

Beyond Exascale Computing

Kathy Yelick

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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

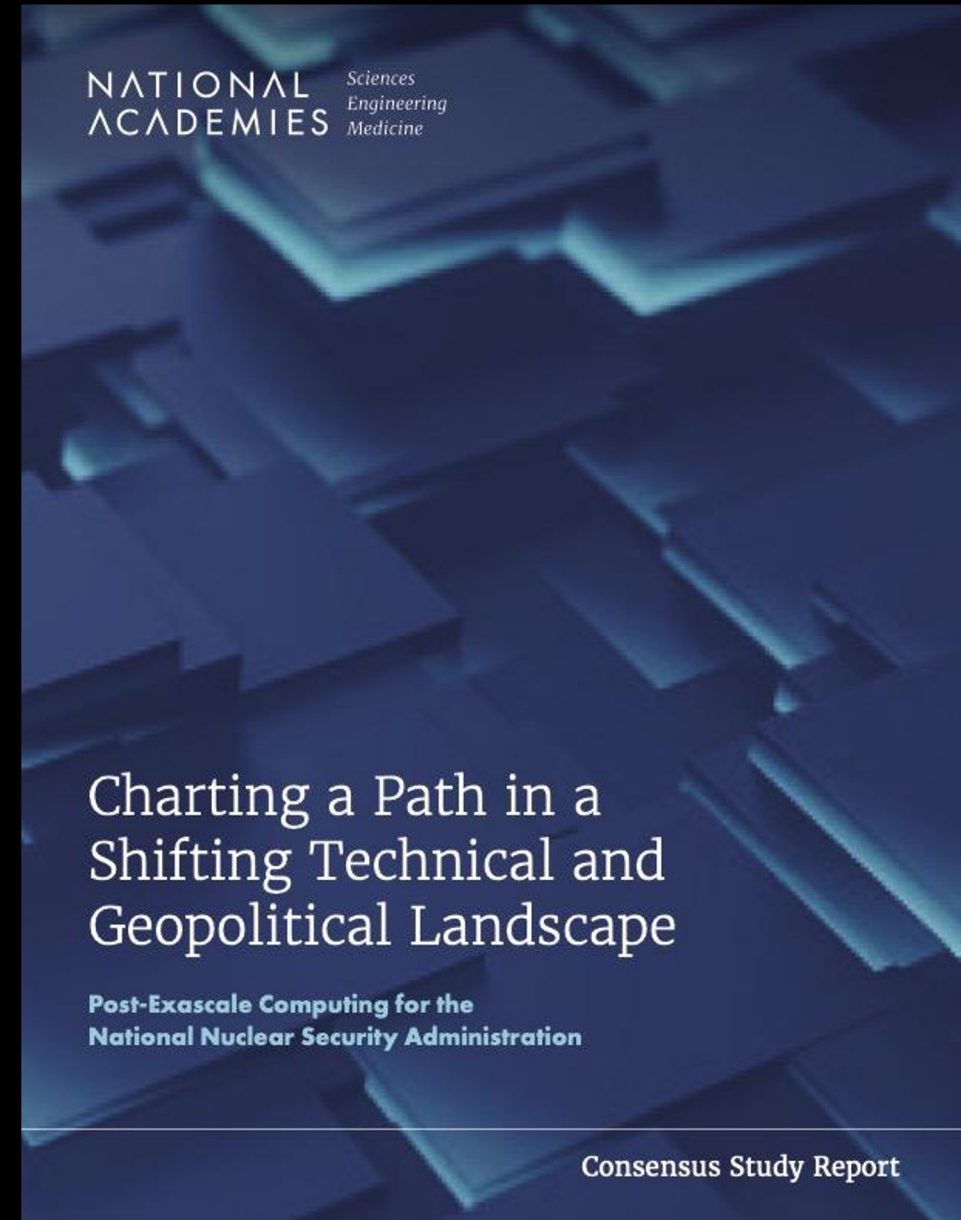
Charlie McMillan

Dan Meiron

Daniel Reed

Karen Willcox

(report at www.cstb.org)



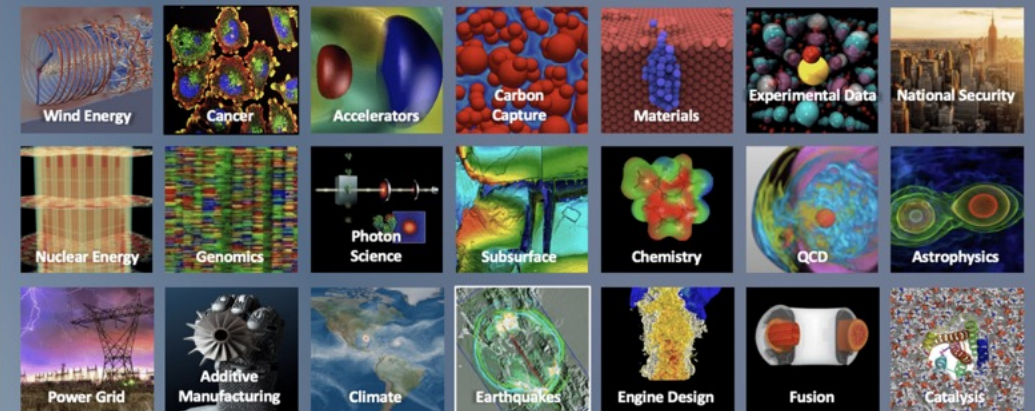
DOE ASCR Report

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

Is this Exascale all over again?



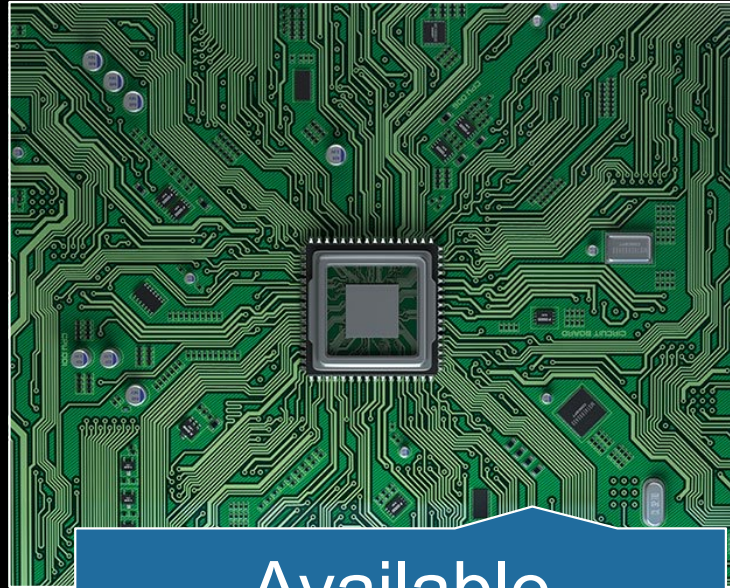
The more things change, the
more they stay the same.

~ Alphonse Karr

Post-Exascale Computing



Computing
demand

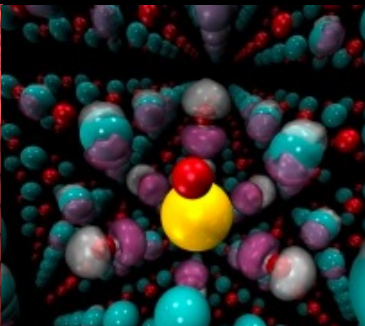
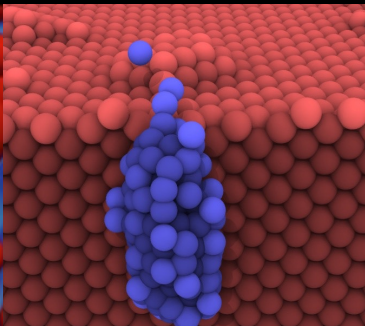
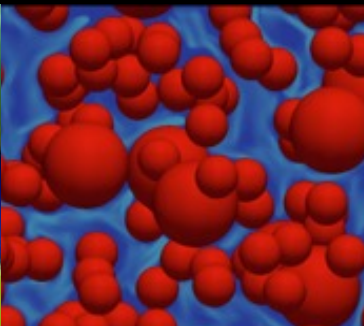
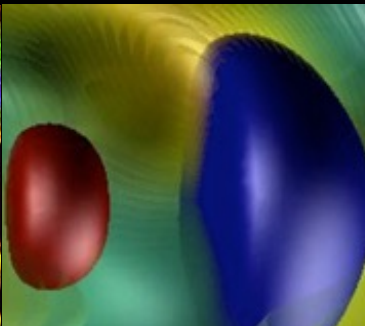
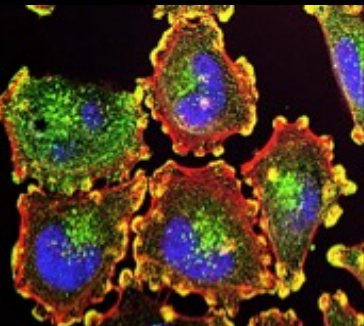
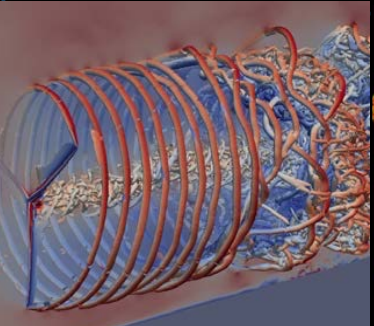


Available
technology

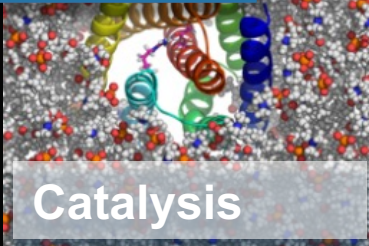
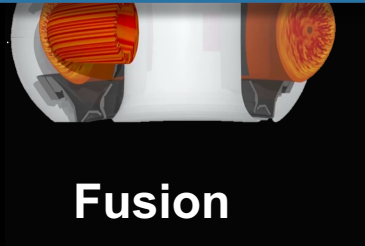
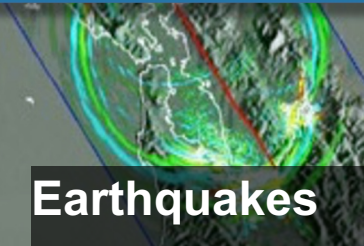
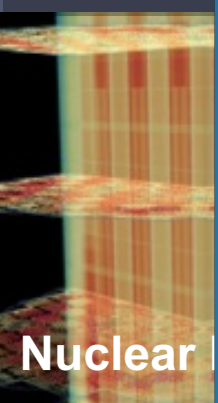


Disruptions

Continue to Rethink Applications



Wind E



- 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

Additive
Manufacturing

Climate

Earthquakes

Combustion

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

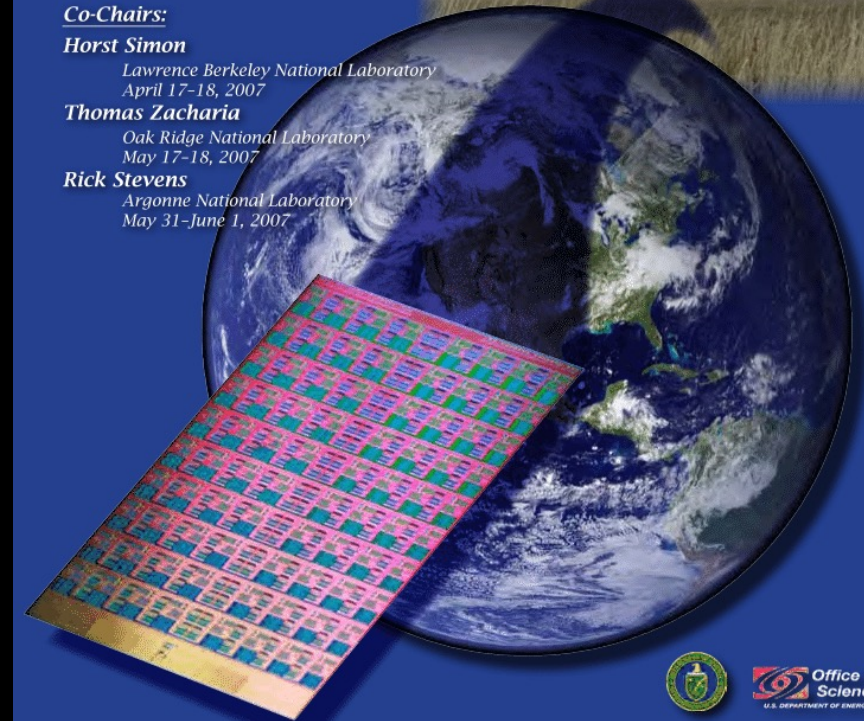
*Lawrence Berkeley National Laboratory
April 17-18, 2007*

