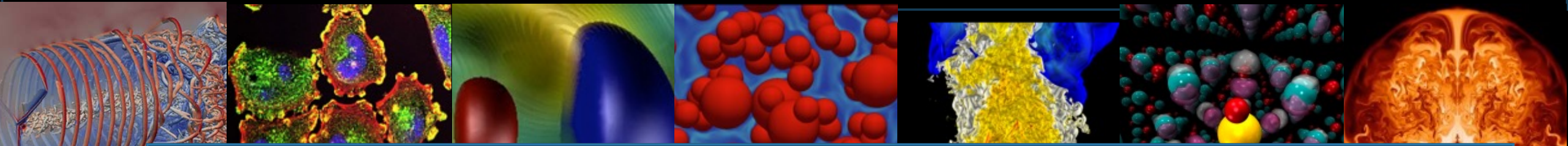


Available
technology

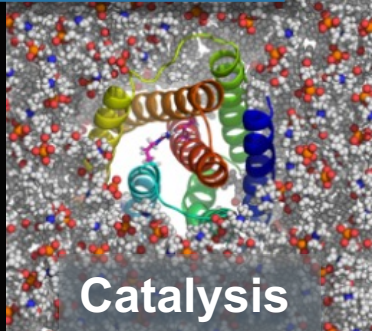
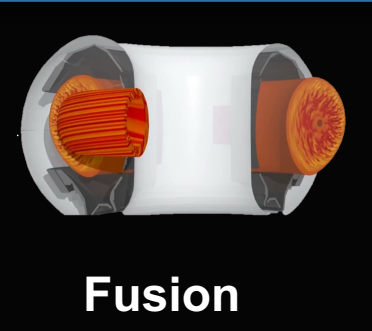
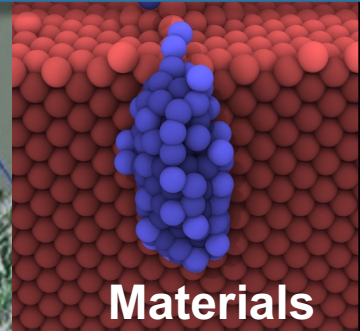
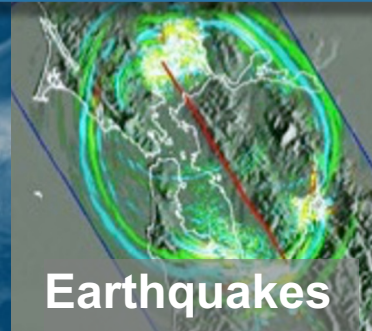
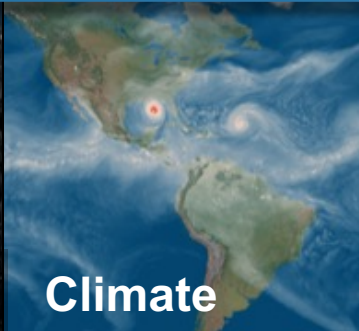
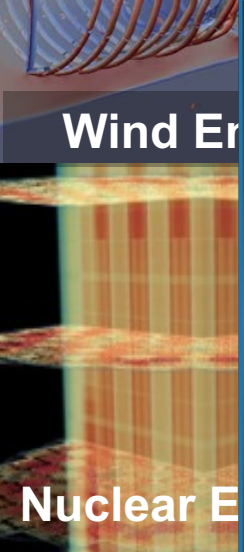


Disruptions

Continue to Rethink Applications



- 24 projects with about 10 people per team
- Rely heavily on hardware features and software teams
- Several new to HPC, all with new capabilities
- We should have another 2 dozen in 10 years!!



Power Grid

Manufacturing

Climate

Earthquakes

Materials

Fusion

Catalysis

Scientific Computing Circa 2007

*Exascale report from 2007 Town Halls
Entirely focused on modeling and
simulation*

~~Scientific Computing is often used
synonymously with Simulation and HPC~~

Simulation \subset Scientific Computing \subset HPC

Modeling and Simulation at the Exascale for Energy and the Environment

Co-Chairs:

Horst Simon

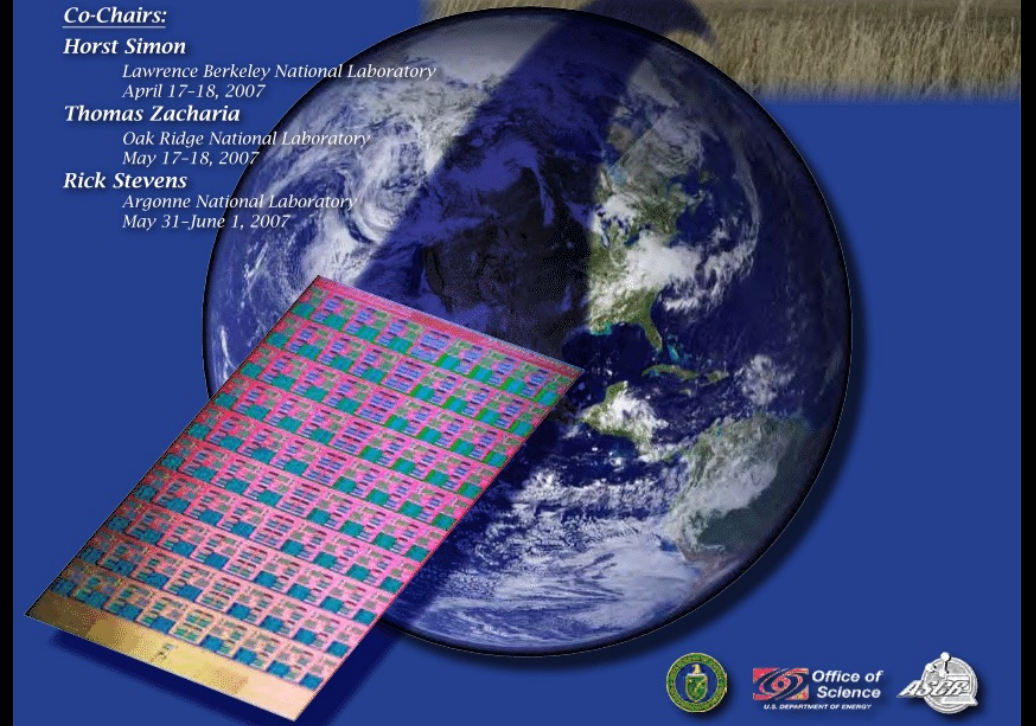
*Lawrence Berkeley National Laboratory
April 17-18, 2007*

Thomas Zacharia

*Oak Ridge National Laboratory
May 17-18, 2007*

Rick Stevens

*Argonne National Laboratory
May 31-June 1, 2007*



Runtime of “hero” calculations are too long

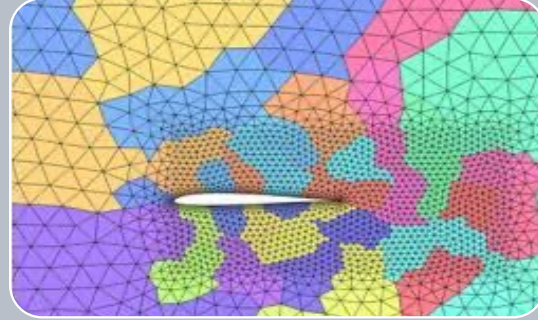
Number of Nodes	Memory Footprint	Wall-Clock Time
2400	~300–400 TB	6 months
4990	~600 TB	3–4 months
288	~20 TB	1 month
3250	104 TB	5.8 days
512	32.8 TB	2 months

Iterative design
does not happen on
6 month cycles

Subset of Application Challenges Beyond Exascale



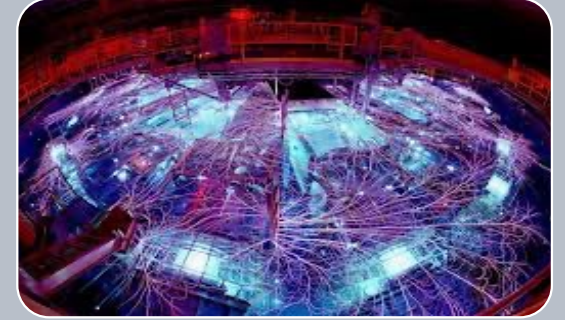
Reentry



Complex geometry

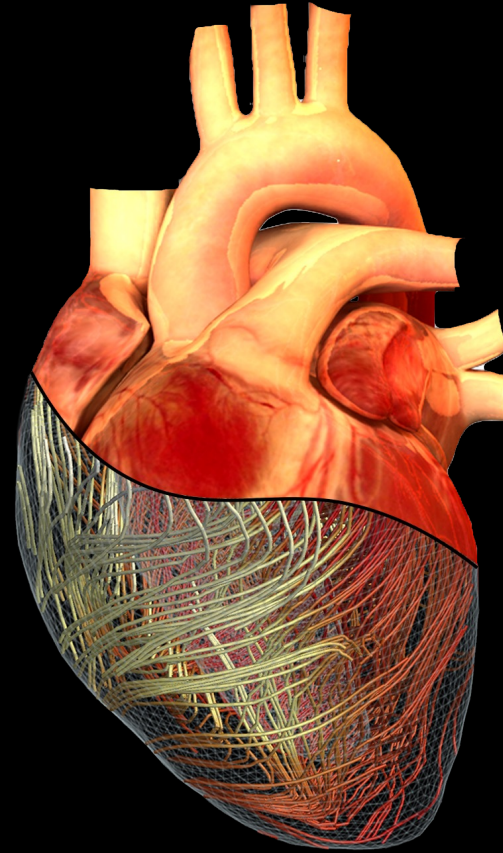


Combustion



Extreme Environs

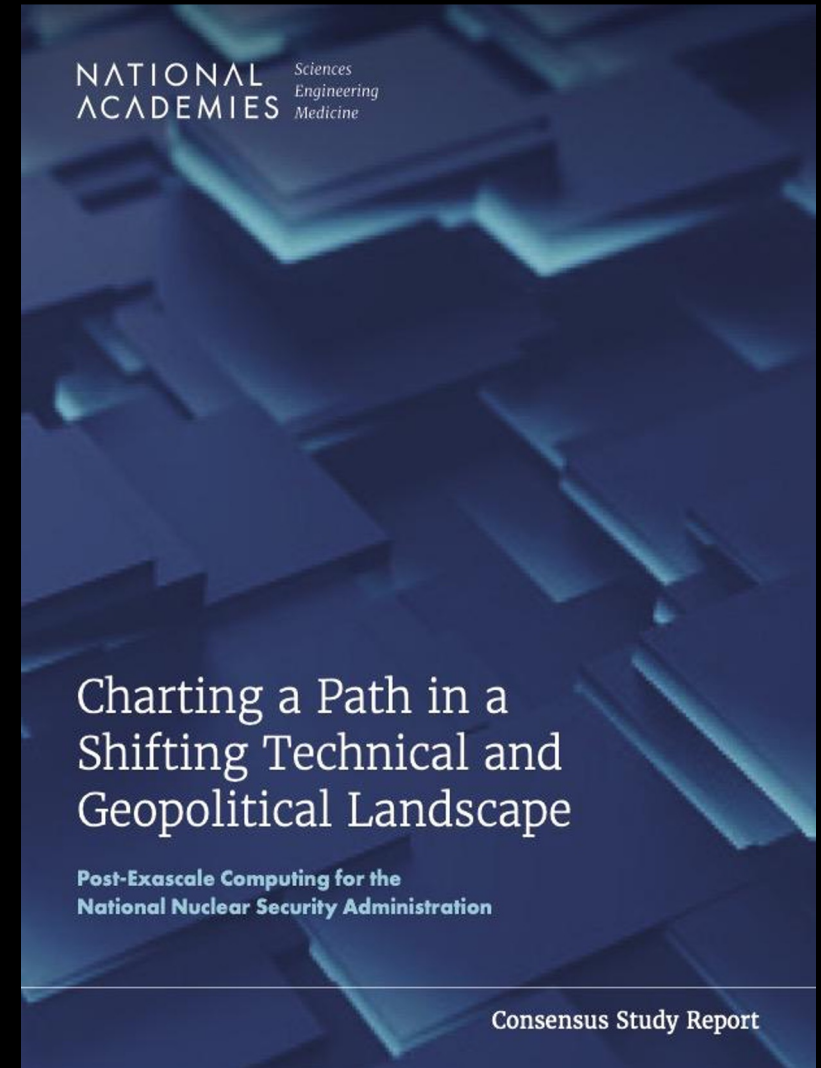
Digital Twins



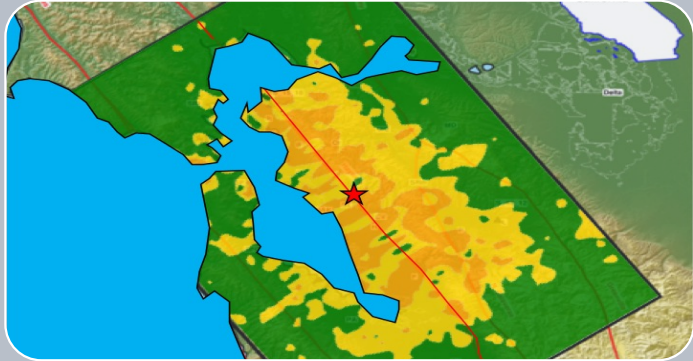
- Simulations
- Sensors / data
- Multi-level
- Real-time

National Academies Study

Finding: The demands for advanced computing continue to grow and will exceed the capabilities of planned upgrades across the NNSA labs.



