More Data, More Science and… Moore's Law

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Three parts

- **Science opportunities**
- **Technology challenges**
- **Productivity approaches**
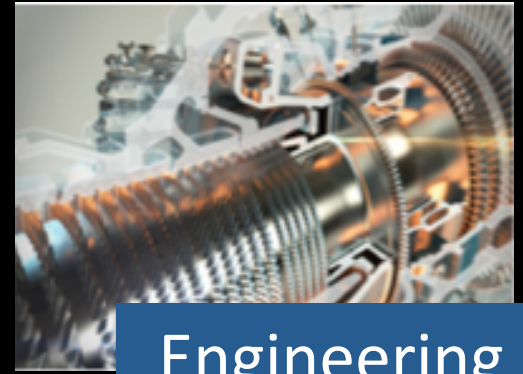
Part I

Science is poised for transformation

and Science in the broadest sense

Medicine

Basic Science

Engineering

Environment

Security

Experimental Science is Changing
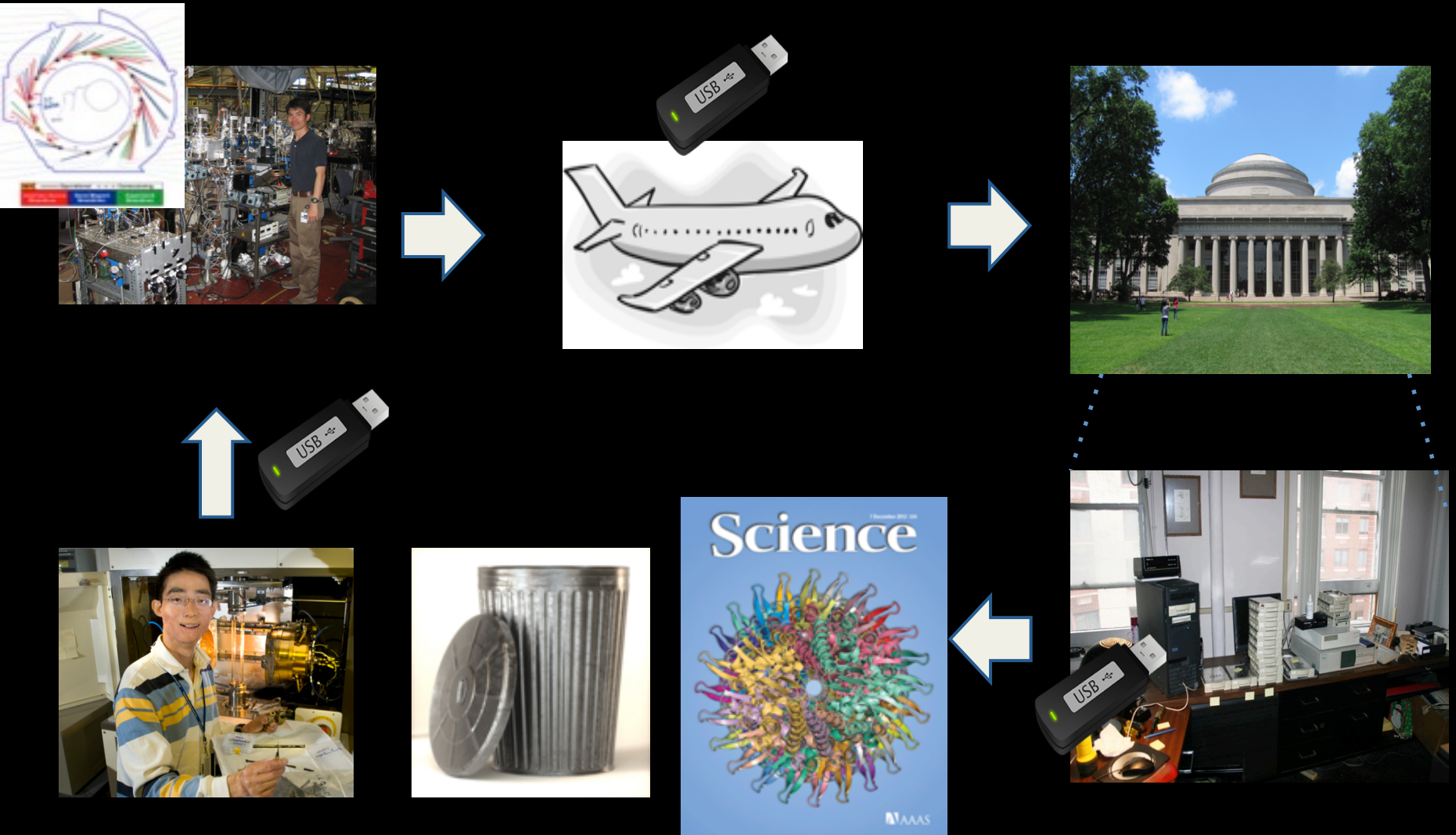
Empowering New Scientists
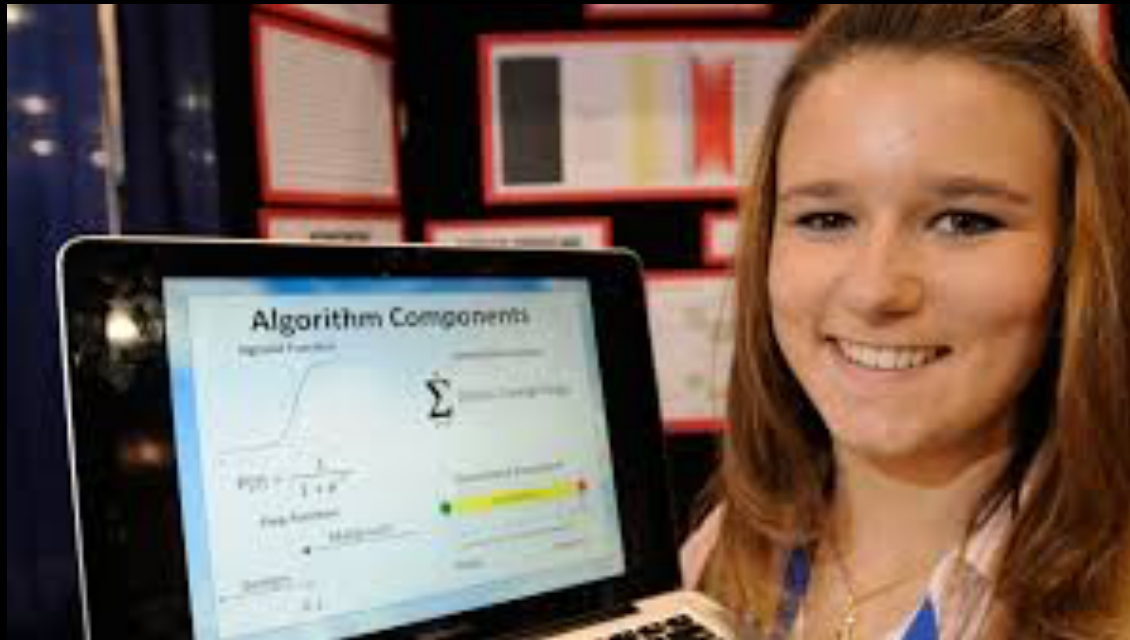
17-year-old Brittany Wegner creates breast cancer detection tool that is 99% accurate on a minimally invasive, previously inaccurate test.