Thomas Zacharia

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

Rick Stevens

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



Office of
Science
U.S. DEPARTMENT OF ENERGY

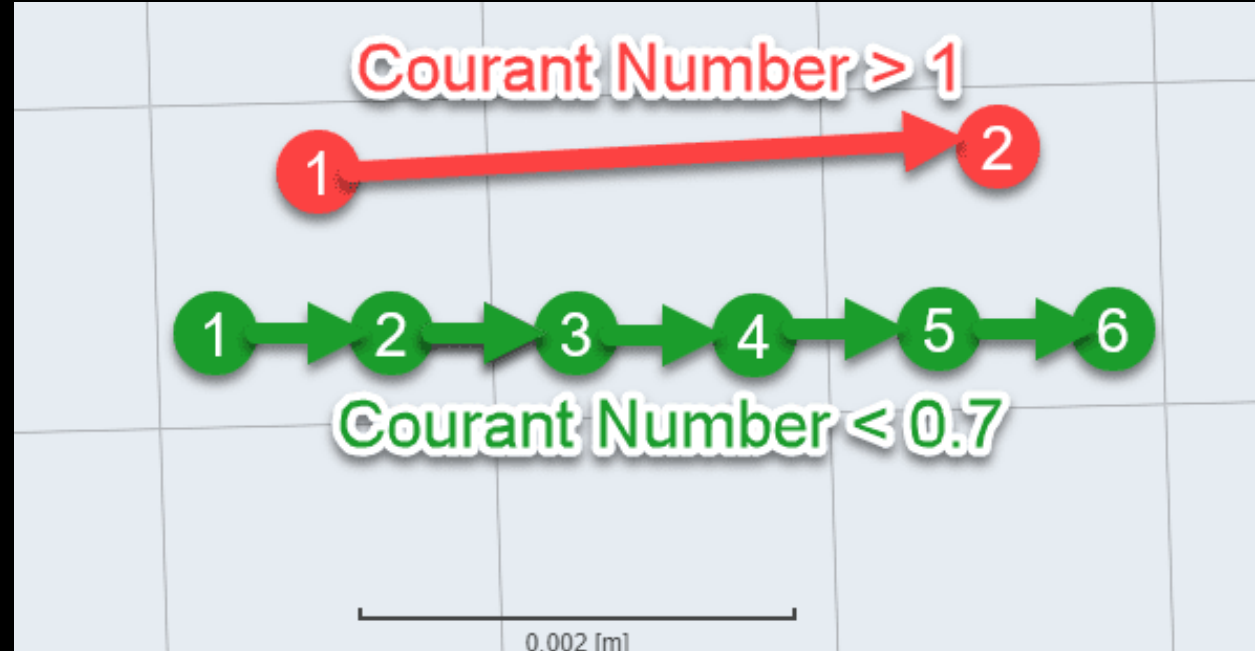
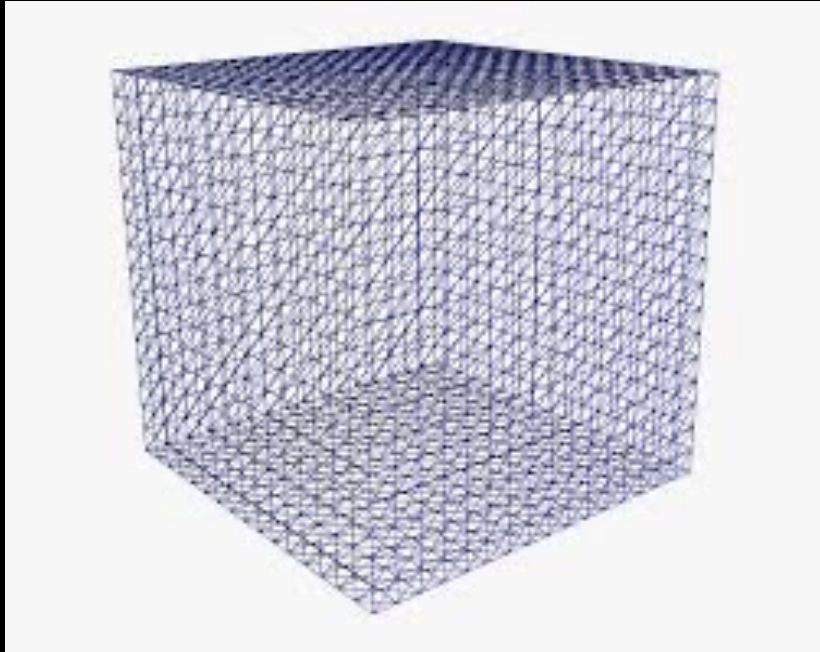


Runtime of “hero” calculations are too long

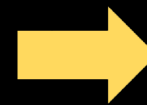
Number of Nodes	Memory Footprint	Wall-Clock Time
2400	~300–400 TB	6 months
4990	~600 TB	3–4 months
288	~20 TB	1 month
3250	104 TB	5.8 days
512	32.8 TB	2 months

Iterative design
does not happen on
6 month cycles

Weak Scaling has Diminishing Returns

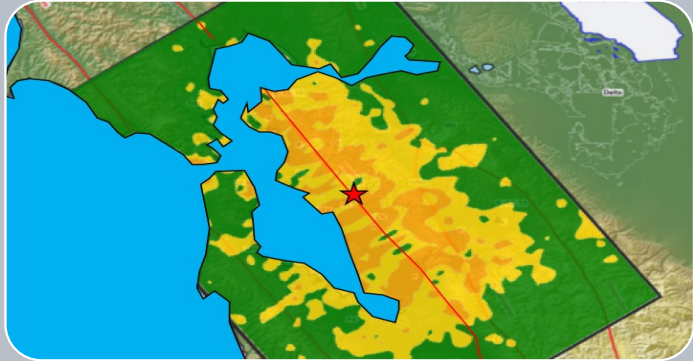


Increase resolution by 10x in each dimension
Increase cores by 1000x



Runtime increases ☹️

New demands for HPC in Science



Simulation

From atoms to the universe



Data

Images, text, to genomes



Learning

Interpret, infer and automate

JGI User Science and ExaBiome's MetaHipMer Assembler

Peatland bog
(0.6 TB)



Mycorrhizal
fungi (1.5 TB)



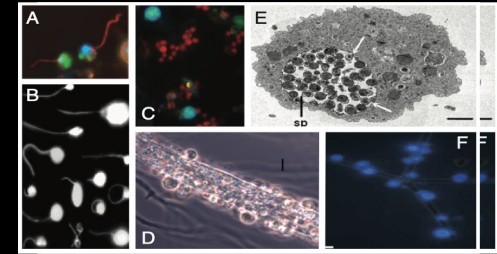
Prescribed fire
(1.5 TB)



Subtropical
soils (1.5 TB)



Dark matter
fungi (1.7 TB)



Coastal
mangroves
(2.1 TB)



Mountainous
watershed (2.7
TB)



Soil carbon
cycle (3.3 TB)



Great Redox
Experiment
(8TB)



Lake Mendota
Time Series (25
TB)

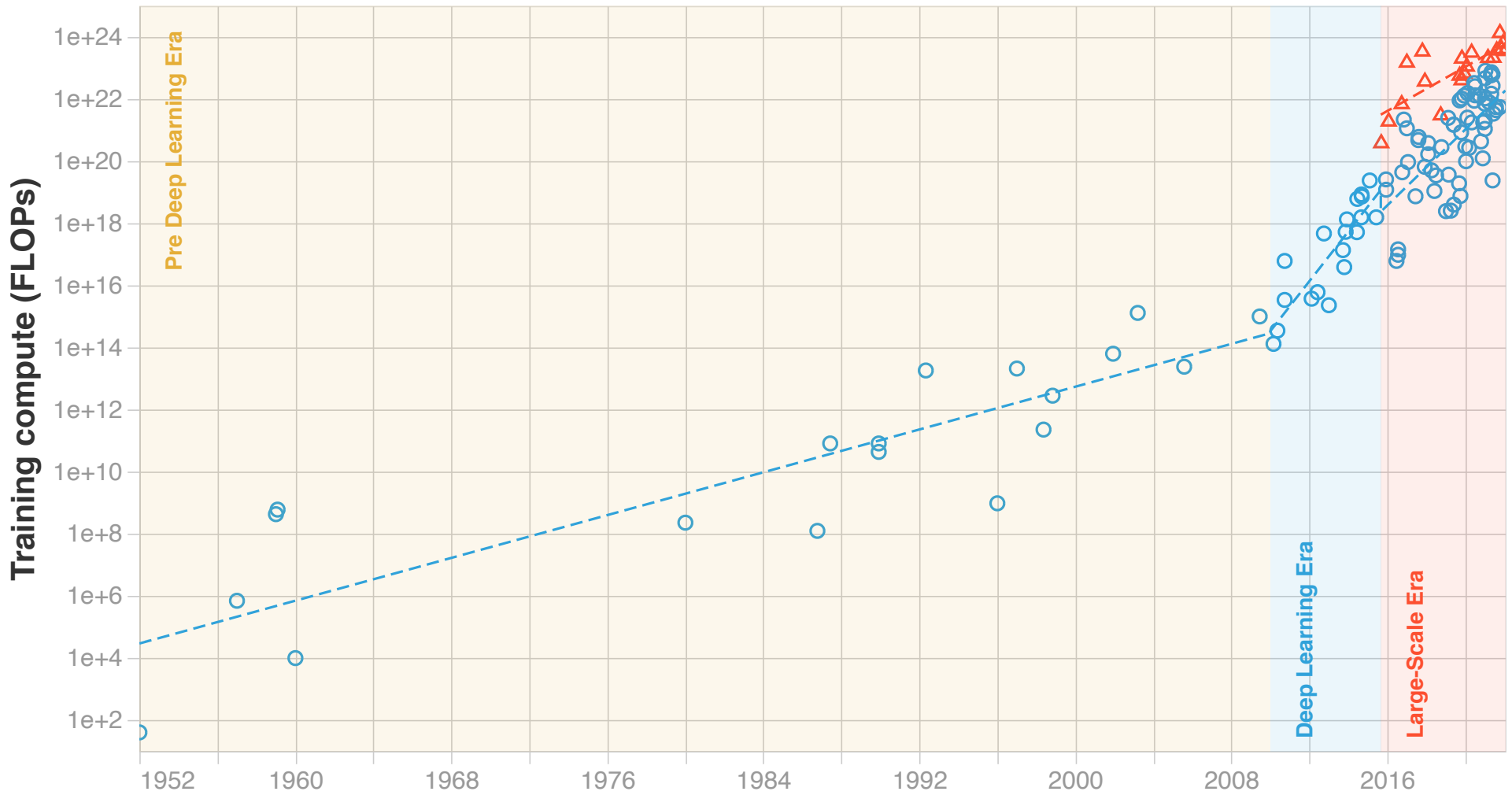


Analyzing huge data sets with exascale tools lead to discovery of new species and protein families ... new science!