New demands for HPC in Science



Simulation
From atoms
to the
universe

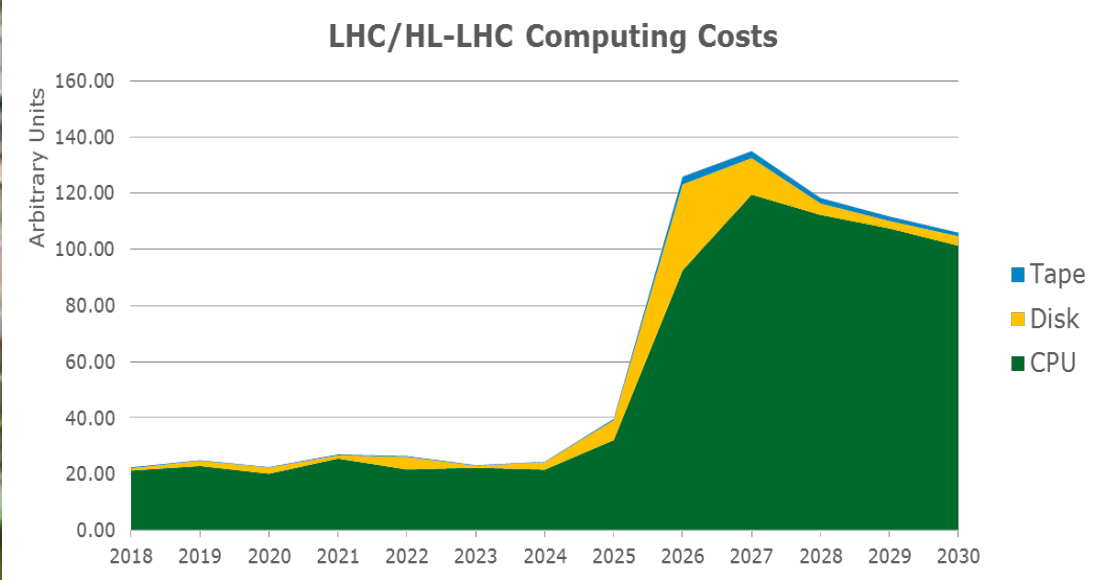
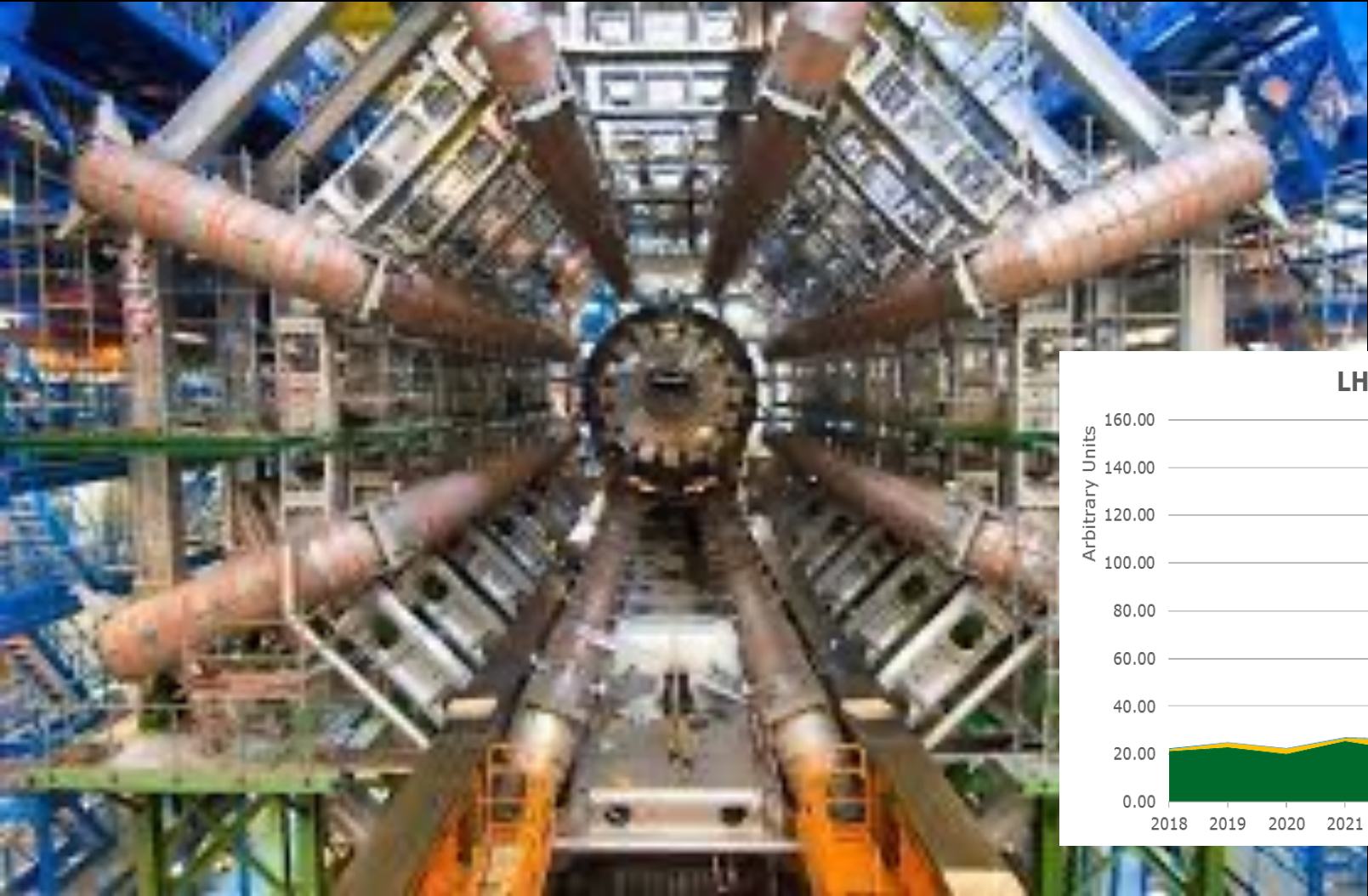


Data
Images, text,
to genomes



Learning
Interpret, infer
and automate

Prediction of Atlas computing +\$1B



Microbial Data in the Environment

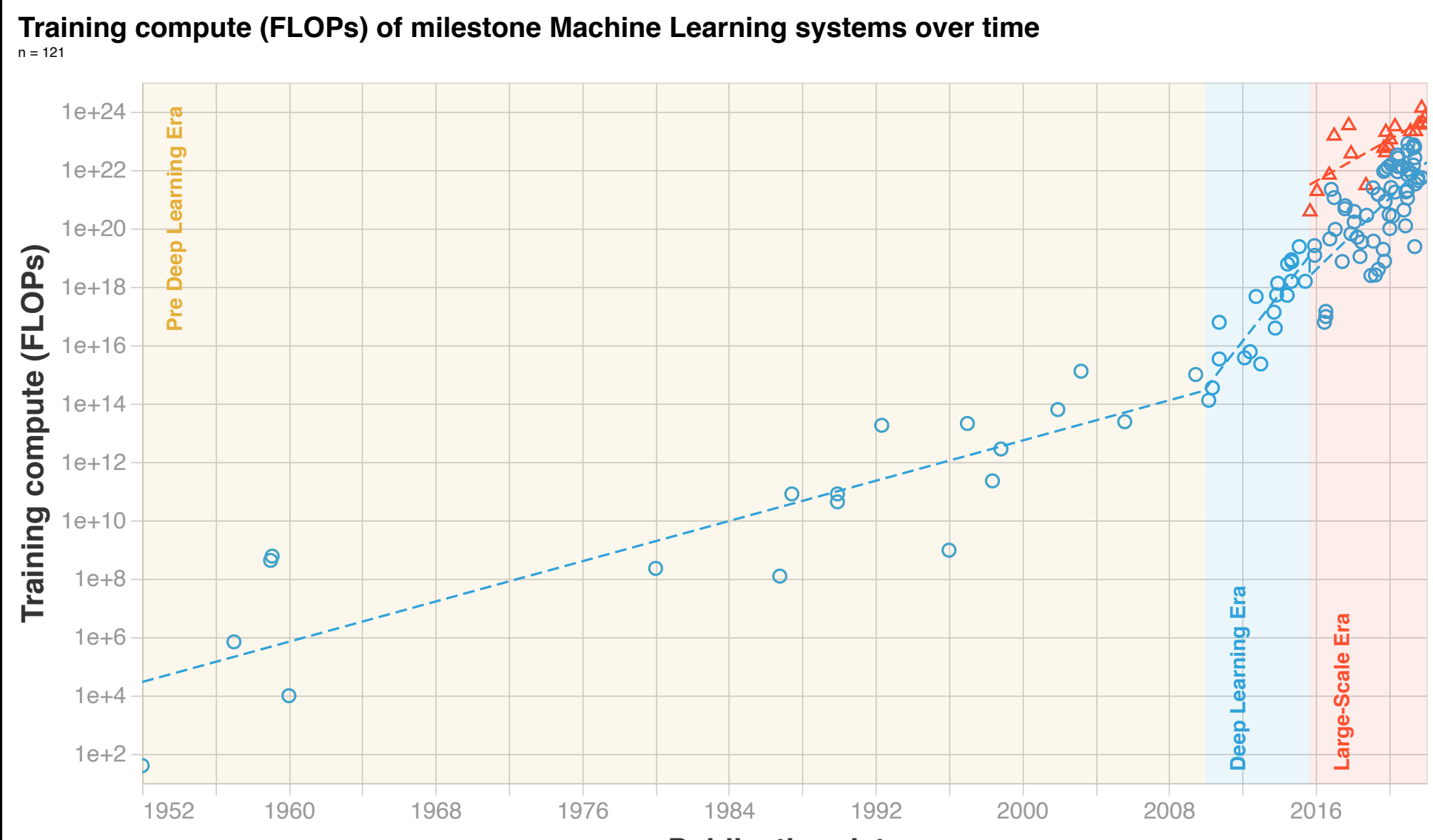


Tara Oceans Microbial data collected from 2009-13

84 Terabytes assembled on 9000 Frontier nodes

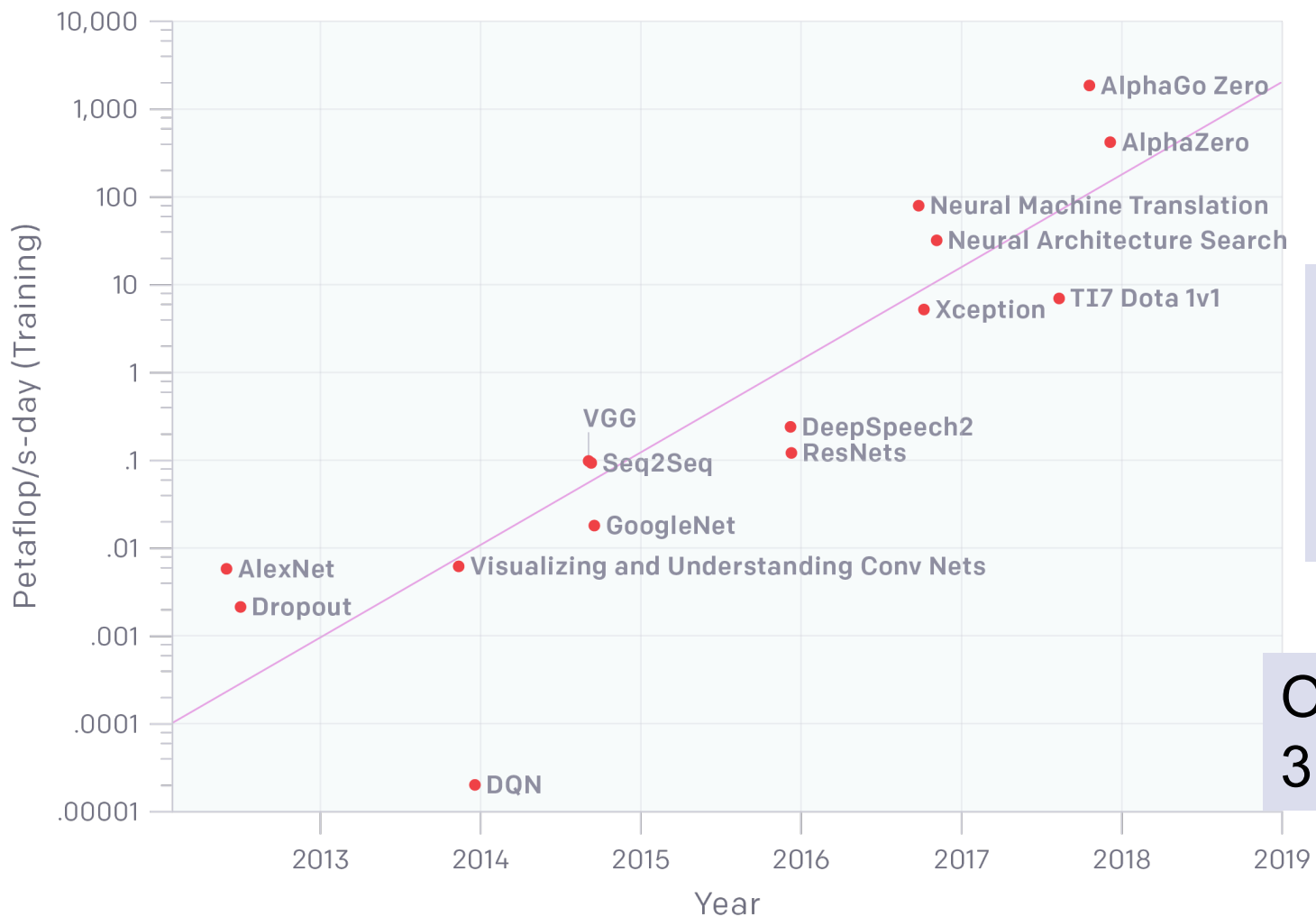
HPC changes observational science

Machine Learning Drives Computational Demand



Computing Requirements in Machine Learning

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



From 2011-2018
the fastest Top500
machine grew <
15x

OpenAI estimates
3.4-month doubling!

*A petaflop/s-day =
10¹⁵ neural net
operations per
second for one
day, ~=
10²⁰ operations*

Is there parallelism?

Always has been

Wait, it's all linear algebra?

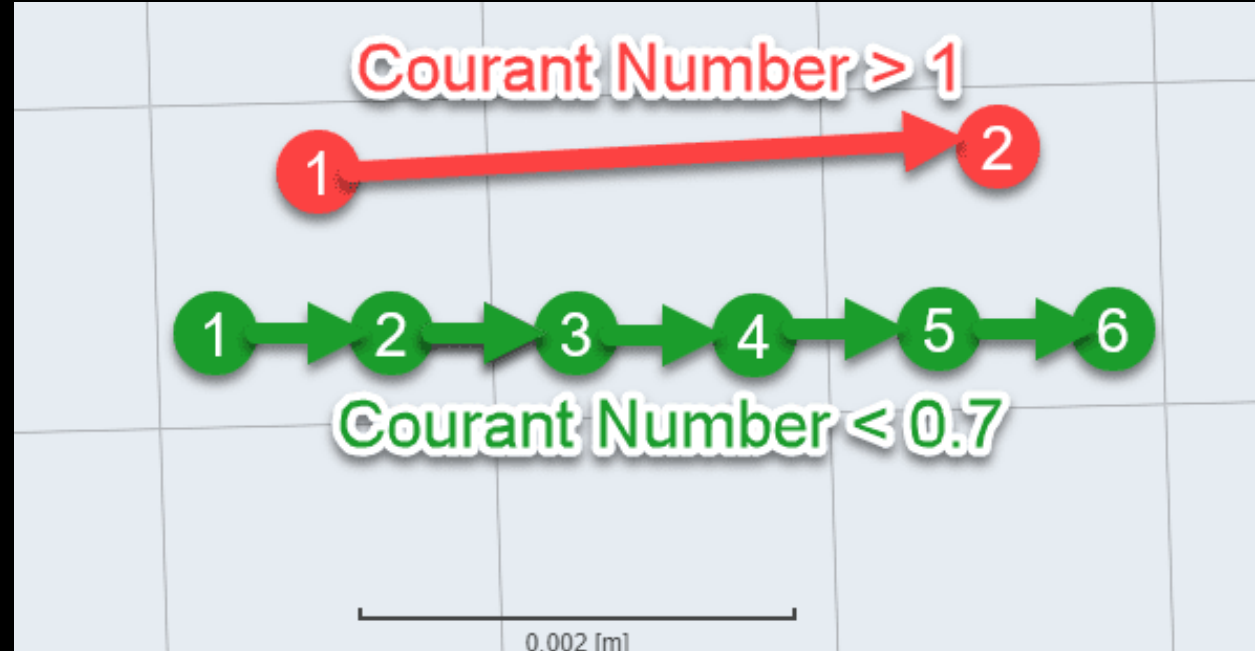
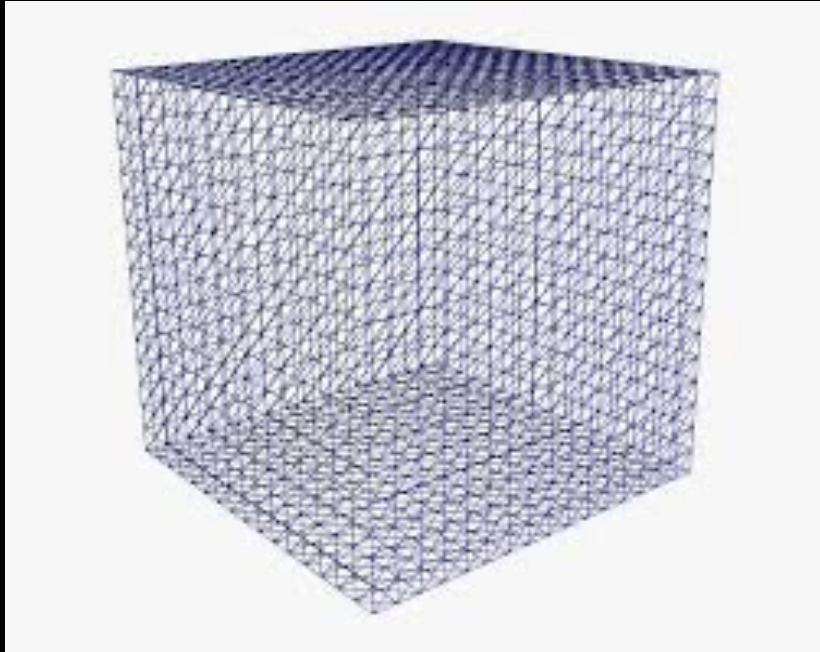
Analytics vs. Simulation Kernels:

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

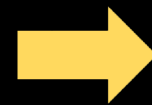
Phil Colella

NRC Report + our paper

Weak Scaling has Diminishing Returns



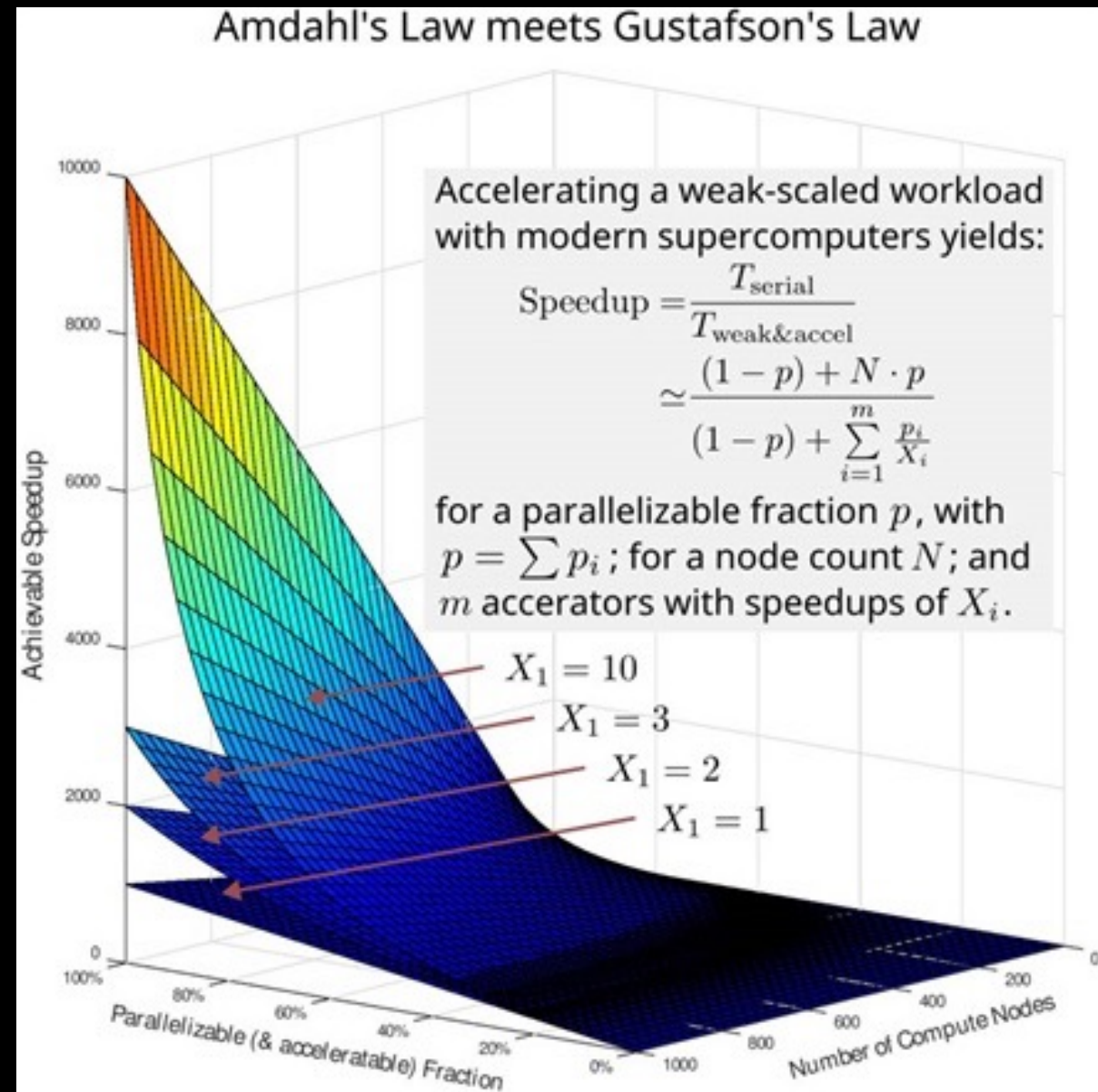
Increase resolution by 10x in each dimension
Increase cores by 1000x



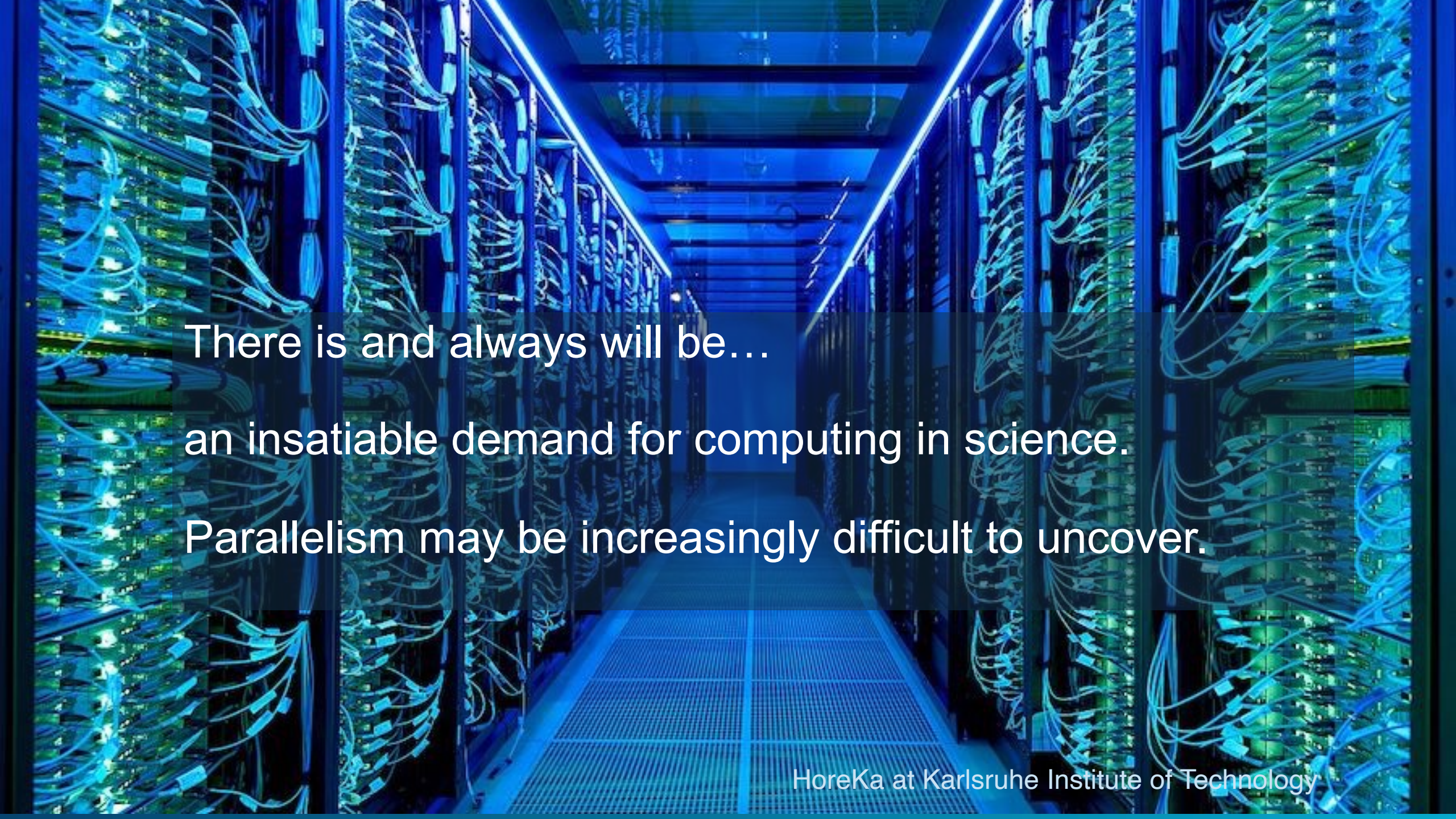
Runtime increases ☹️

Strong and weak scaling

- Strong scaling
 - Most desirable for users
 - Harder to find (Amdahl)
- Weak scaling
 - Limited for super-linear algorithms
 - Needs memory capacity to scale
 - Data problems also need I/O



See SIAM News, 9/22 [Satoshi Matsuoka](#) and [Jens Domke](#)

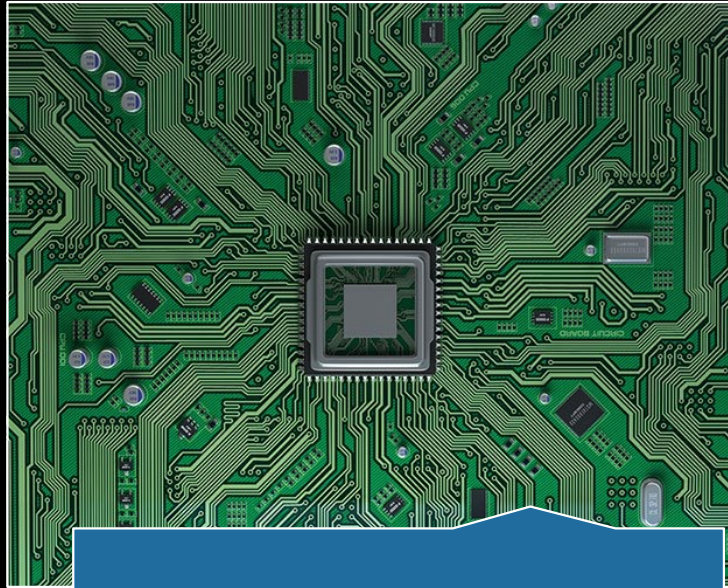


There is and always will be...
an insatiable demand for computing in science.
Parallelism may be increasingly difficult to uncover.

Post-Exascale Computing



Computing
demand



Disruptions



Technology

Disruptions

AI

Quantum

Cloud

Implied question: Do these make HPC obsolete?

AI for Science

AI FOR SCIENCE

RICK STEVENS
VALERIE TAYLOR
Argonne National Laboratory
July 22–23, 2019

JEFF NICHOLS
ARTHUR BARNEY MACCABE
Oak Ridge National Laboratory
August 21–23, 2019

KATHERINE YELICK
DAVID BROWN
Lawrence Berkeley National Laboratory
September 11–12, 2019

U.S. DEPARTMENT OF ENERGY U.S. DEPARTMENT OF ENERGY Office of Science
February 2020

ANL-22/91

ADVANCED RESEARCH DIRECTIONS ON
AI FOR SCIENCE, ENERGY, AND SECURITY

Report on Summer 2022 Workshops

Jonathan Carter
Lawrence Berkeley National Laboratory

John Feddema
Sandia National Laboratories

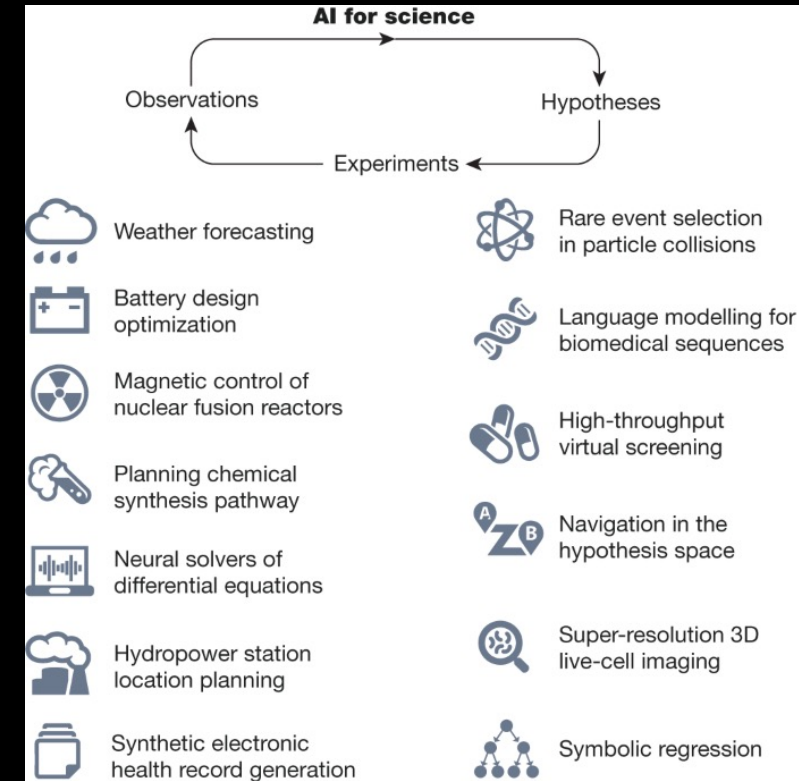
Doug Kothe
Oak Ridge National Laboratory

Rob Neely
Lawrence Livermore National Laboratory

Jason Pruet
Los Alamos National Laboratory

Rick Stevens
Argonne National Laboratory

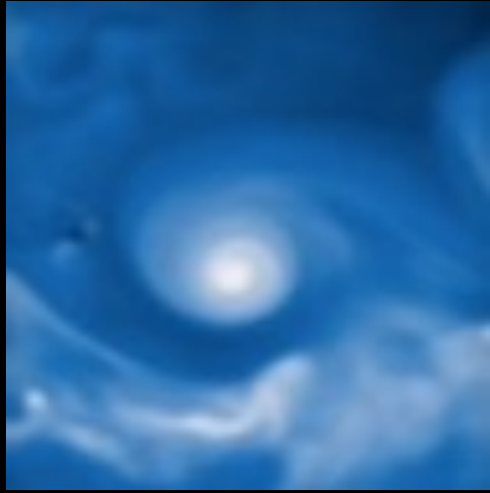
U.S. DEPARTMENT OF ENERGY U.S. DEPARTMENT OF ENERGY Office of Science NIS
May 2023



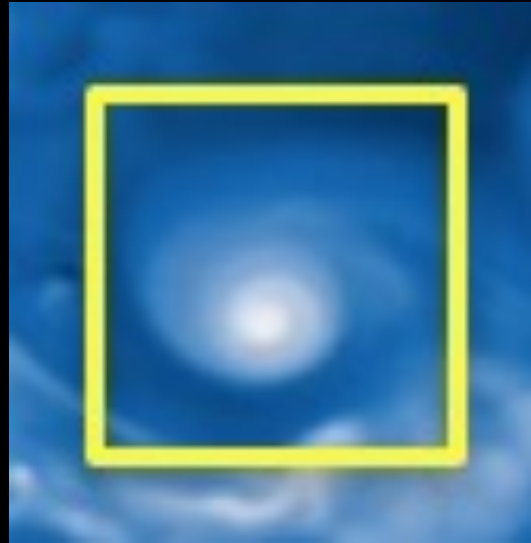
Scientific discovery in the age of artificial intelligence, 2023