Machine Learning Drives Computational Demand

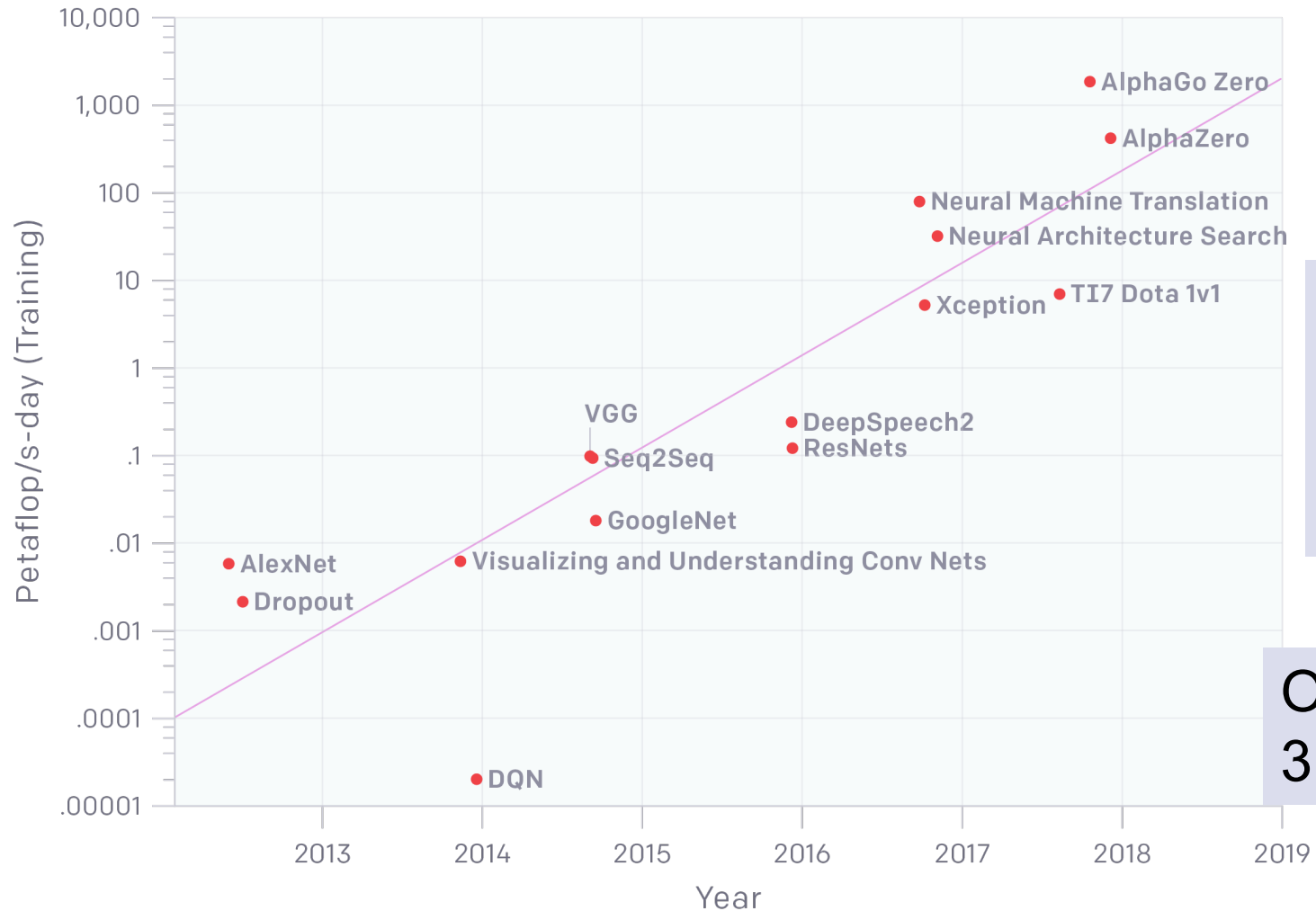
Training compute (FLOPs) of milestone Machine Learning systems over time

n = 121



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 =
 10^{15} neural net
operations per
second for one
day, \sim
 10^{20} operations

Reproducibility and Efficiency in Science through Cloud Labs



“Plugging an experiment into a browser forces researchers to translate the exact details of every step into unambiguous code”

<https://www.theguardian.com/>

Automation in Self-Driving Laboratories



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

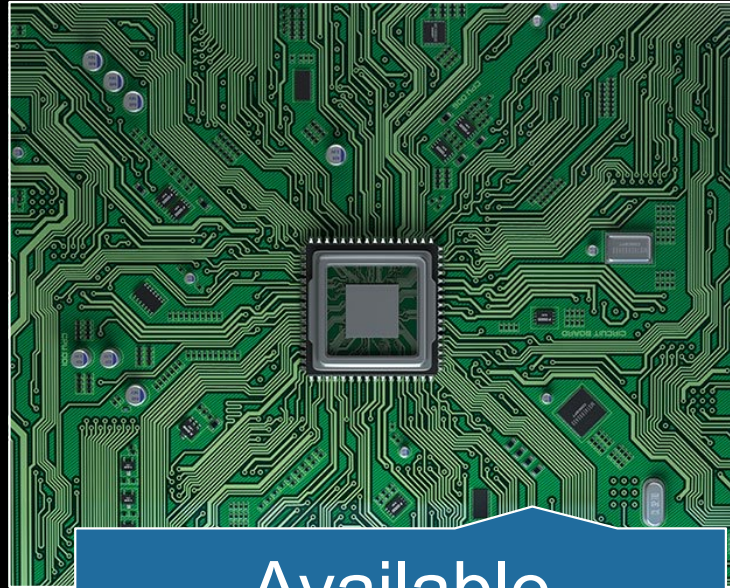


I sense an insatiable demand for computing in science.
This was true pre-exascale and will persist indefinitely.

Post-Exascale Computing



Computing
demand

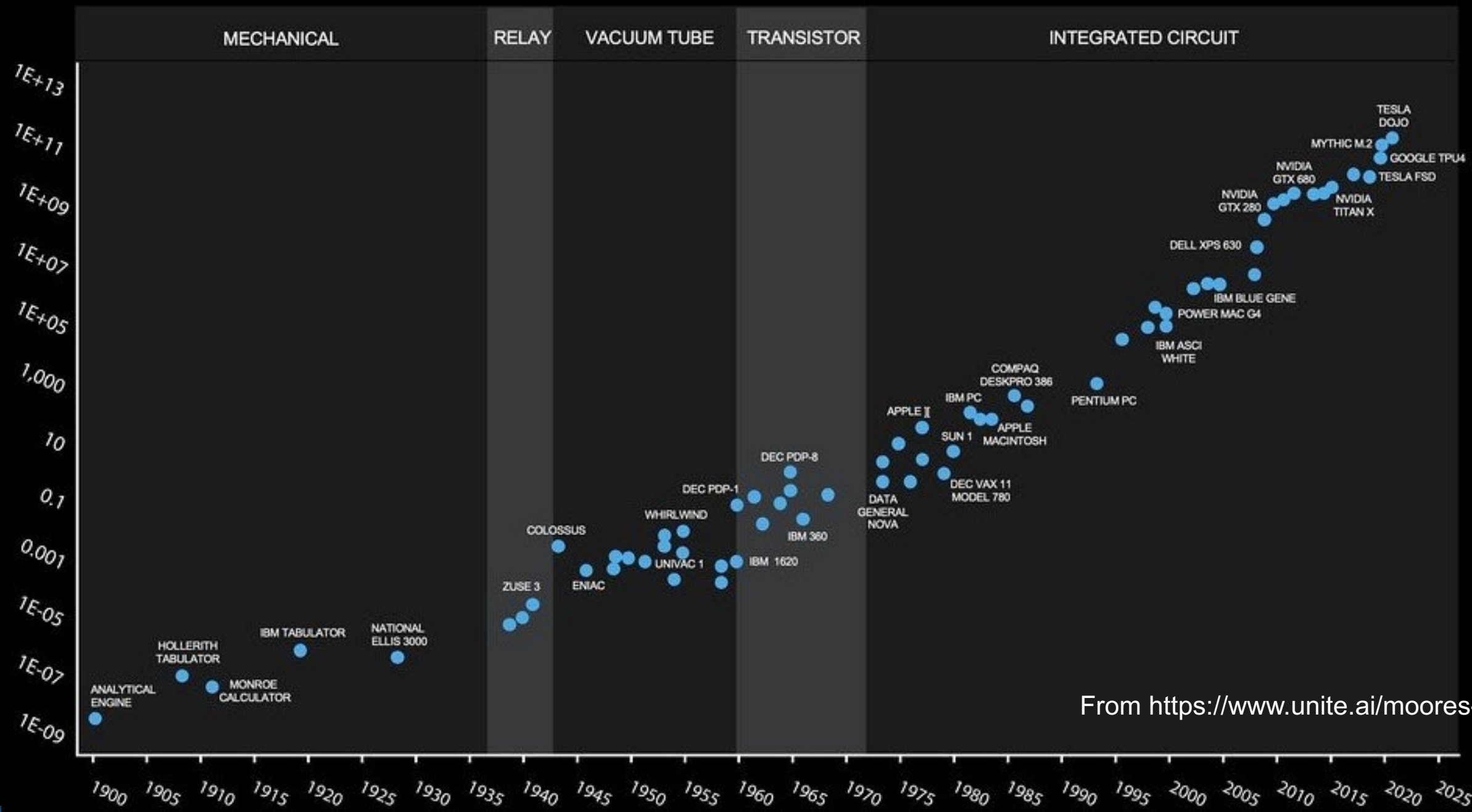


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technology



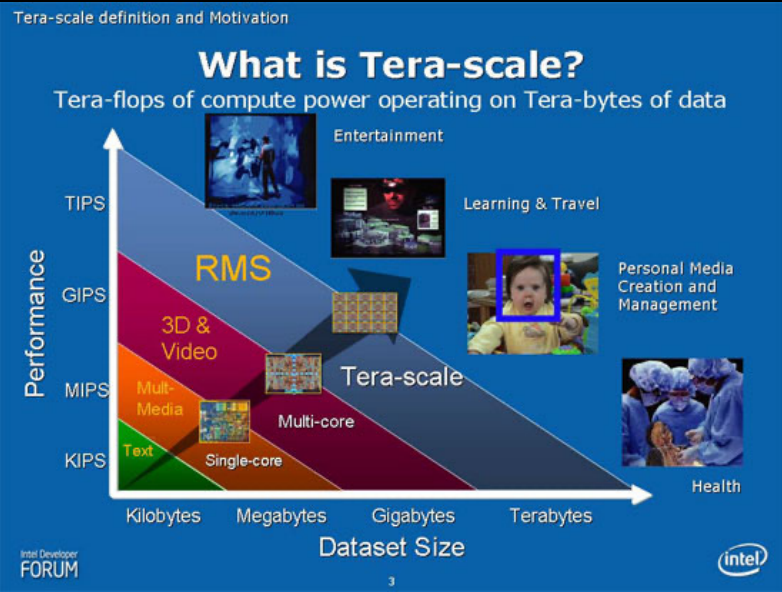
Disruptions

122 YEARS OF MOORE'S LAW



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

It's hard to think exponentially



Scientific Grand Challenges

CROSSCUTTING TECHNOLOGIES FOR COMPUTING AT THE EXASCALE

February 2-4, 2010 • Washington, D.C.

The image shows a perspective view of a long row of server racks in a data center. A large white circle is overlaid on the center, containing a 3D visualization of a complex, interconnected grid or mesh structure, possibly representing a simulation or data visualization. The U.S. Department of Energy logo is in the bottom right.

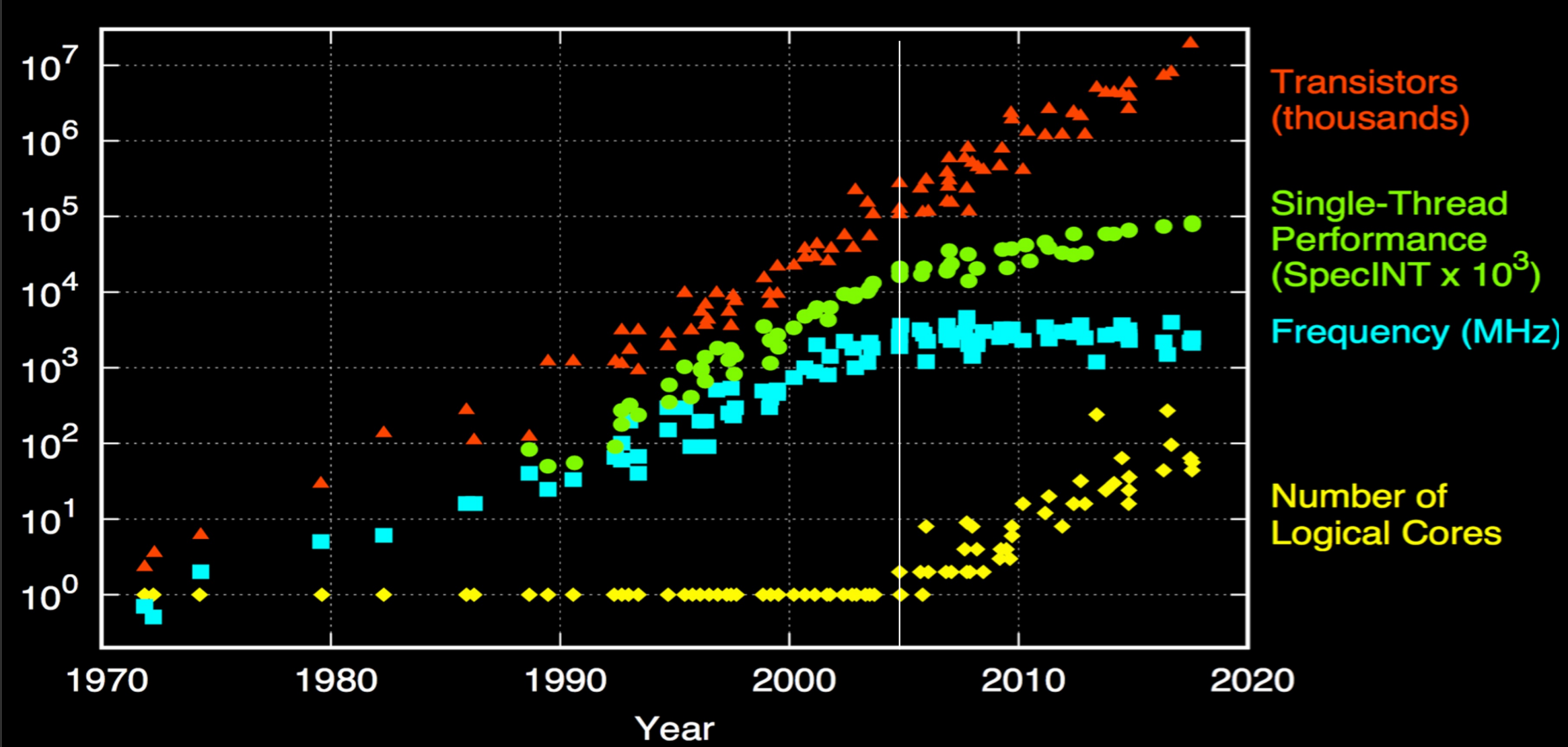
U.S. DEPARTMENT OF ENERGY

Sponsored by:
Office of Advanced Scientific Computing Research, Office of Science
Office of Advanced Simulation and Computing, National Nuclear Security Administration

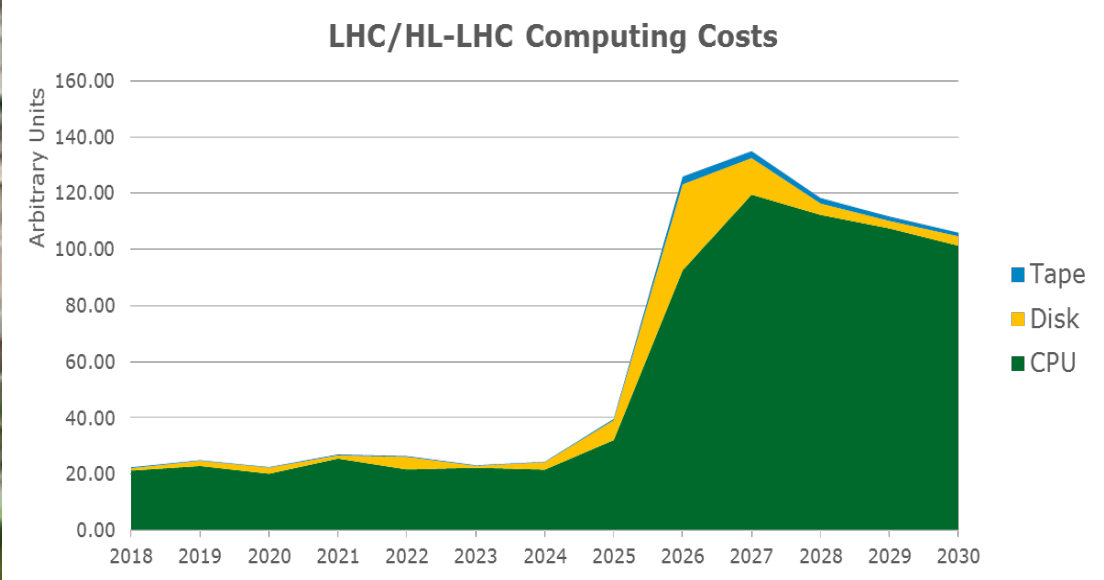
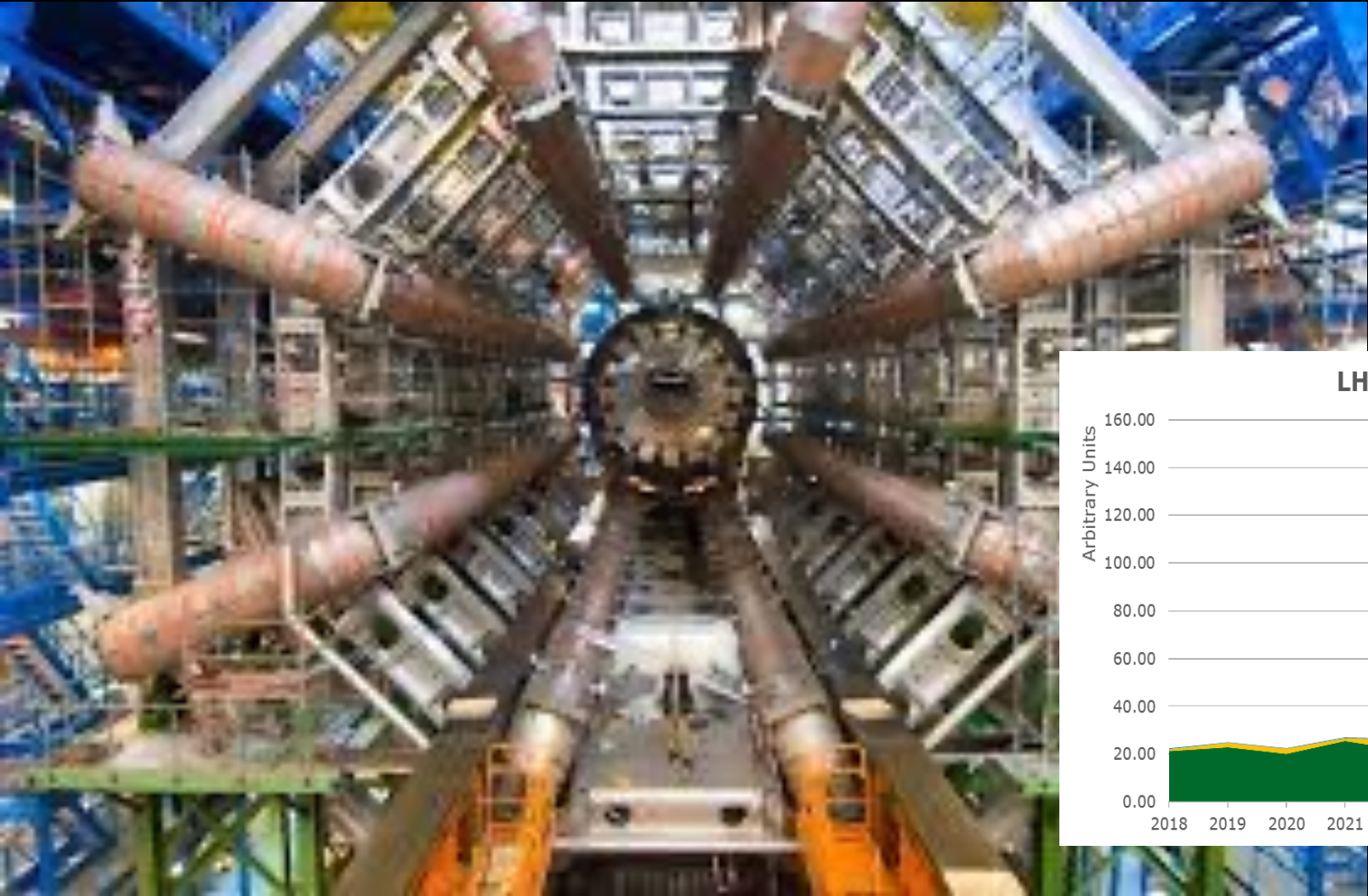


But it's also hard to stop

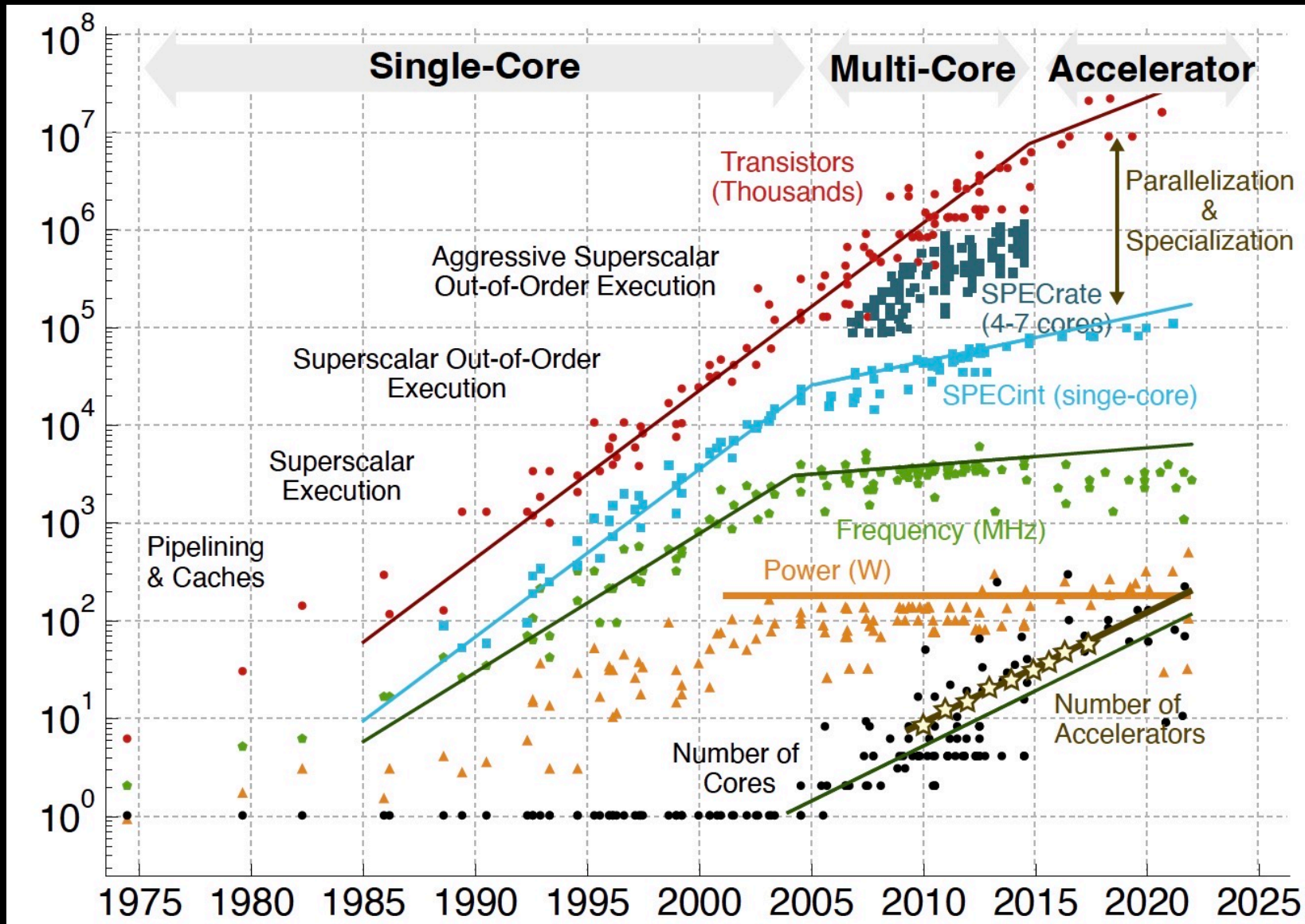
Dennard Scaling is Dead; Moore's Law Will Follow