Analyze Simulations to Find Hurricanes

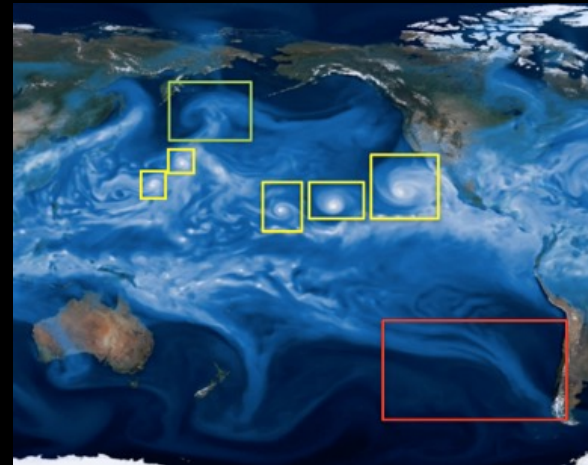
Classification



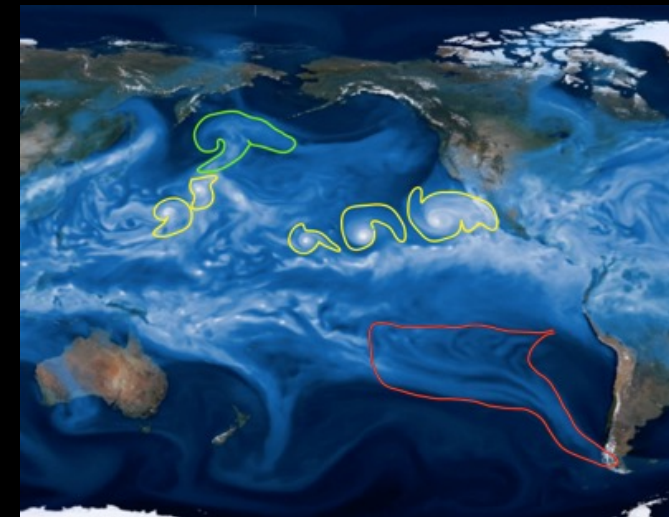
Localization



Detection



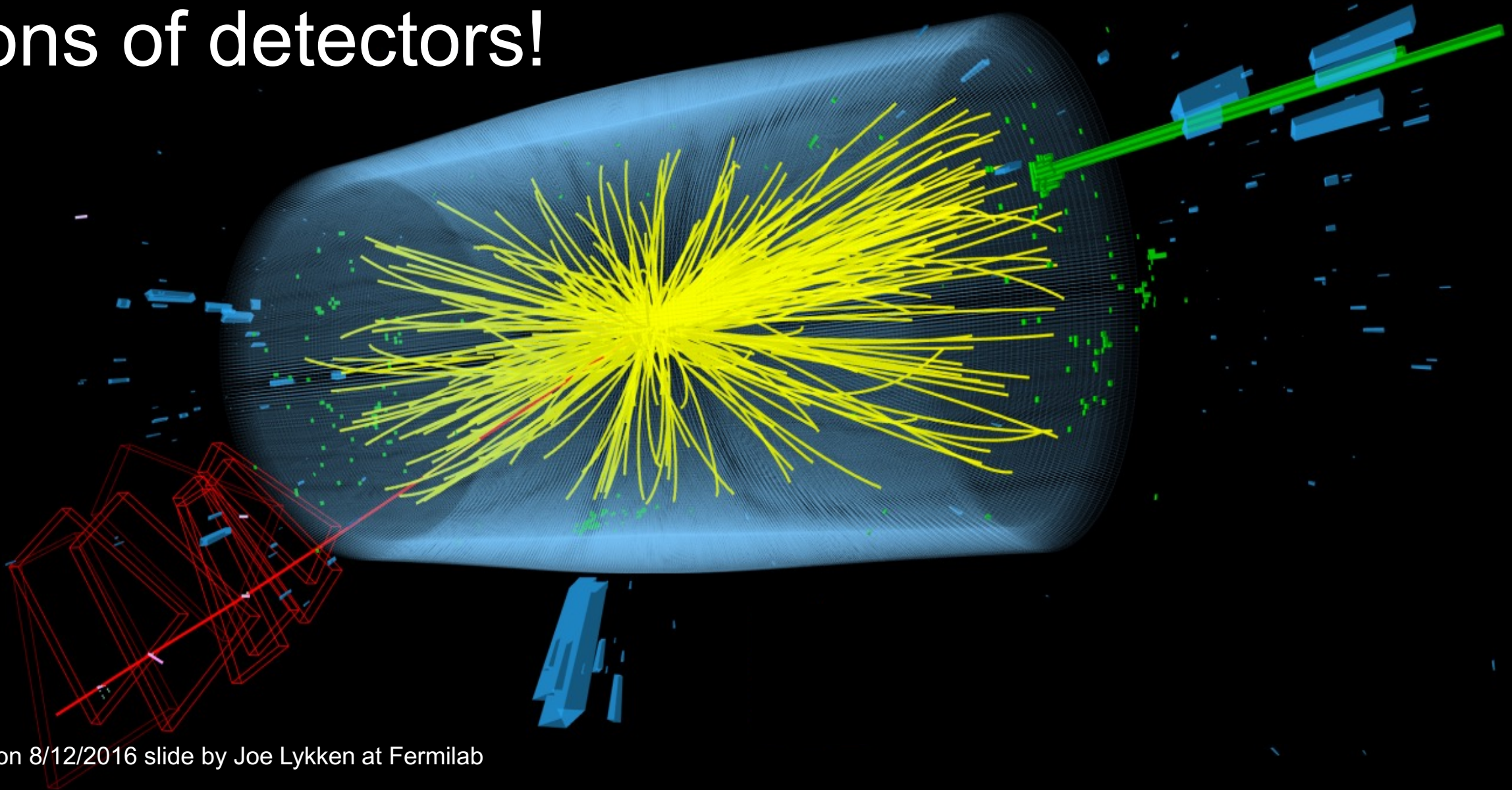
Segmentation



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

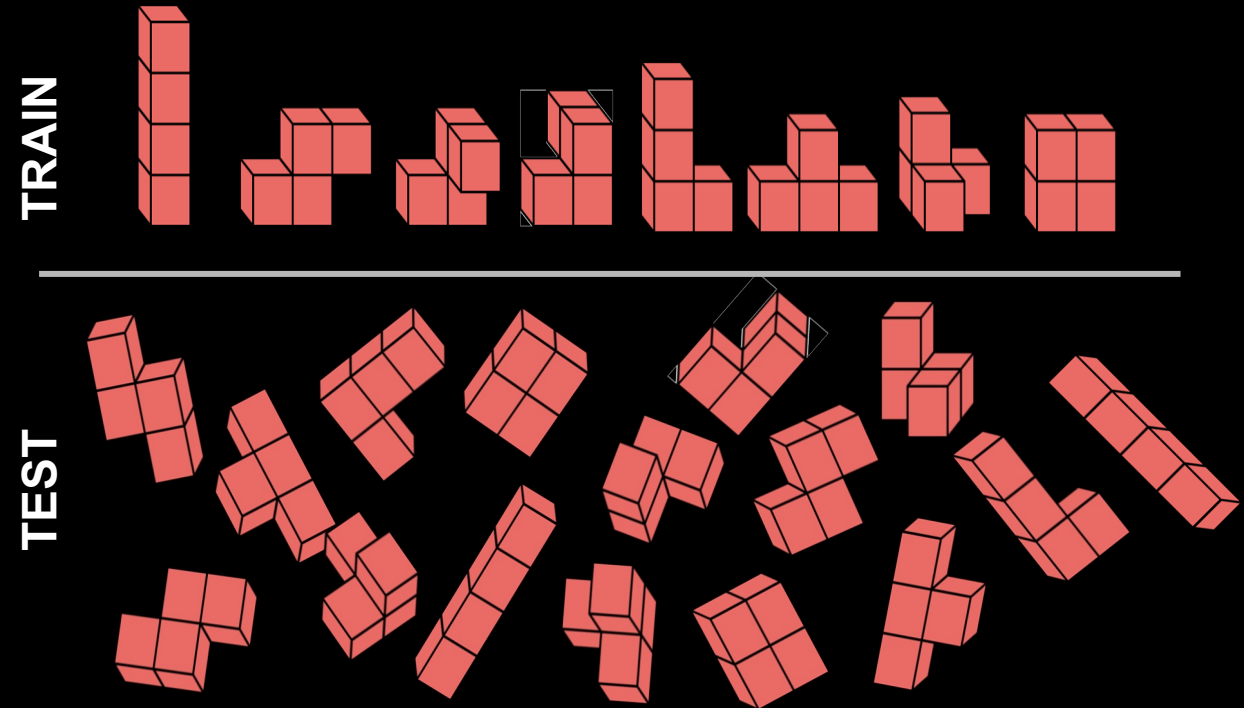
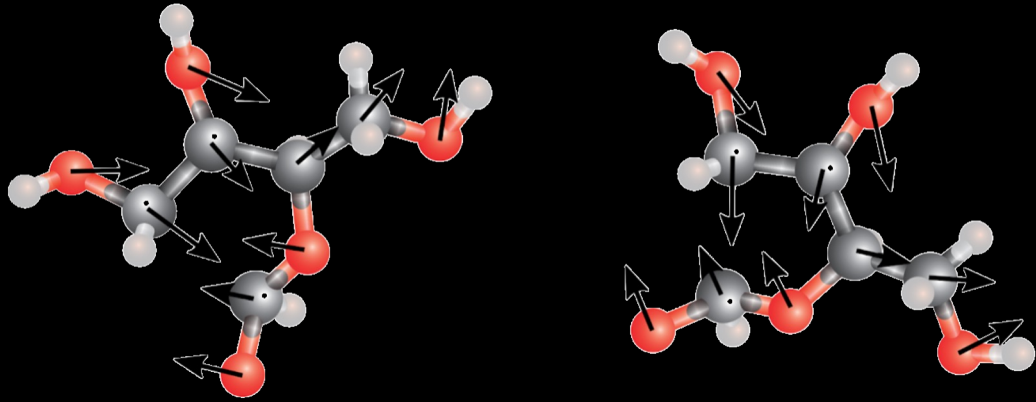
Source: Prabhat

Deep Learning: like adding 4,000 extra tons of detectors!



Deep Learning with Physical Laws

Physics-aware learning



A network with 3D translation- and 3D rotation-equivariance

Automation in Self-Driving Laboratories



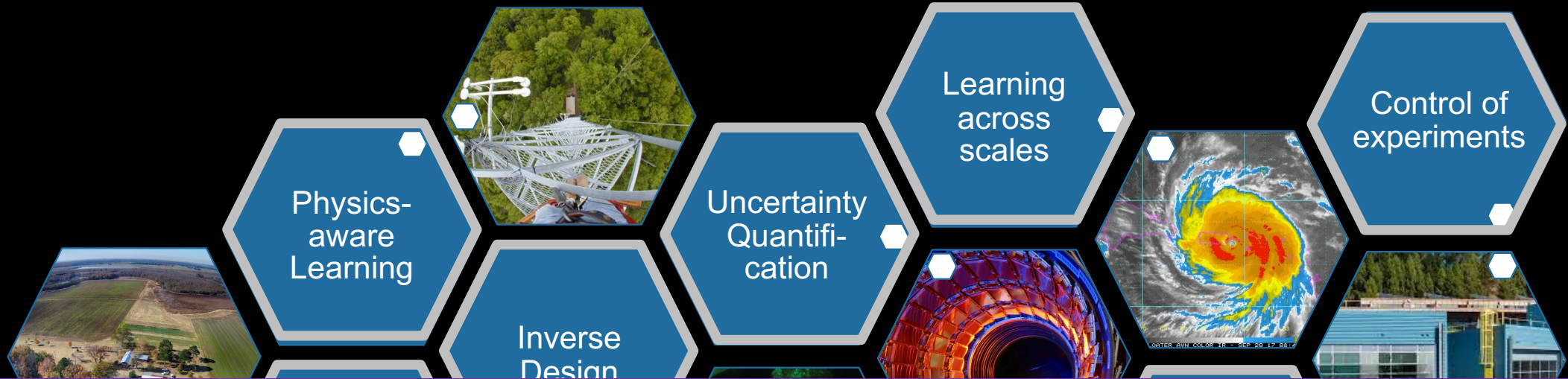
E.g., Strateos Cloud Lab
14K square feed
200+ instruments

Five Stages of AI

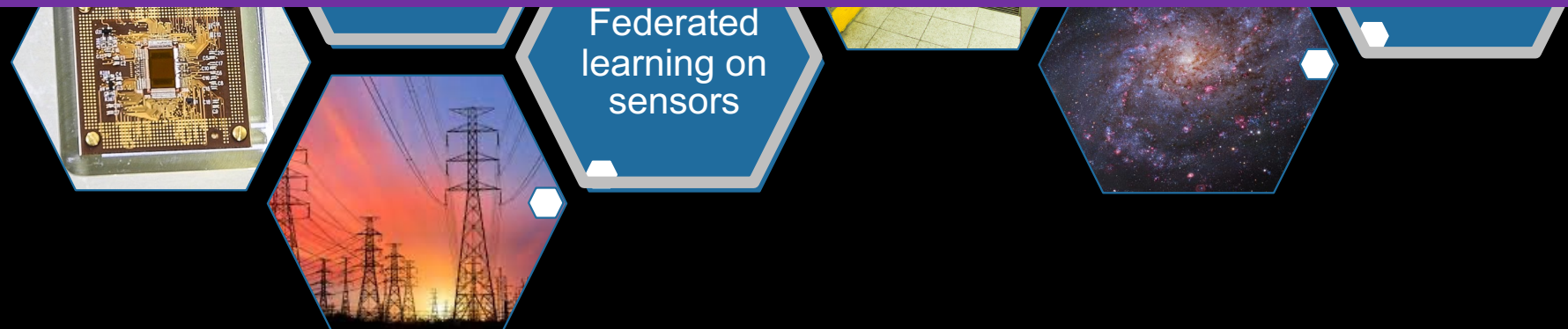


And this includes AI researchers!

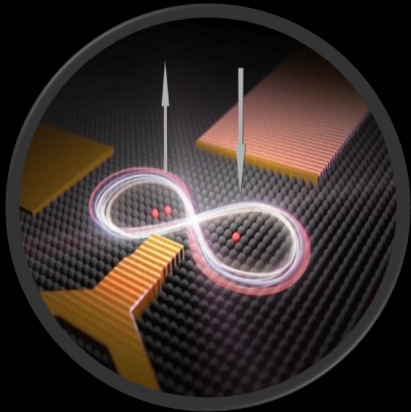
AI in Science



The Computational Science and Engineering community (including NNSA) should have a leadership role in addressing UQ, safety, alignment, and explainability in AI for science and engineering