Prediction of Atlas computing +\$1B



End Game for Moore's Law: Parallelization and Specialization



From Chris Batten, Cornell ENGRI 1210 citing

C. Batten, M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, K. Rupp & [Y. Shao, IEEE Micro'15] & [C. Leiserson, Science'20]

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



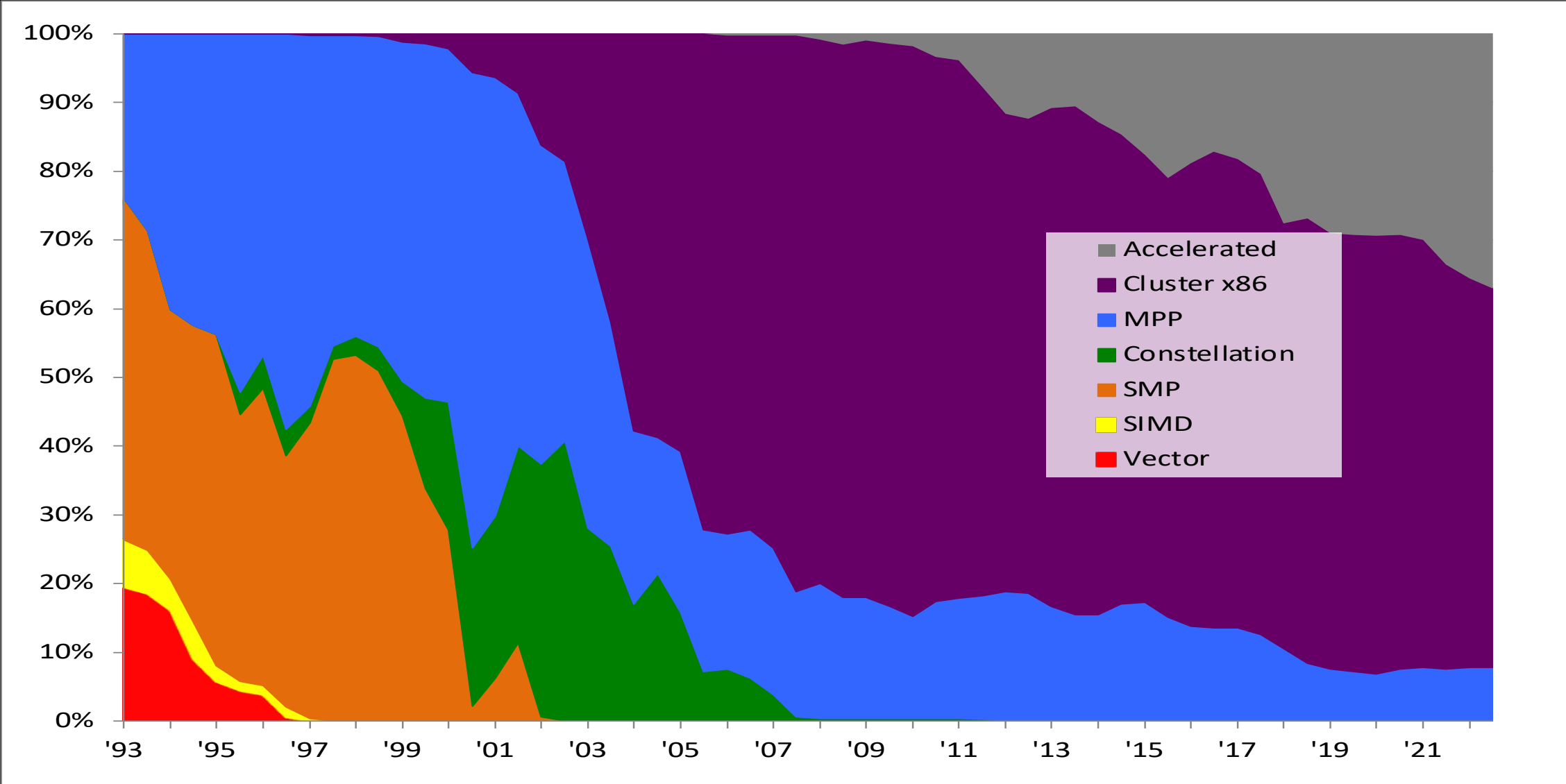
Exascale
HPE Intel+Intel



Pre-exascale
HPE AMD+NVIDIA

1 Architecture (3 GPUs), 1 Integrator!

Growth of Accelerators in HPC



AI Chip Landscape

More on <https://basicmi.github.io/AI-Chip/>

Tech Giants/Systems



IC Vender/Fabless



IP/Design Service



Startup in China



Startup Worldwide



扫码访问AI芯片文章

Compiler



Benchmarks



Everyone is Making AI Chips

NVIDIA

AMD

Intel

IBM

Traditional
chip makers

“Software”
companies

Facebook + Intel

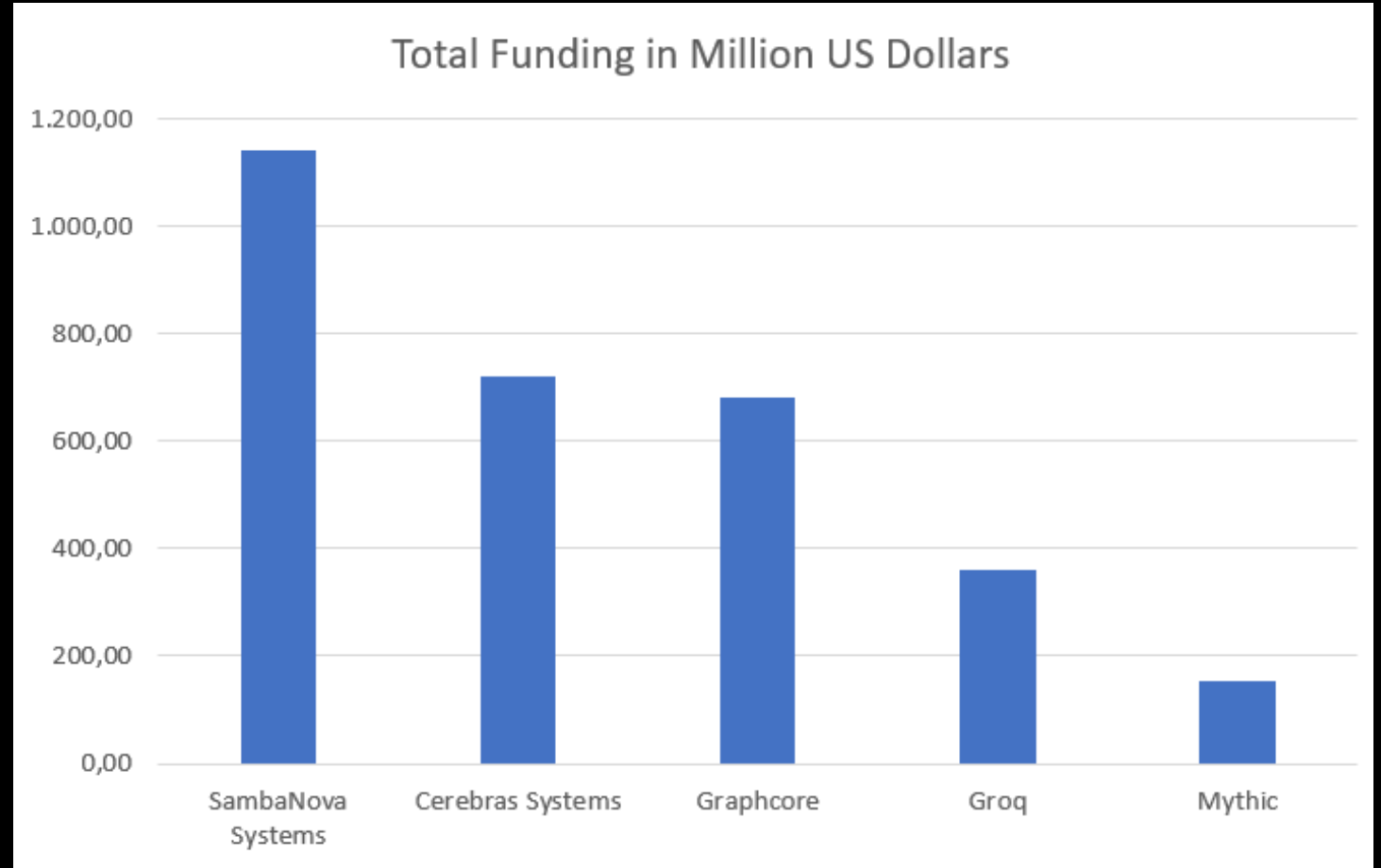
Amazon (Echo, Oculus)

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

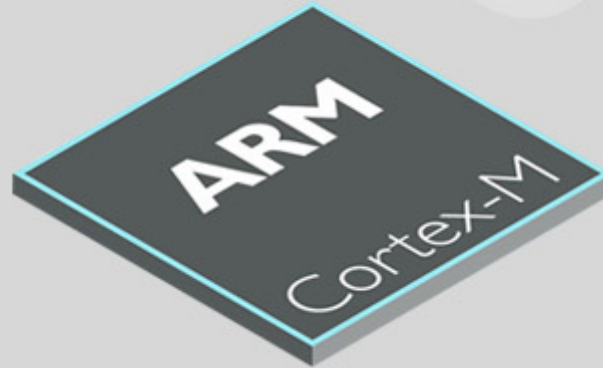
Specialization for the masses?