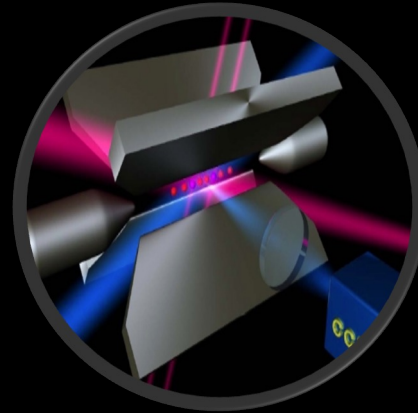


Types of Quantum Bits Diversity & Progress



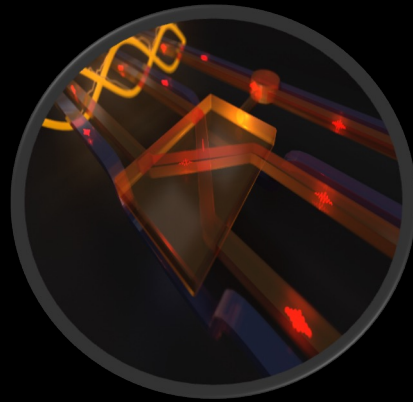
Dopants in Silicon / Diamond

www.sciencedaily.com



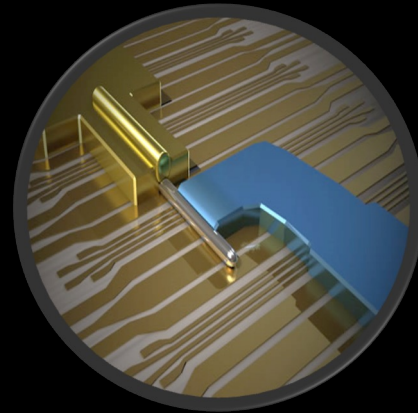
Trapped Ions

www.quantumoptics.at



Photonic Circuits

www.phys.org



Topological Wires

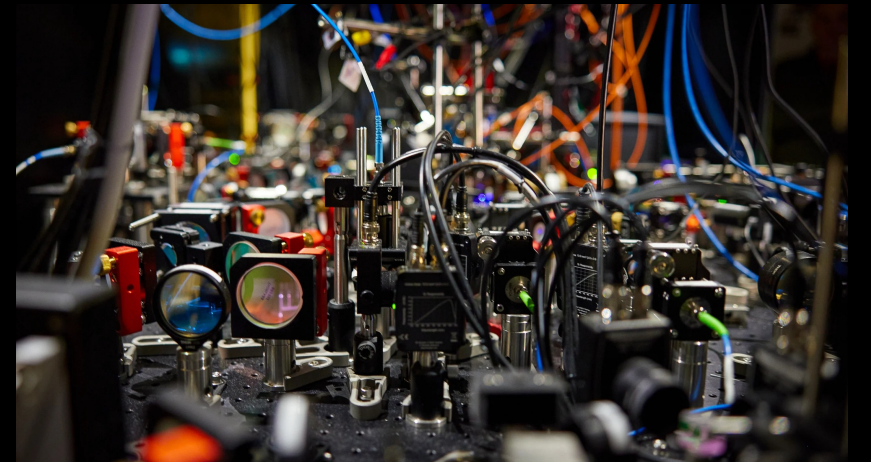
www.microsoft.com



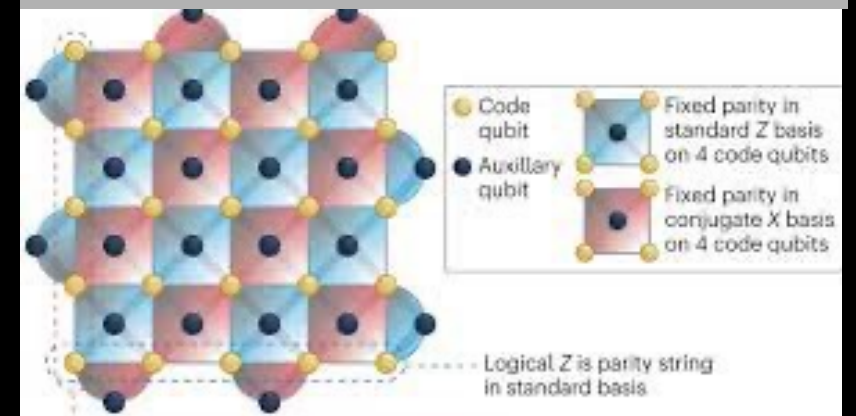
Superconducting Circuits

www.qnl.berkeley.edu

High-fidelity parallel entangling gates on a neutral-atom quantum computer



A series of fast-paced advances in Quantum Error Correction

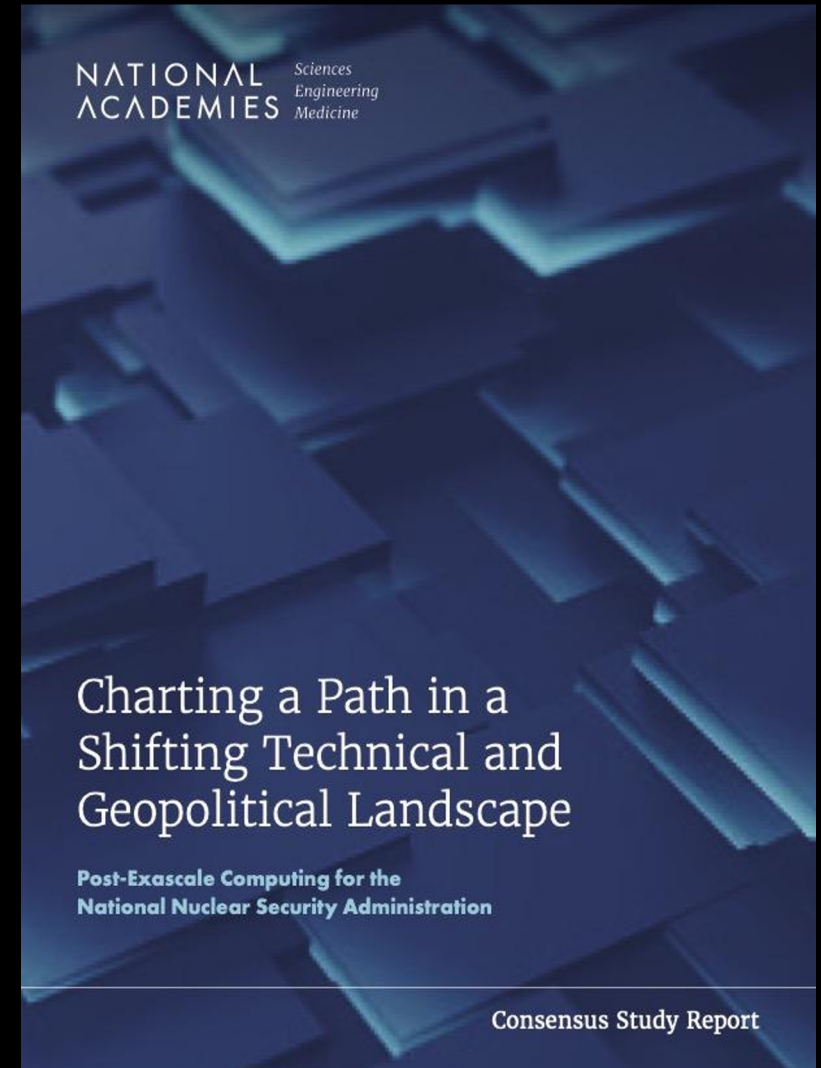


National Academies Study

Finding: **Quantum technology** has the potential to improve the fundamental understanding of material properties.

However, **breakthroughs in quantum algorithms and systems are needed** to make quantum computing practical for multiphysics stockpile modeling.

Quantum computing is more likely to serve as a **special-purpose accelerator** than to replace leading-edge computing.



Cloud Computing



Lessons Learned from Clouds



- Availability
- Cost vs price
- Higher level programming

Old programming models never die, they just get buried under layers!

The screenshot shows a Jupyter Notebook interface in a browser. The title bar reads "Lorenz Differential Equations". The notebook content includes:

Exploring the Lorenz System of Differential Equations

In this Notebook we explore the Lorenz system of differential equations:

$$\begin{aligned} \dot{x} &= \sigma(y - x) \\ \dot{y} &= \rho x - y - xz \\ \dot{z} &= -\beta z + xy \end{aligned}$$

This is one of the classic systems in non-linear differential equations. It exhibits a range of different behaviors as the parameters (σ, β, ρ) are varied, including what are known as *chaotic* solutions. This system was originally developed as a simplified mathematical model for atmospheric convection in 1963.

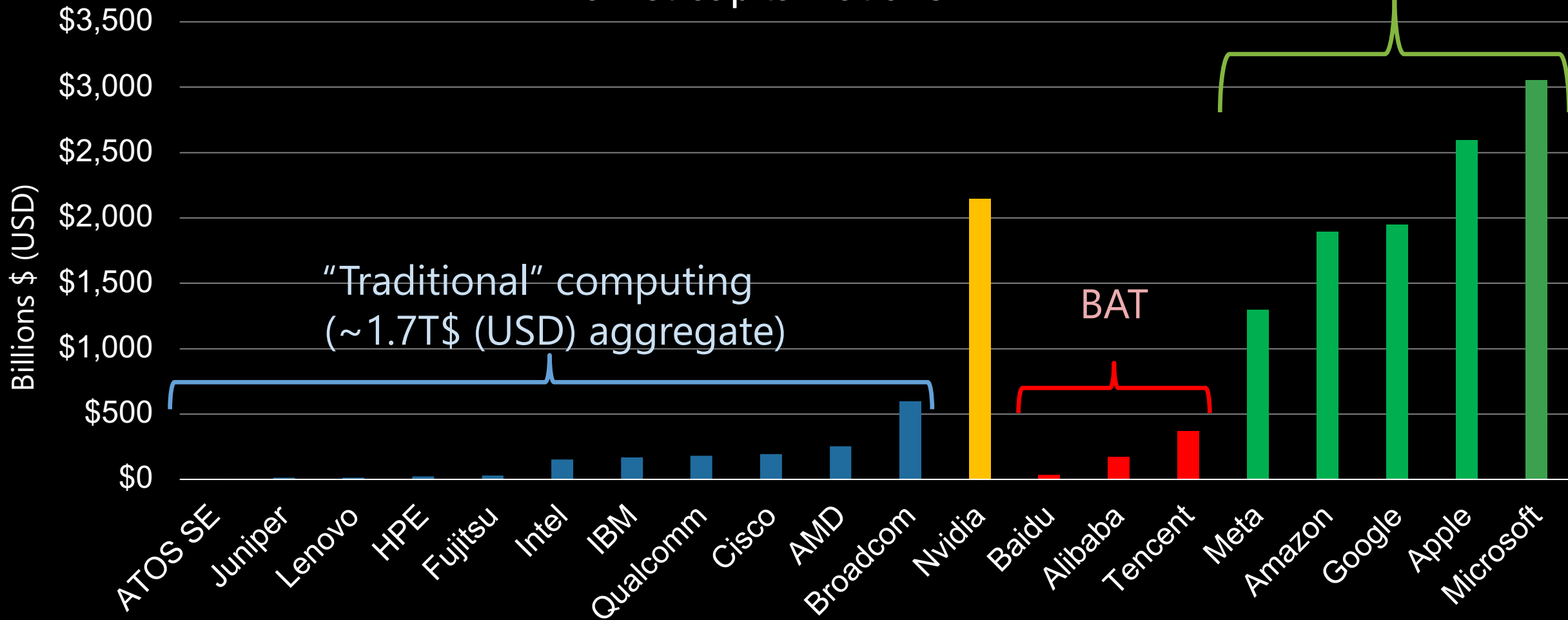
```
In [12]: interact(solve_lorenz, N=fixed(10), angle=(0.,360.),
                 sigma=(0.0,50.0), rho=(0.0,50.0));
```

angle	308.90
max_time	12.00
σ	10.00
β	2.63
ρ	28.00

A 3D plot of the Lorenz attractor, showing the characteristic butterfly-like shape of the system's trajectory. The plot is rendered with a blue wireframe and a colorful surface.

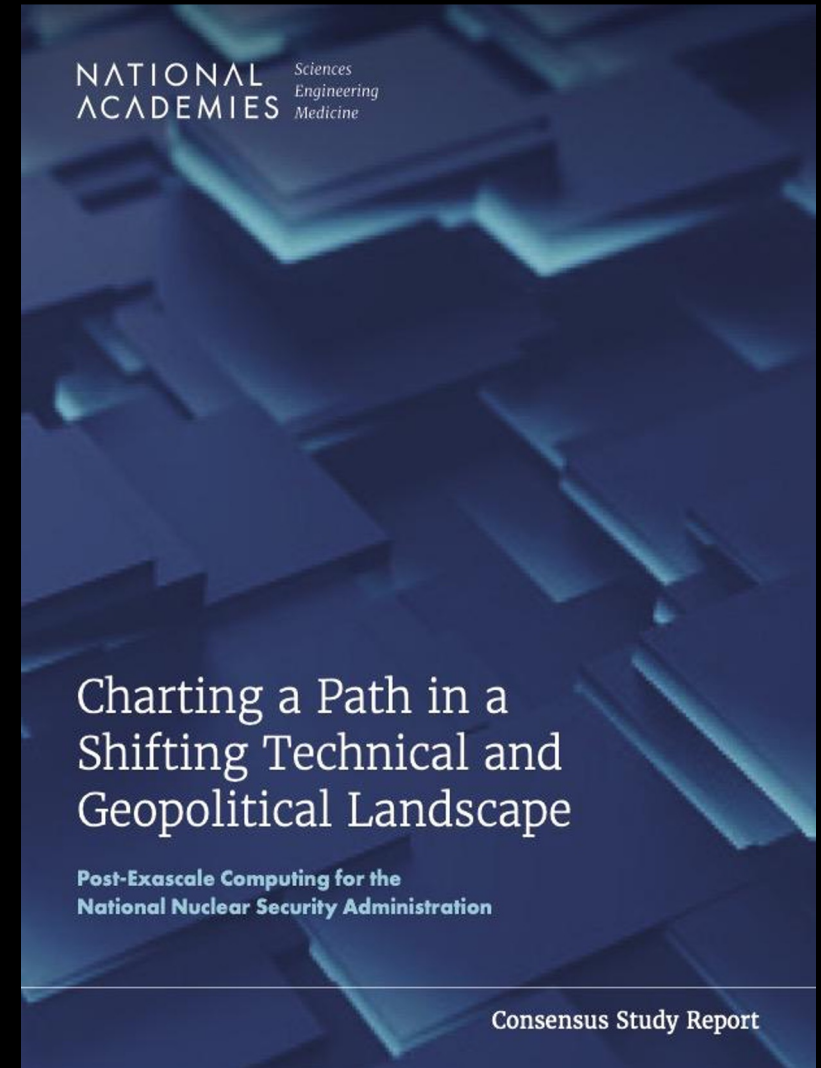
Follow the money, understand the implications

Market capitalizations



National Academies Study

Finding: **Cloud providers are engaged in hardware and software innovations** and will have more market influence in **technology and talent** but are **not aligned with NNSA requirements**.



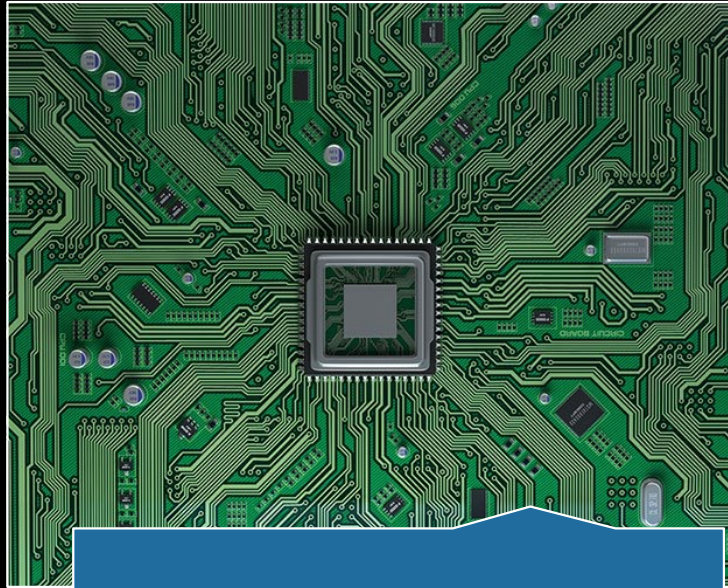
HPC community has always punched above its weight



Post-Exascale Computing



Computing
demand

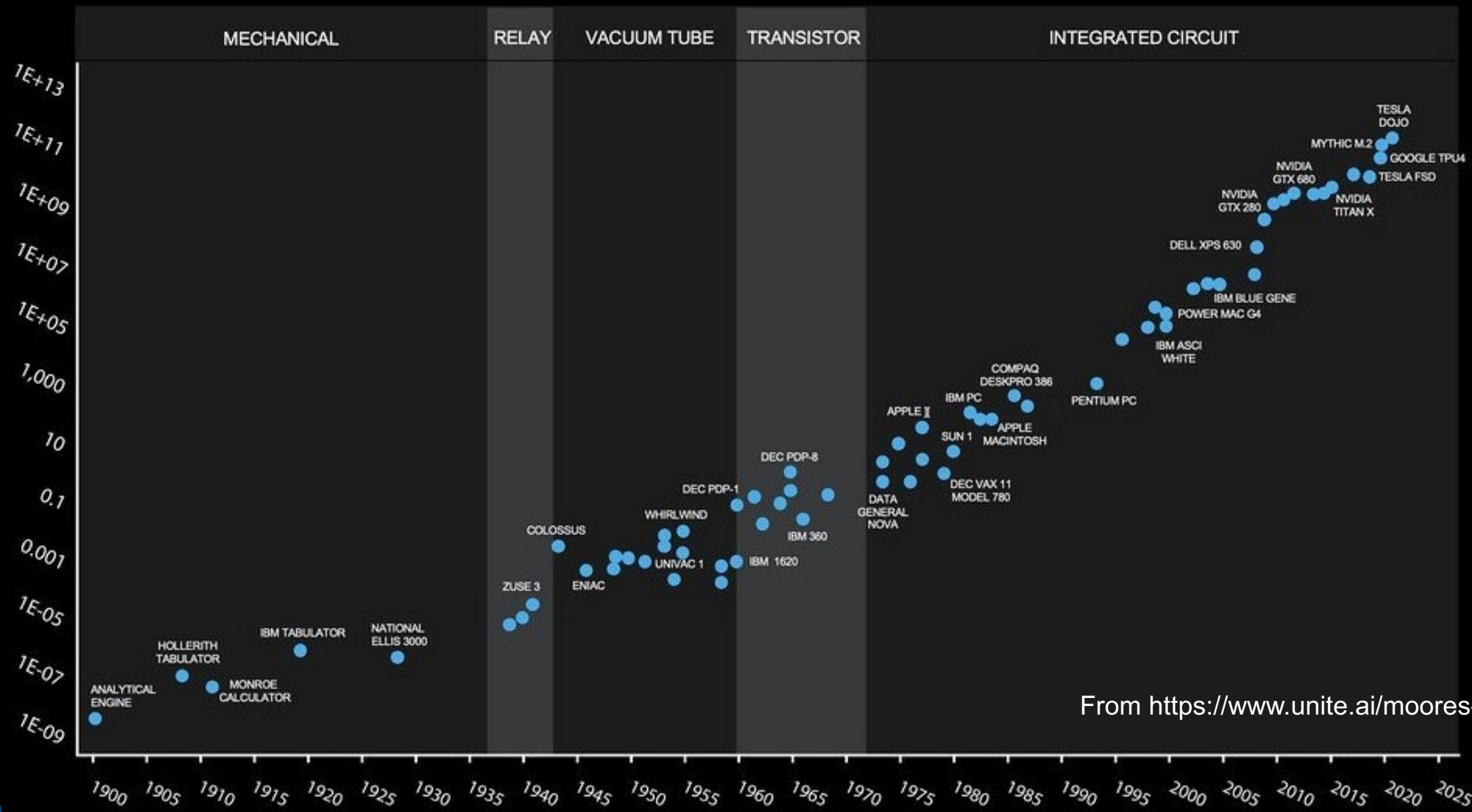


Disruptions



Technology

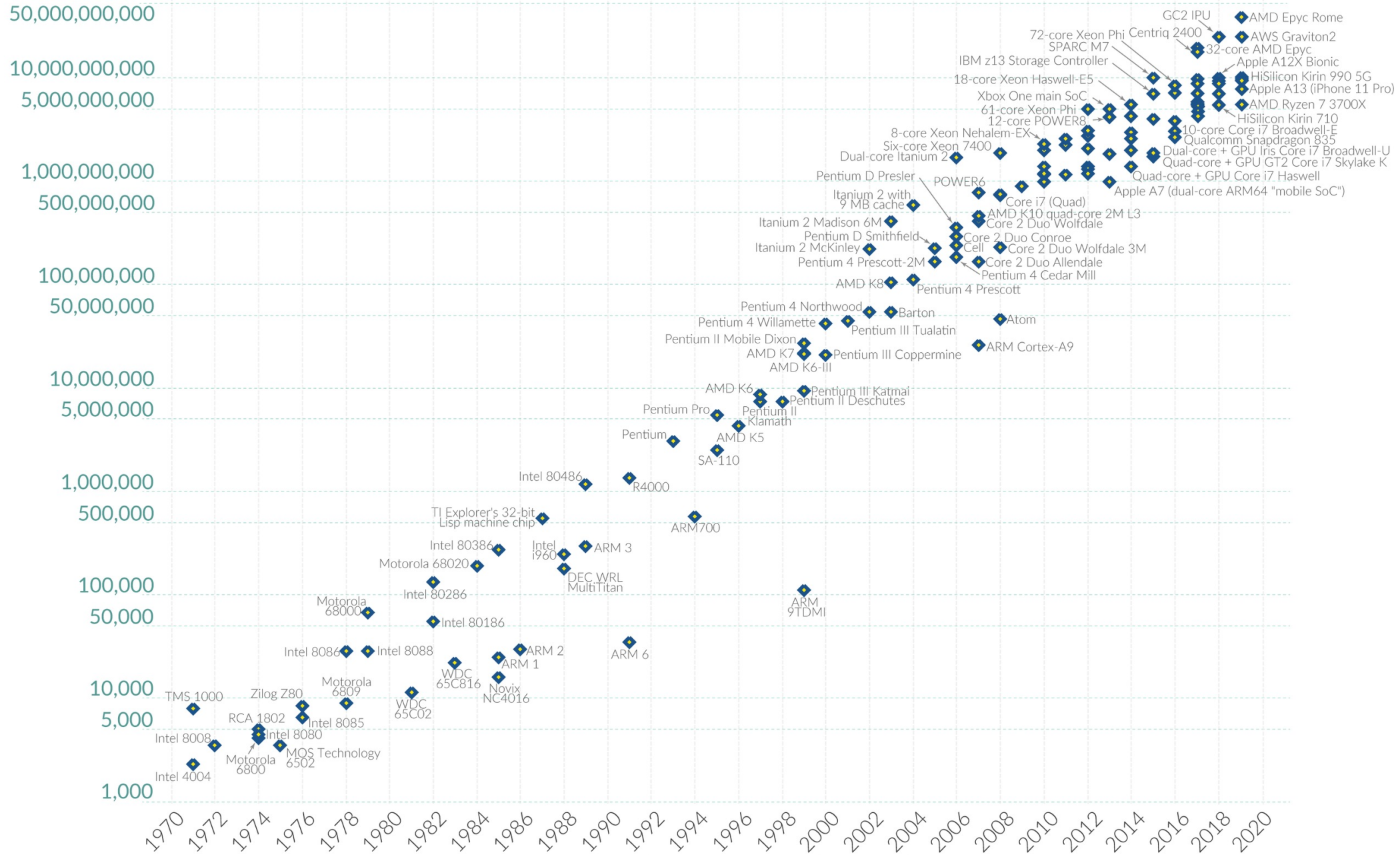
122 YEARS OF MOORE'S LAW



From <https://www.unite.ai/moores-law/>

10 μm	6 μm	3 μm	1.5 μm	1 μm	800 nm	600 nm	350 nm	250 nm	180 nm	130 nm	90 nm	65 nm	45 nm	32 nm	22 nm	14 nm	10 nm	7 nm	5 nm	3 nm
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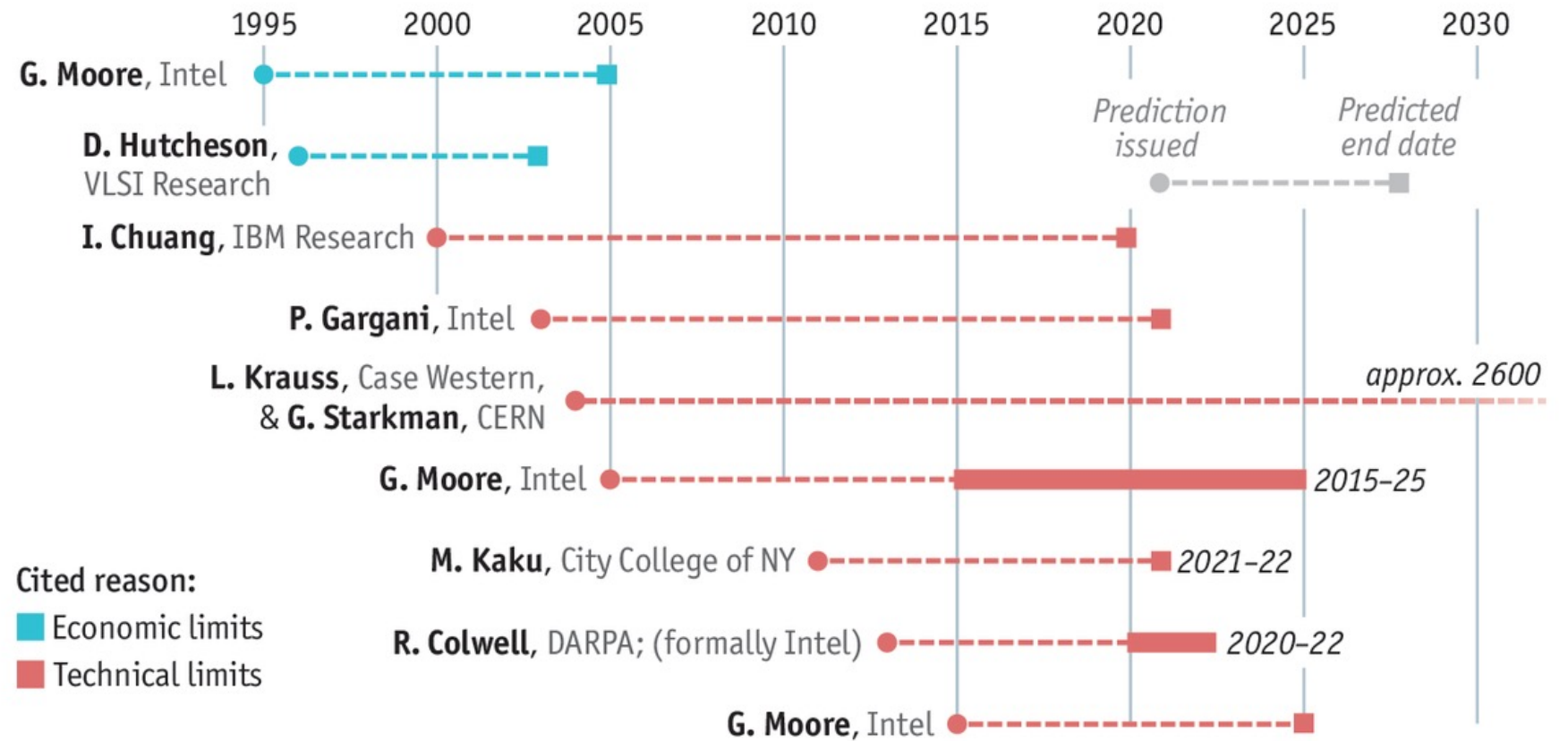
Transistor count



<https://www.economist.com/technology-quarterly/2016/03/10/horses-for-courses>

Faith no Moore

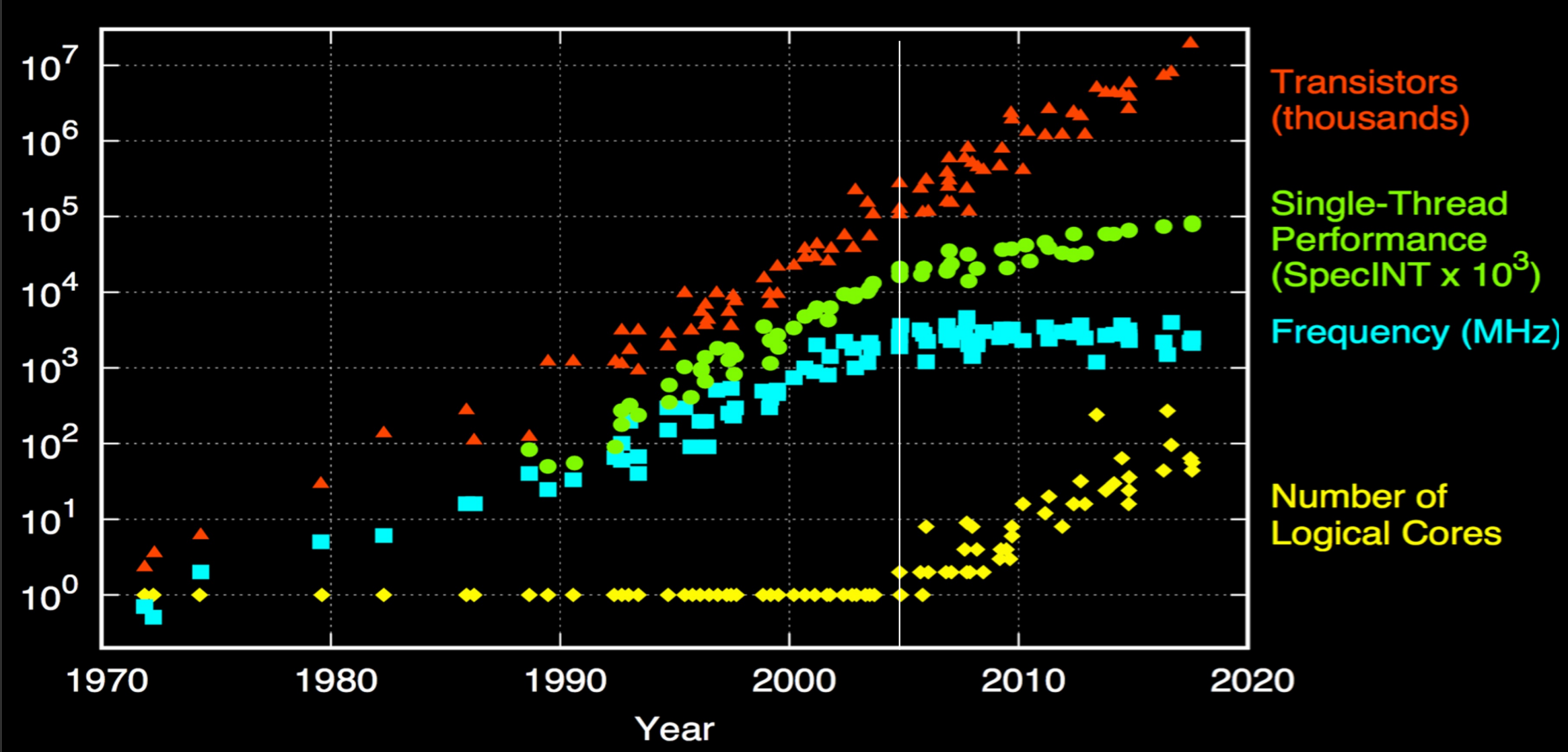
Selected predictions for the end of Moore's law



Sources: Intel; press reports; *The Economist*

Economist.com

Dennard Scaling is Long Dead; Moore's Law Will Follow



Performance Programming pre 2005



Exascale Architecture Plans (2008)

Petascale X 10x more energy X 100x more Performance per Joule = Exascale

**Accelerators
(GPUs)**

**100x
more
cores**

**Faster
clocks +
SIMD**

Exascale Era Architectures (US DOE Office of Science)

US DOE Office of Science Systems



Exascale
HPE AMD+AMD



Exascale
HPE Intel+Intel



Pre-exascale
HPE AMD+NVIDIA

1 Architecture (3 GPUs), 1 Integrator!

First-in-Class HPC Systems (Top500)

	First TF	First PF	First EF
	ASCI Red	Roadrunner	Frontier
Month-Year	Jun-97	Jun-08	Jun-22
Best Tech (nm)	500	65	6
Peak (PF/s)	0.001453	1.38	1686
Sustained (PF/s)	0.001068	1.04	1102
Power (MW)	0.85	2.35	21.1
Efficiency (GF/W)	0.00125647	0.44	52.2
Memory (PB)	0.001212	0.04	9.4
FPU's (K)	9	464	534,000
Cabinets	104	296	74
Floorspace (m ²)	150	557	678

Kogge and Dally: Frontier vs the Exascale Report: Why so long? and Are We Really There Yet?
+Wikipedia for ASCI Red

Energy efficiency didn't track technology scaling

Gate Length (nm)	65	32	16	6
Metal 1 pitch (nm)	180	100	64	40
Energy ⁻¹	1	1.8	2.8	4.5
Area ⁻¹	1	3.2	7.9	20.3

Rumors of 2nm fabs, but how much will it help?

Kogge and Dally: Frontier vs the Exascale Report: Why so long? and Are We Really There Yet?

The “Aggressive” Strawman was a bit early, but close to Summit

	Strawman	Summit
Year	2015	11/2018
Best Tech	32nm	16nm
Peak (PF/s)	2,000	201
Sustained (PF/s)	1,000	148
Power (MW)	67.7	9.8
Efficiency (GF/W)	14.9	14.7
Memory (PB)	3.5	2.8
Bandwidth/flop (B/F)	0.08	0.13
Mem BW (PB/s)	158	27
Bisection(TB/s)	210	105
FPUUs (M)	664	144
Cabinets	583	256
Floorspace (m^2)	1195	520

Resilience would have been a bigger problem with a 7x larger Summit

Post-Exascale Architecture Plans 2024 (Strawperson-v0)

Exascale X 2x more energy X 500x more Performance per Joule ??

GPUs

Influenced to make AI better (e.g., sparsity)?