 RISC-V

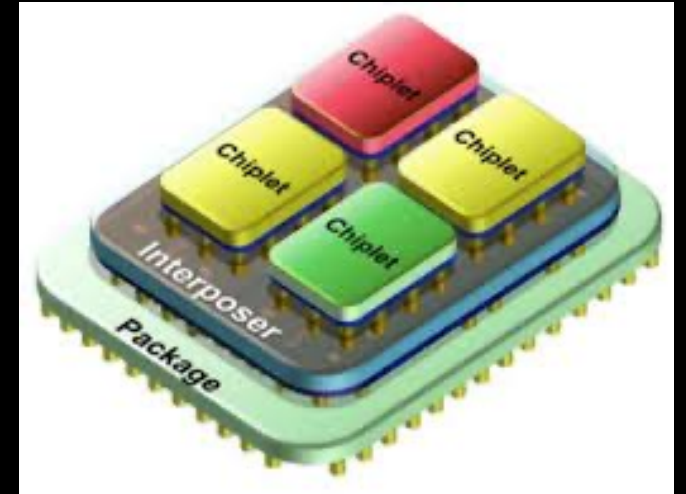


RISC-V Architecture

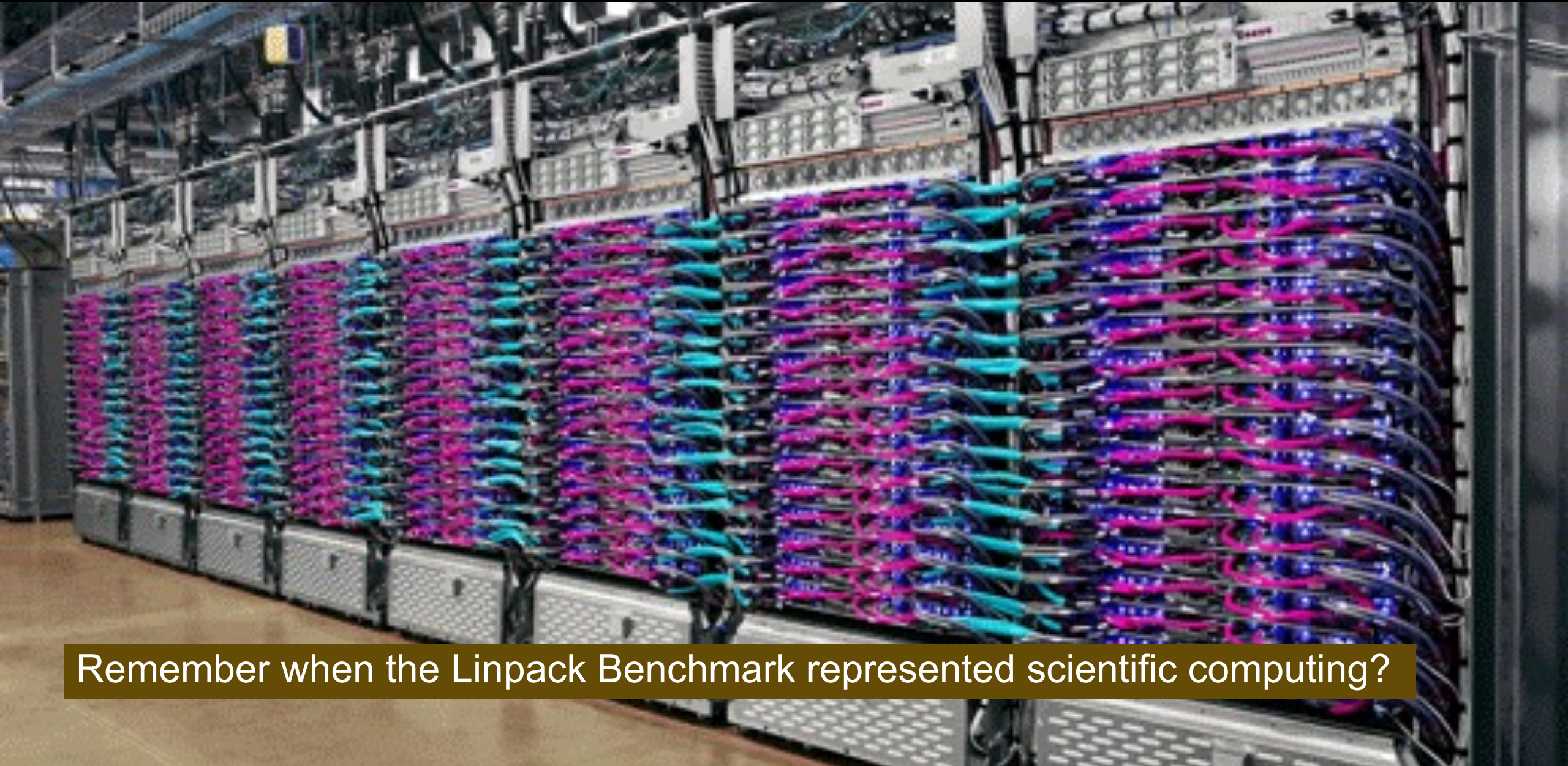
ARM[®]



ARM Architecture



Specialization: Is deep learning the only application?



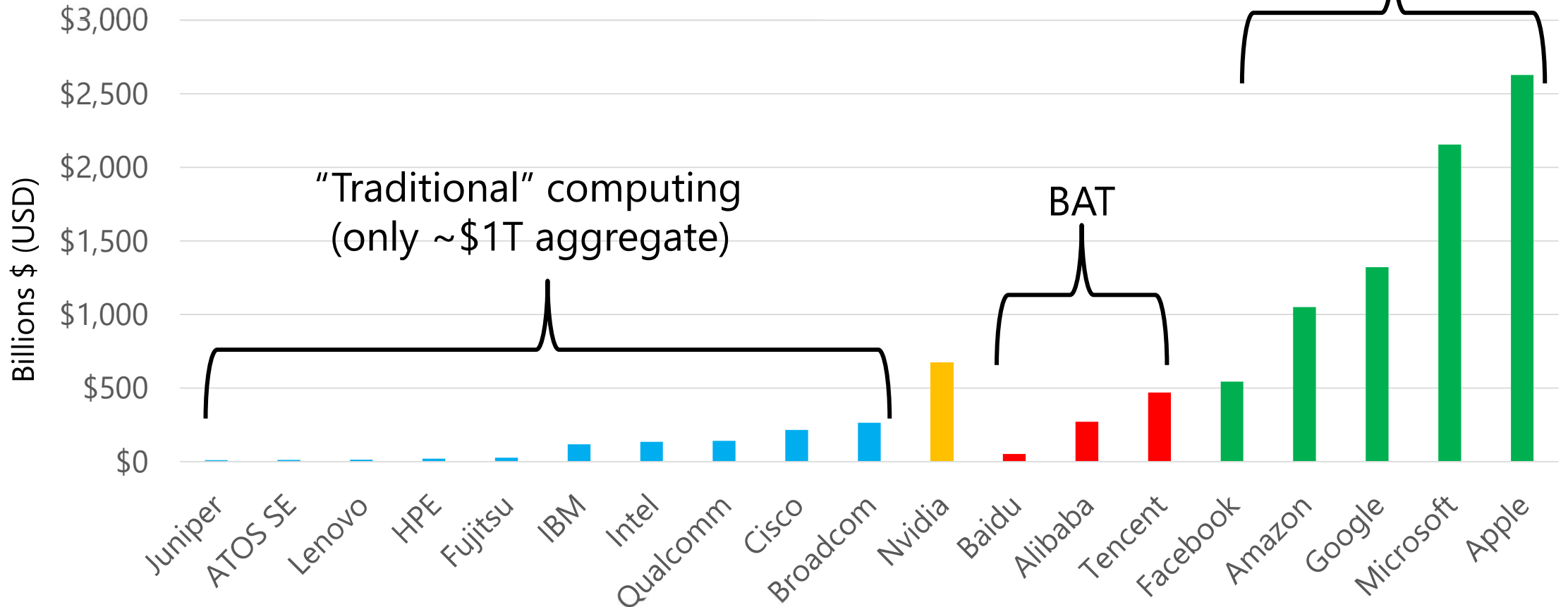
Remember when the Linpack Benchmark represented scientific computing?

Cloud "Hyperscalars" dominate computing

Market capitalizations

One measure of market influence

AI/cloud computing ecosystem
Trillion+ \$ (USD) companies



Source: Dan Reed, U. Utah



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

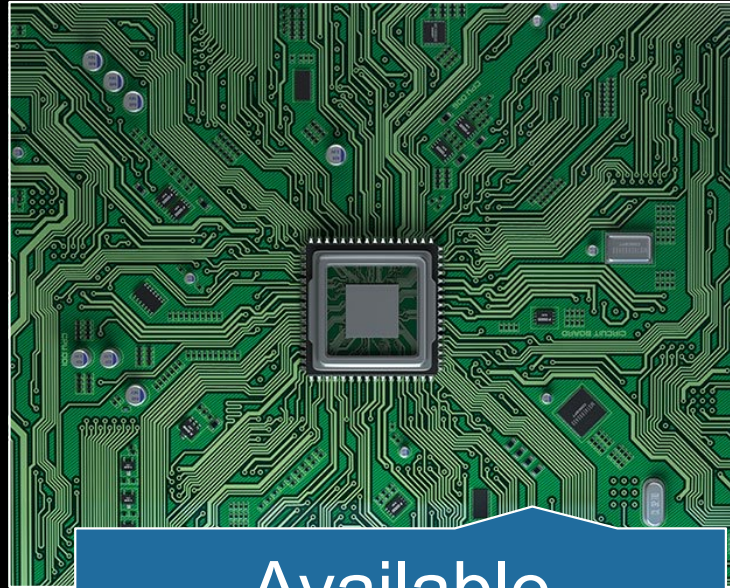
*for AI in Science
and Simulation ?*



Post-Exascale Computing



Computing
demand



Available
technology



Disruptions

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 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

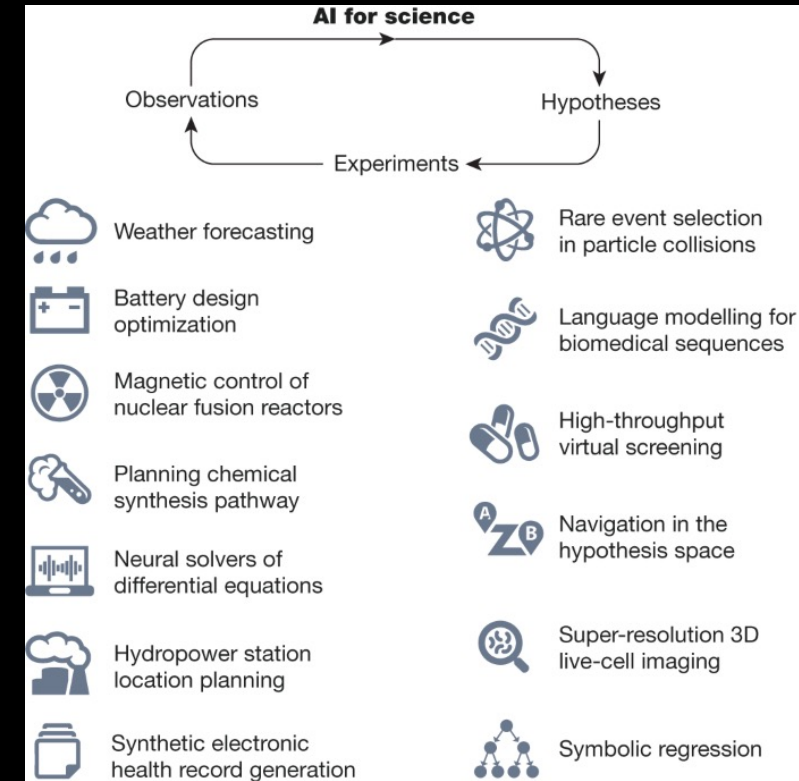
Doug Kothe
Oak Ridge National Laboratory