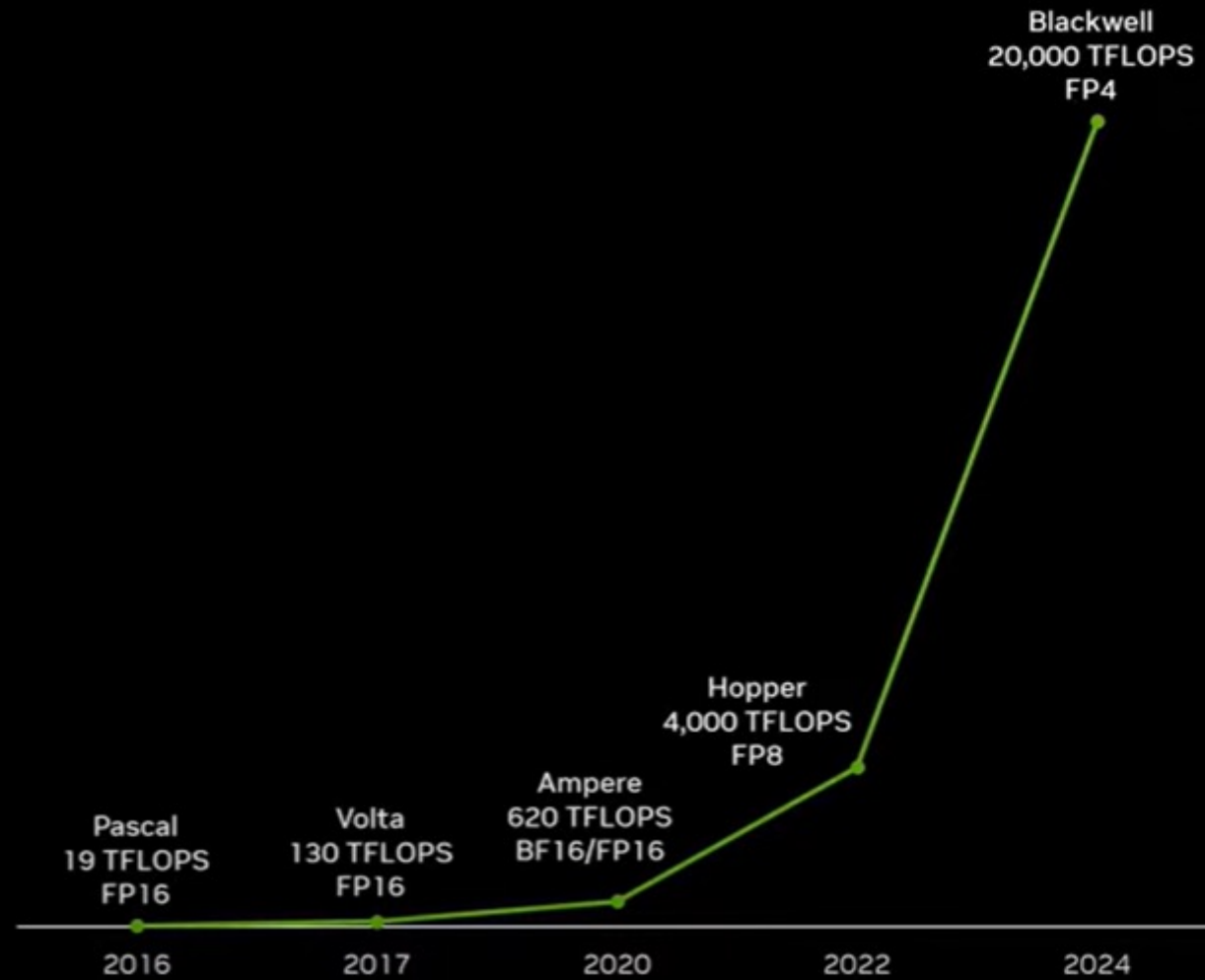
Specialized for AI

Specialized for Simulation

Designed by DOE, DoD, ...?

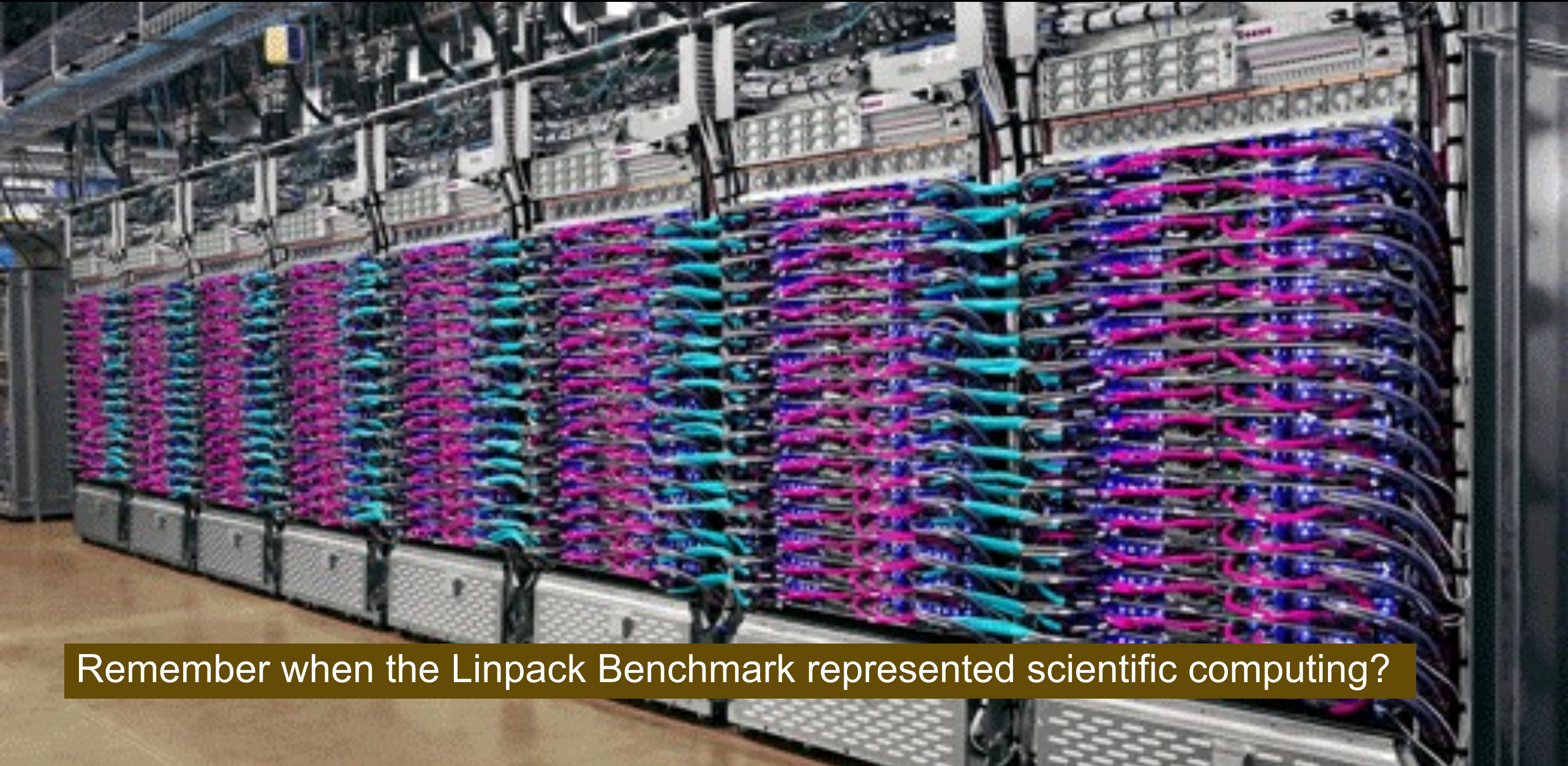
Another Exponential?

1000X AI Compute in 8 Years



Jensen Huang's Nvidia GTC Keynote

Specialization: Is deep learning the only application?



Remember when the Linpack Benchmark represented scientific computing?

Everyone is Making AI Chips

NVIDIA

AMD

Intel

IBM

Traditional
chip makers

“Software”
companies

Facebook + Intel

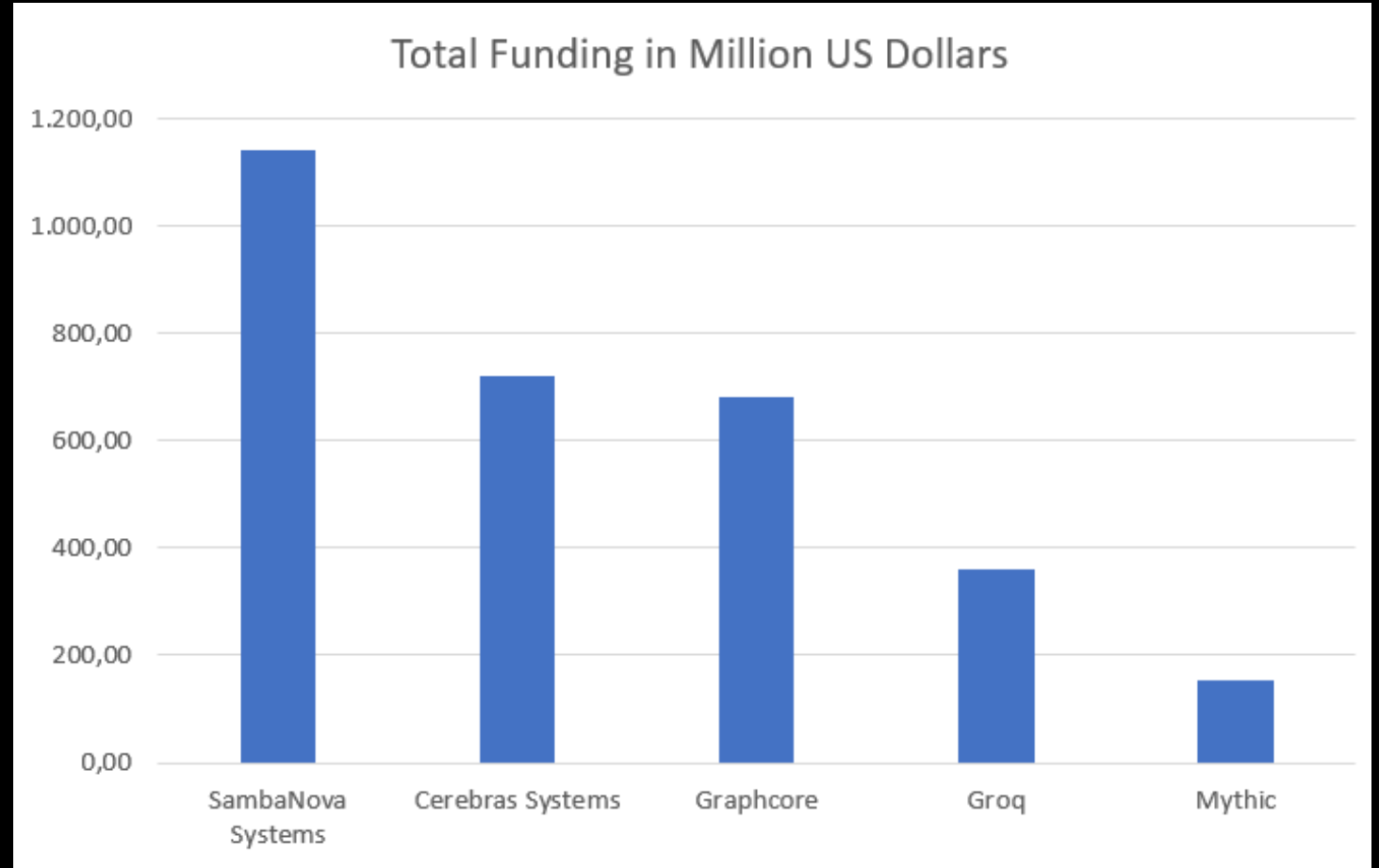
Amazon (Echo, Oculus)

Google (TPU, Pixel)

Apple (SoCs)

Microsoft (“AI chip”)

Not everyone is selling those chips!



Graphcore, Nervana Cerebras, Wave Computing, Horizon Robotics, Cambricon, DeePhi, Esperanto, SambaNova, Eyeriss, Tenstorrent, Mythic, ThinkForce, Groq, Lightmatter

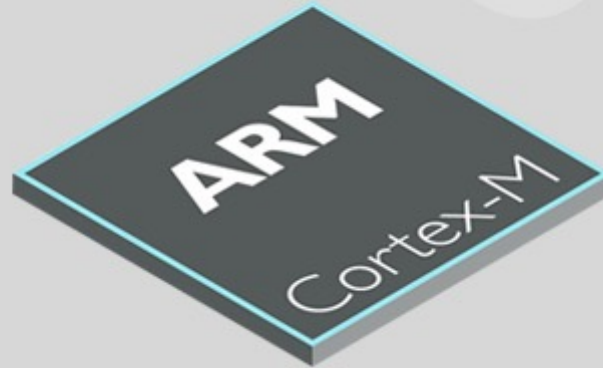
Specialization for the masses?

 **RISC-V**



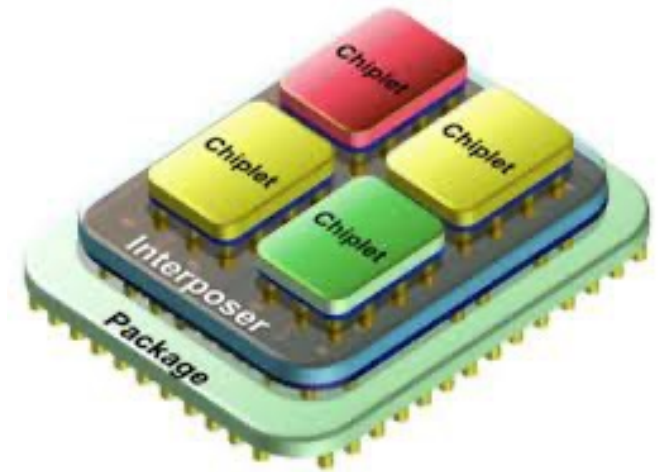
RISC-V Architecture

ARM[®]



ARM Architecture

Chipllets



Technology and Marketplace: Radically Different!

What's a post-Exascale strategy for the science community?

Beat them

- Design processors for science

*More Co-Design and
don't forget the math and software*

Join them

- Leverage AI Hardware

*for AI in Science
and Simulation ?*

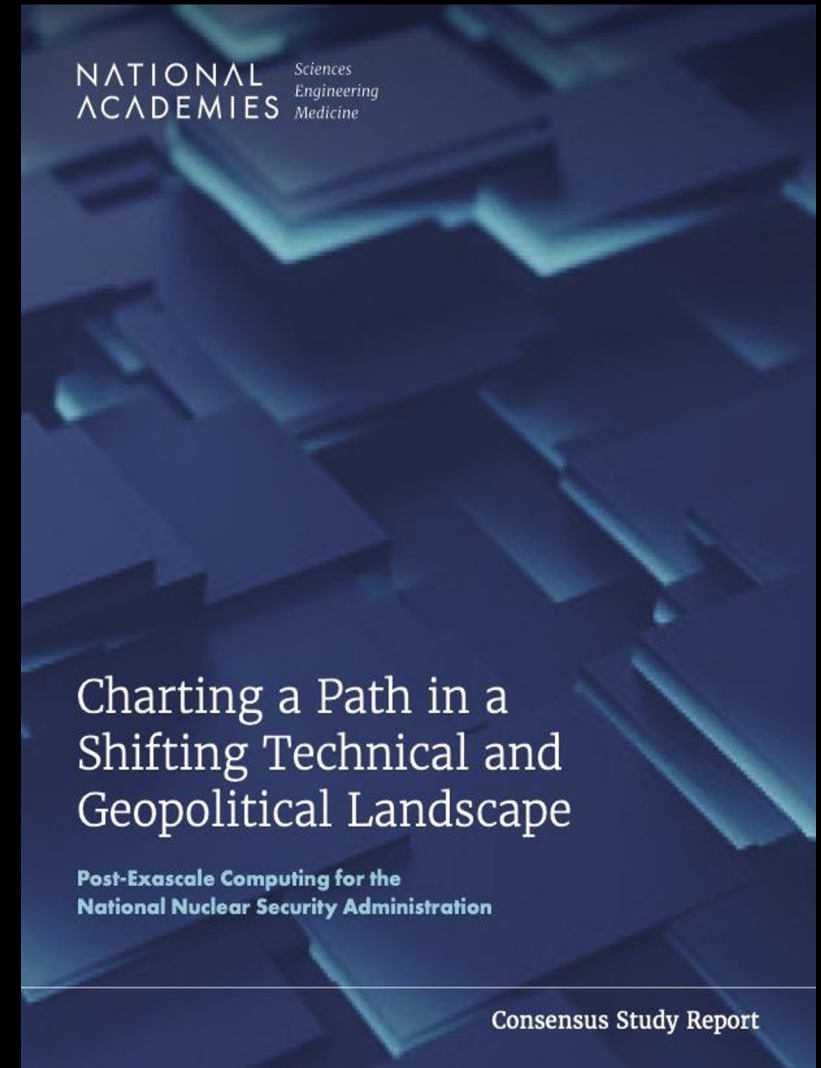


Workforce



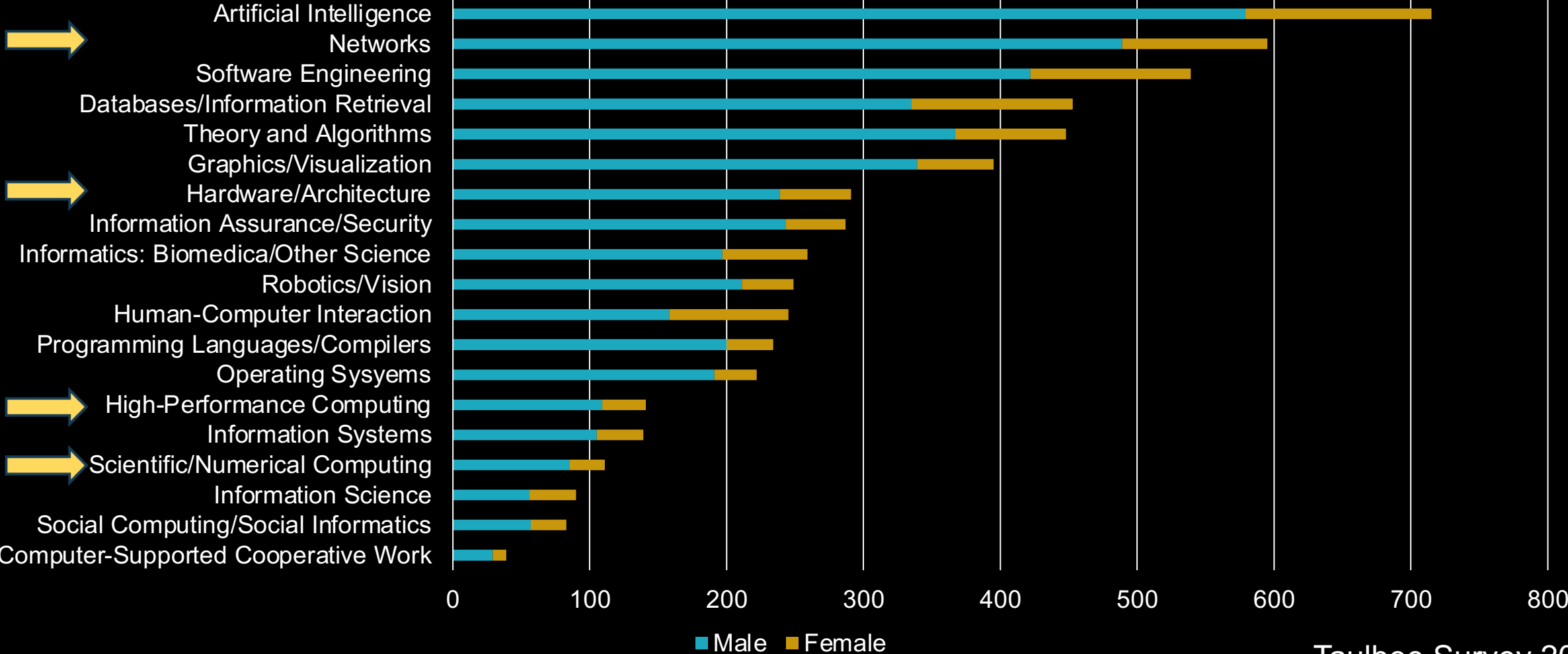
Finding: The NNSA laboratories face significant challenges in recruiting and retaining the highly creative workforce that NNSA needs, owing to competition from industry, a shrinking talent pipeline, and **challenges in hiring diverse and international talent.**

- The U.S. national security enterprise has benefited enormously from **inclusion of global talent.**



Where are the US Computer Science PhDs student doing?

PhDs by Specialty



STEM Graduates Around the World

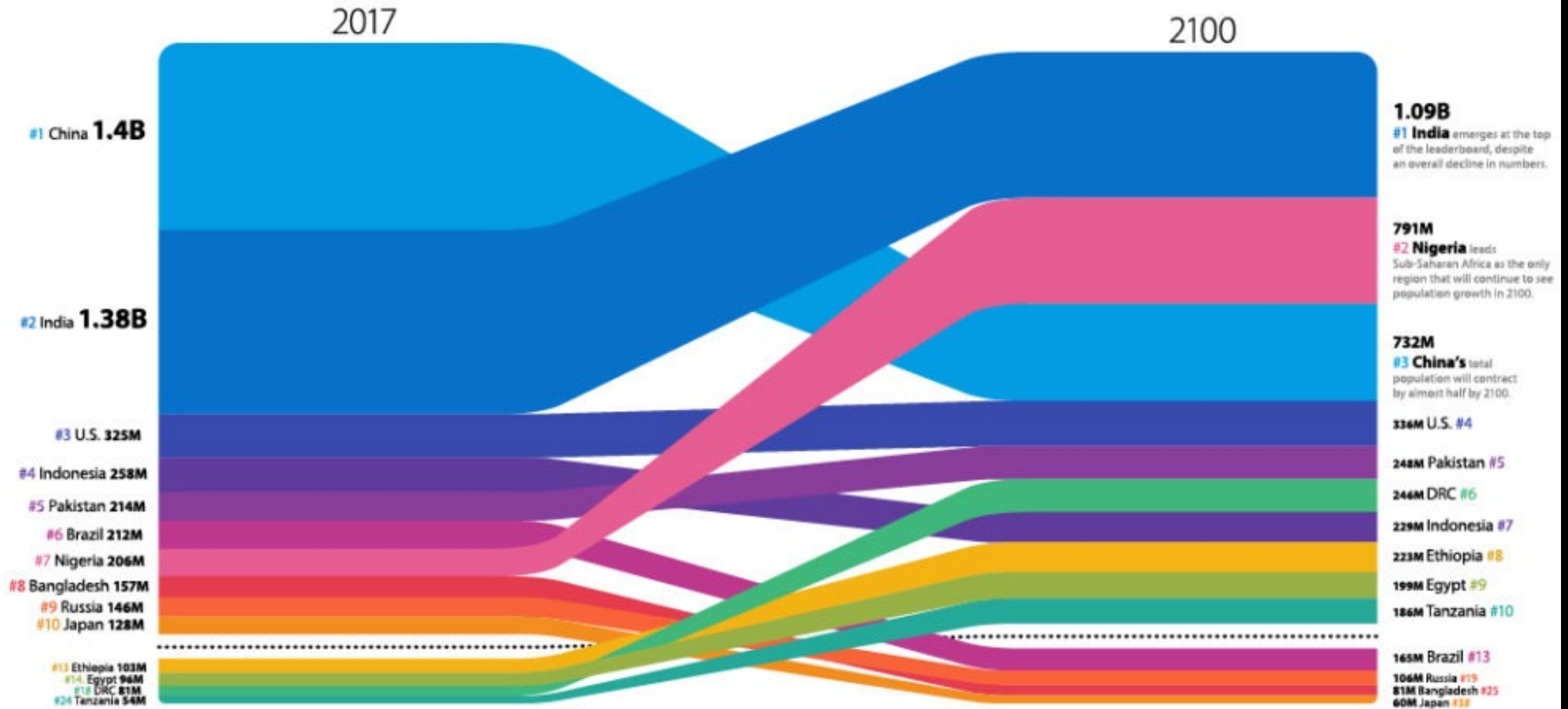
THE COUNTRIES WITH THE MOST STEM GRADUATES

Recent graduates in Science, Technology, Engineering & Mathematics (2016)

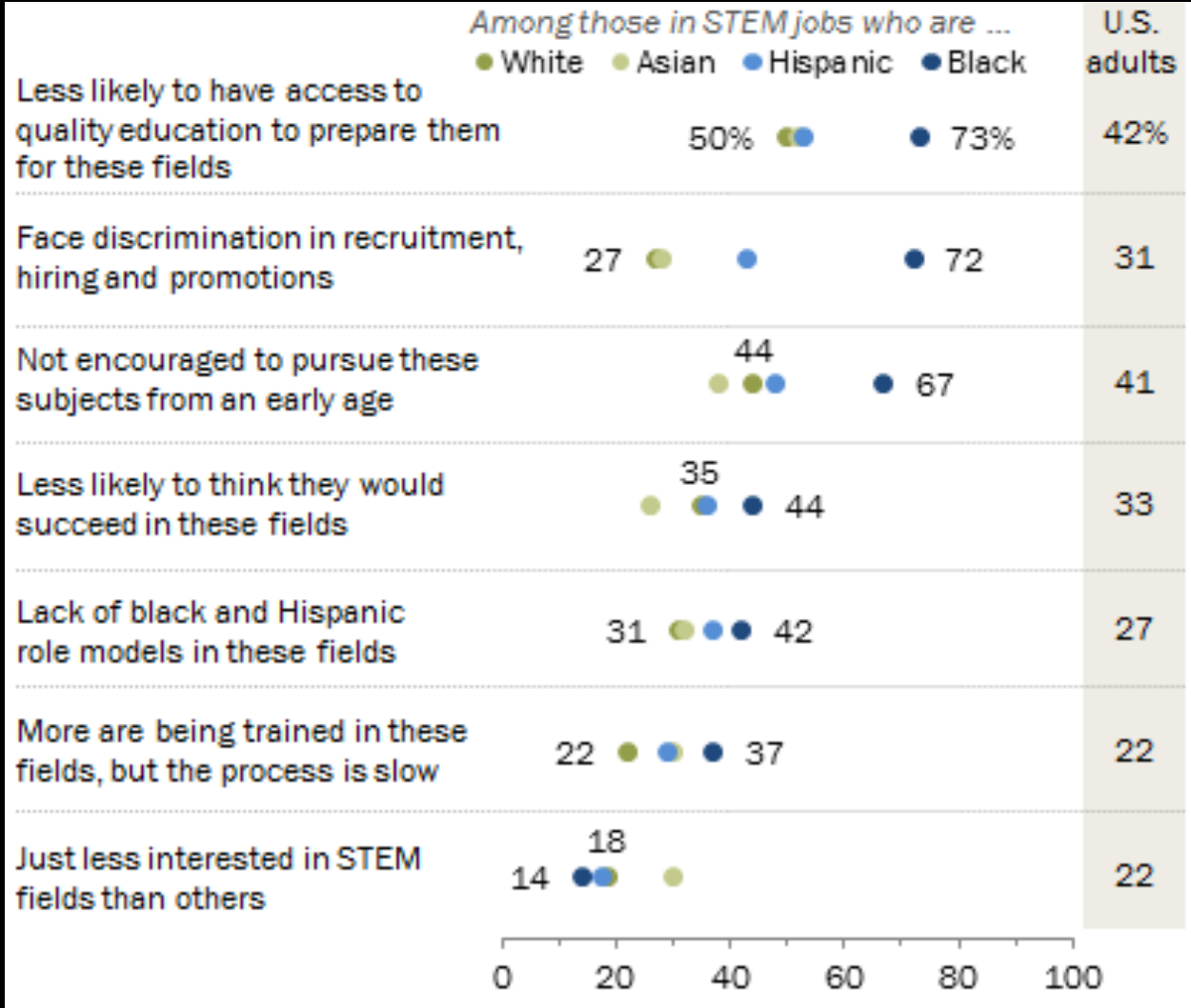


Source: World Economic Forum

Top 10 Countries by Population



Reasons are Systemic



Wide racial and ethnic gaps among STEM employees on why so few blacks and Hispanics work in the field

% of those in science, technology, engineering and math jobs who say each of the following is a major reason why blacks and Hispanics are underrepresented in STEM jobs in this country

Note: Whites, blacks and Asians are non-Hispanic only; Hispanics are of any race. Respondents who gave other responses or who did not give an answer are not shown. Source: Survey of U.S. adults conducted July 11-Aug. 10, 2017.

"Women and Men in STEM Often at Odds Over Workplace Equity"

PEW RESEARCH CENTER

Using Scientific Computing (Broadly) to Attract and Retain Talent



UC Berkeley
EECS
Lecturer SOE
Dan Garcia

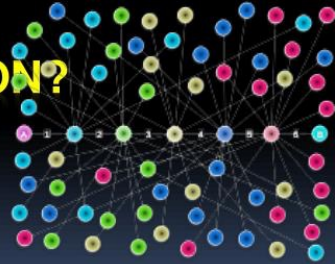
CS10 The Beauty and Joy of Computing

Lecture #23 : Limits of Computing

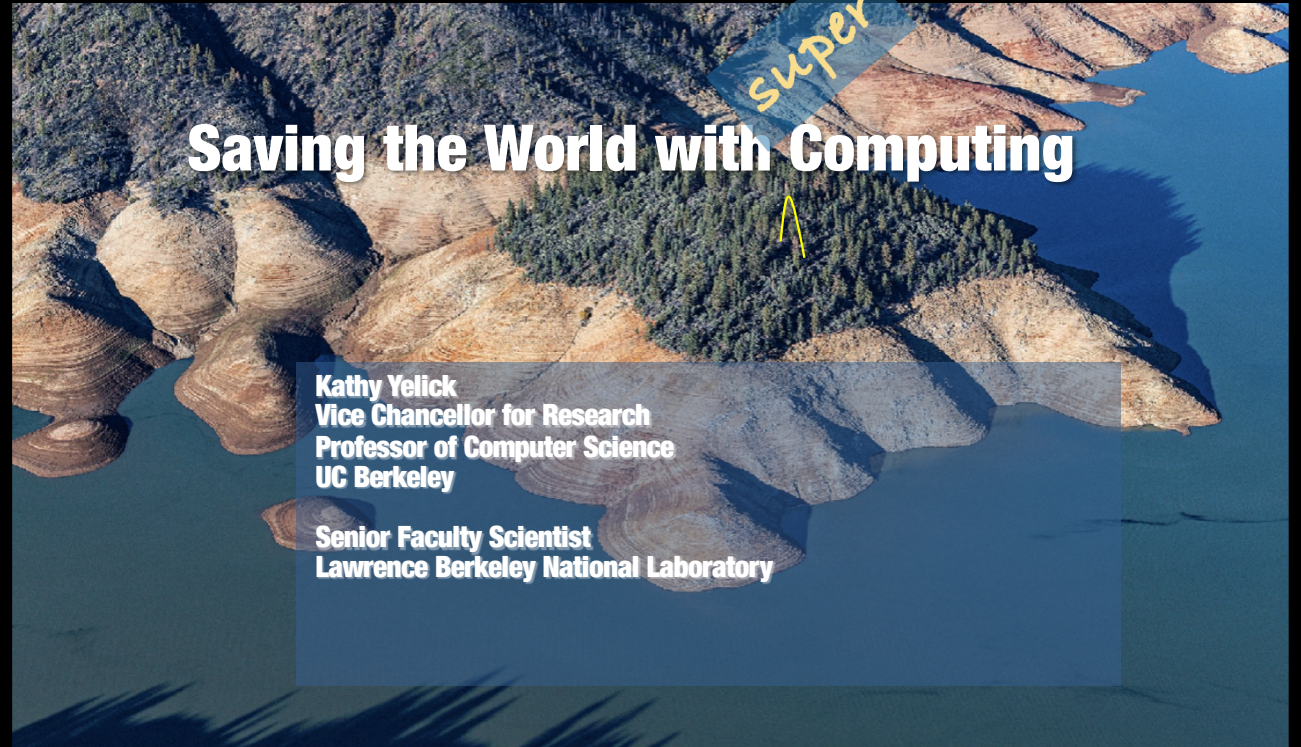
2011-11-23

4.74 DEGREES OF SEPARATION?

Researchers at Facebook and the University of Milan found that the avg # of “friends” separating any two people in the world was < 6 .



<http://www.nytimes.com/2011/11/22/technology/between-you-and-me-4-74-degrees.html>



Often over 50% women with (relatively) high representation of other historically underserved groups

Post Exascale Computing: Not Business as Usual

- **Computing demands** continue to grow
- The benefits of more **weak scaling** are limited
- **Computing technology** has hit several “walls”
- The **computing industry** has changed dramatically
- **AI methods** are having huge impacts elsewhere
- **Quantum computing** potential for science still unknown
- **Cloud computing** is dominating the computing industry
- **Global supply chain** issues present uncertainties