Rob Neely
Lawrence Livermore National Laboratory

Jason Pruet
Los Alamos National Laboratory

Rick Stevens
Argonne National Laboratory

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



Scientific discovery in the age of artificial intelligence, 2023

Analyze Images to Find Cats

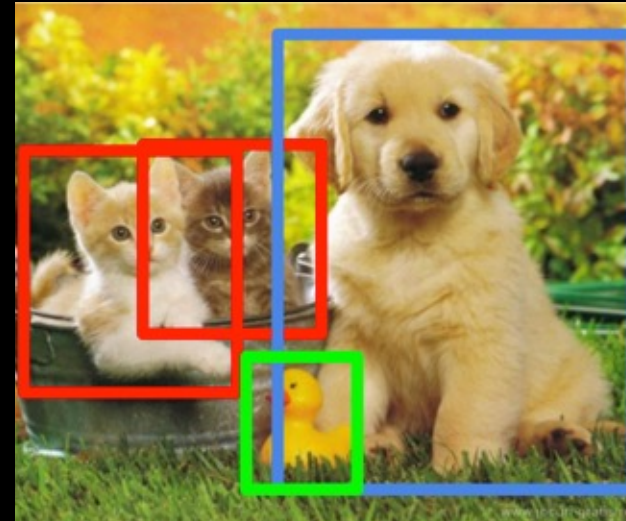
Classification



Localization



Detection

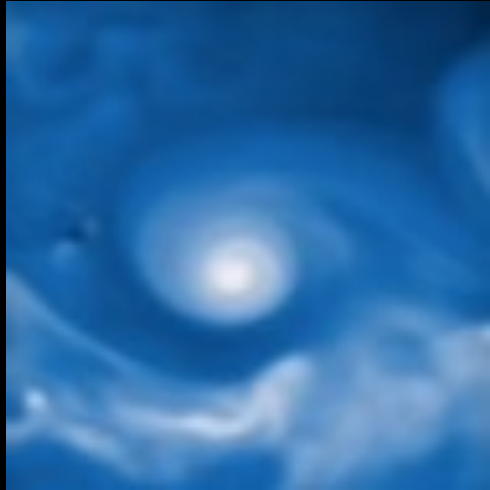


Segmentation

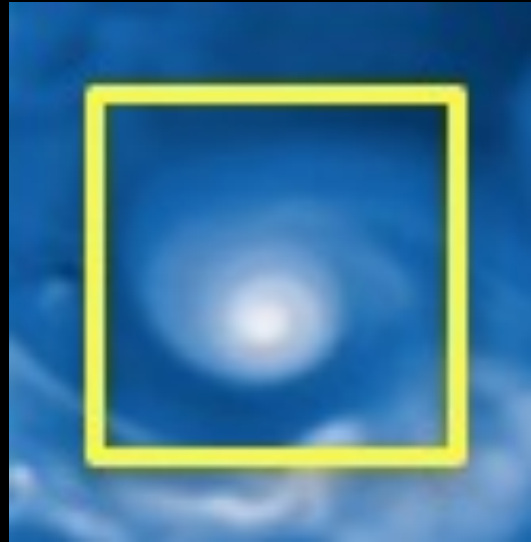


Analyze Simulations to Find Hurricanes

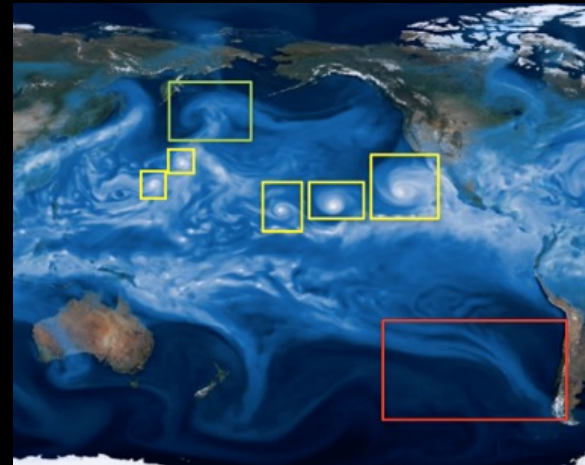
Classification



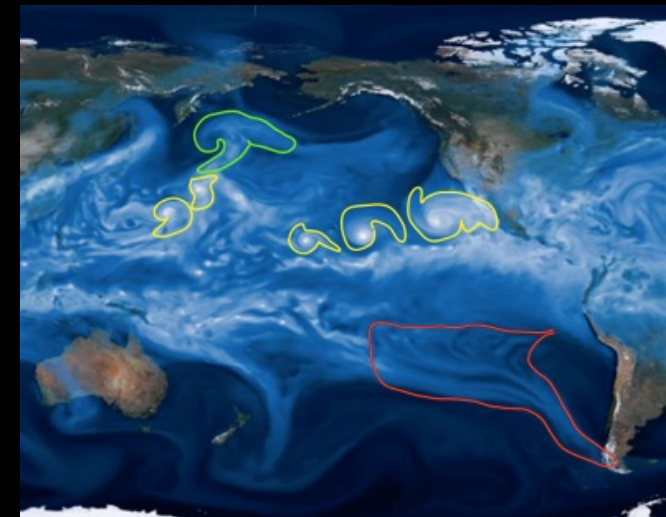
Localization



Detection



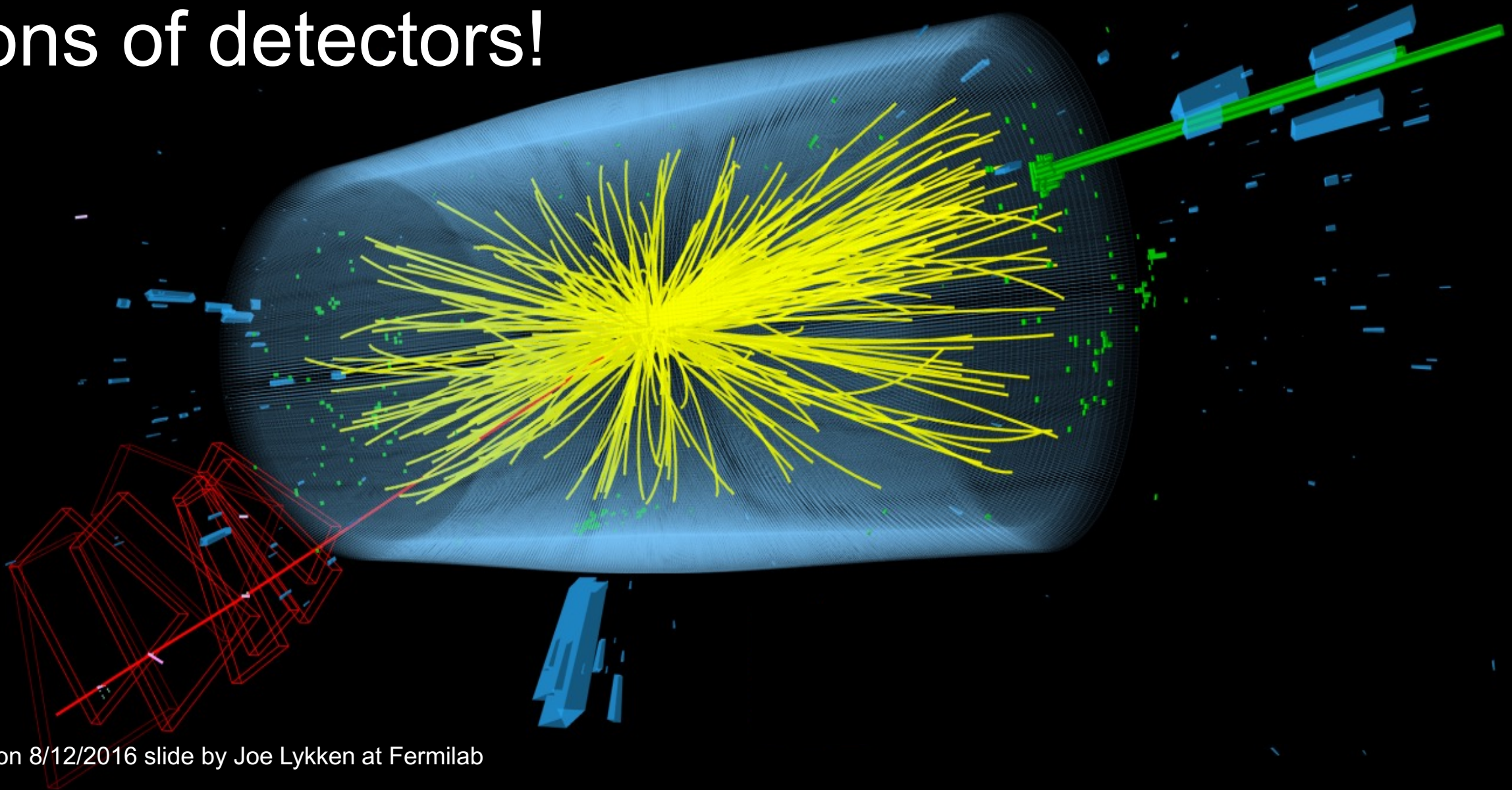
Segmentation



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

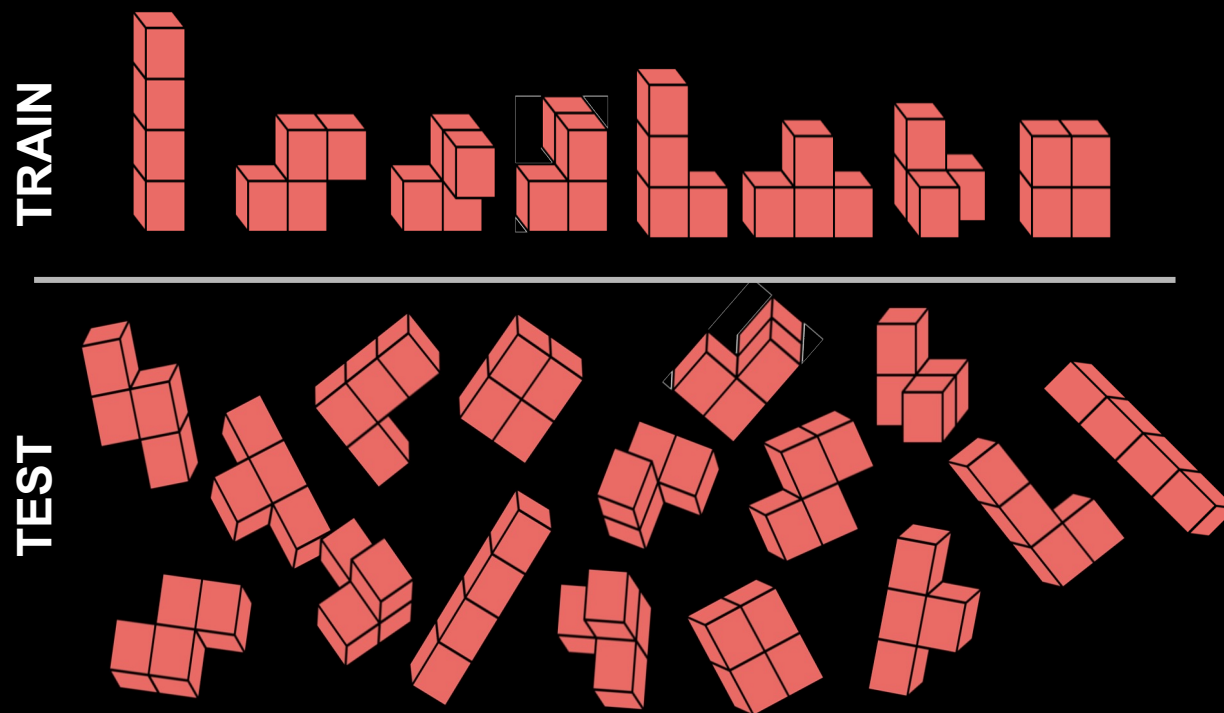
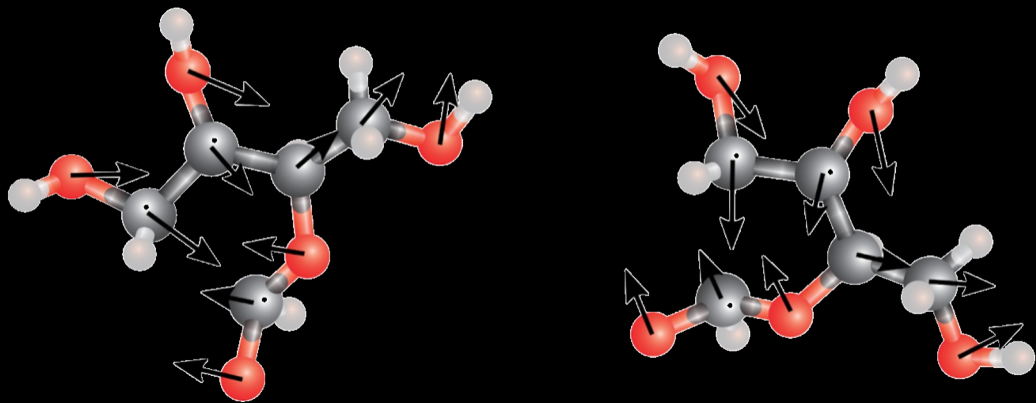
Source: Prabhat

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



CNNs for Materials with Physical Laws

Physics-aware learning



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

Filtering, De-Noise and Curating Data

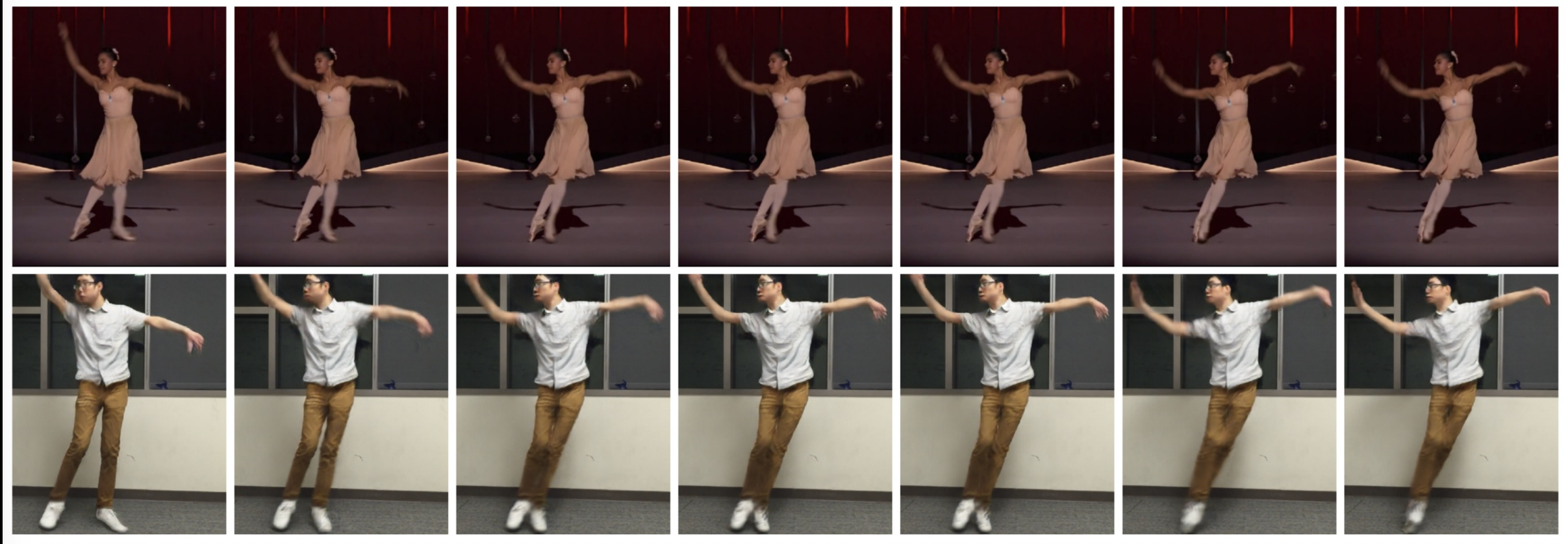


AmeriFlux & FLUXNET: 750 users access carbon sensor data from 960 carbon flux data years; Developing ML to denoise data.



Arno Penzias and Robert Wilson discover Cosmic Microwave Background in 1965

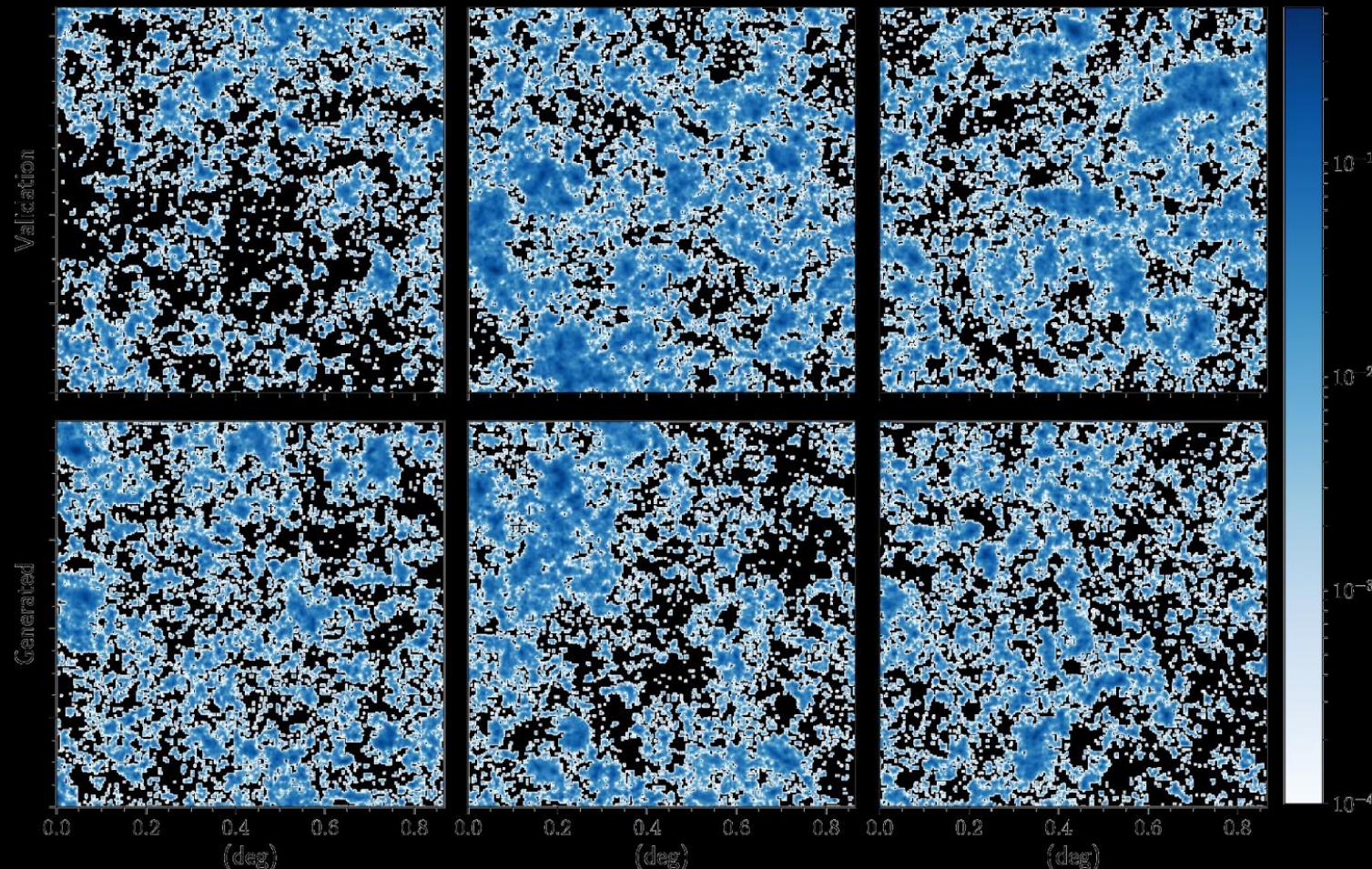
Generate Videos



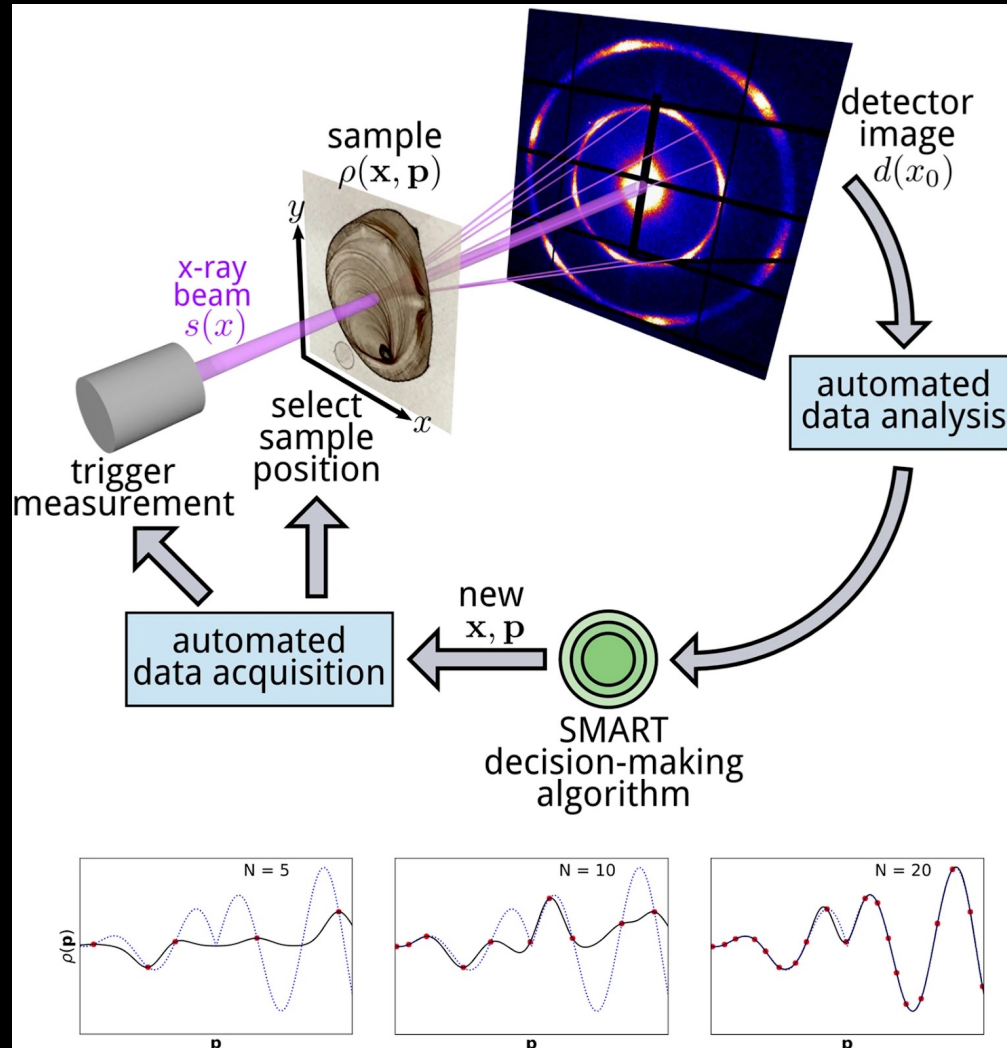
Caroline Chan, Shiry Ginosar, Tinghui Zhou, Alexei A. Efros, UC Berkeley

Generate Data from Expensive Experiments

Generate convergence maps of weak gravitational lensing, to help in understanding the physical laws governing the universe.



Automated experiments

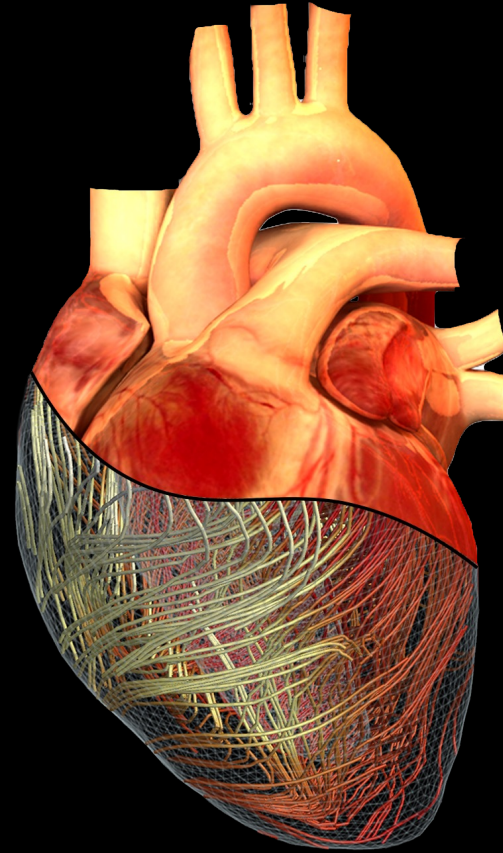


Utilization and robustness

- AI-based autonomous discovery
- Decisions based on small datasets
- Uncertainty estimates

Source: CAMERA Project, PI James Sethian
Slide input: Lavanya Ramakrishna

Digital Twins



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



The economic model is key



Cloud vs HPC : It's all about the Business Model in '35

Cloud	HPC
Focus on storage	Focus on computing (flop/s)
Cheap(est) commodity component	High end components (some specialization)
Commodity networks	High performance networks
Pay as you go	Purchased for mission; pay in non-fungible "hours"
< 50% utilization	> 90% utilization
On-demand access	Large jobs wait in queues
Multiple jobs per node	Dedicated set of nodes
On-node disks (air cooled)	Separate storage (compute liquid cooled)

**Policy and
business
model**

Rethink software

Transform publishing, research, teaching!

- Higher level
- Different interaction



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

A screenshot of a Jupyter Notebook interface. The browser address bar shows "127.0.0.1:8888/notebooks/talks/slides/1607-nersc/Lorenz%20Differential%20Equations...". The notebook title is "Lorenz Differential Equations". The interface includes a menu bar (File, Edit, View, Insert, Cell, Kernel, Widgets, Help) and a toolbar with icons for file operations and code execution. The main content area has the following text:

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));`

Below the code is an interactive control panel with sliders for:
- angle: 308.90
- max_time: 12.00
- σ : 10.00
- β : 2.63
- ρ : 28.00

At the bottom is a 3D plot of the Lorenz attractor, showing its characteristic butterfly shape with multiple colored trajectories.

How did we get here?

- **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

We need a new strategy for post-exascale computing