Machine Learning + Online Data + Cloud Computing
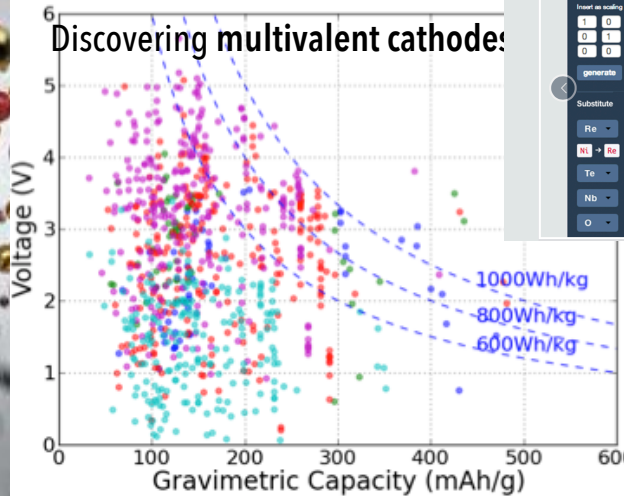
Old School Experimental Science

Computing, experiments, networking and expertise in a "Superfacility" for Science

Special Purpose processing here?

GISAX

Slot-die printing of Organic photovoltaics

HipGISAXS & RMC

CAMERA
Applied Math

Computational Scientists May Never Login

Novel computing technology here?

- **Over 10,000 users of the Materials Project since 2011**
- **1000x more computing needed for more materials, environments, and details**

Simulations both consume and produce massive data
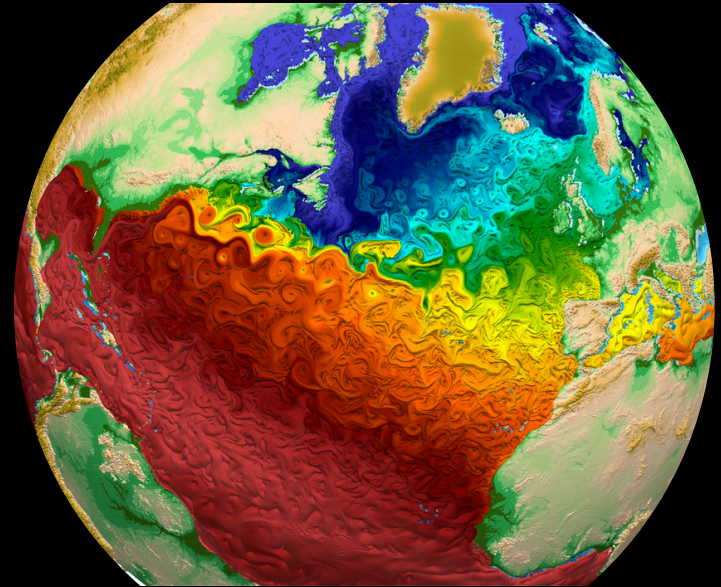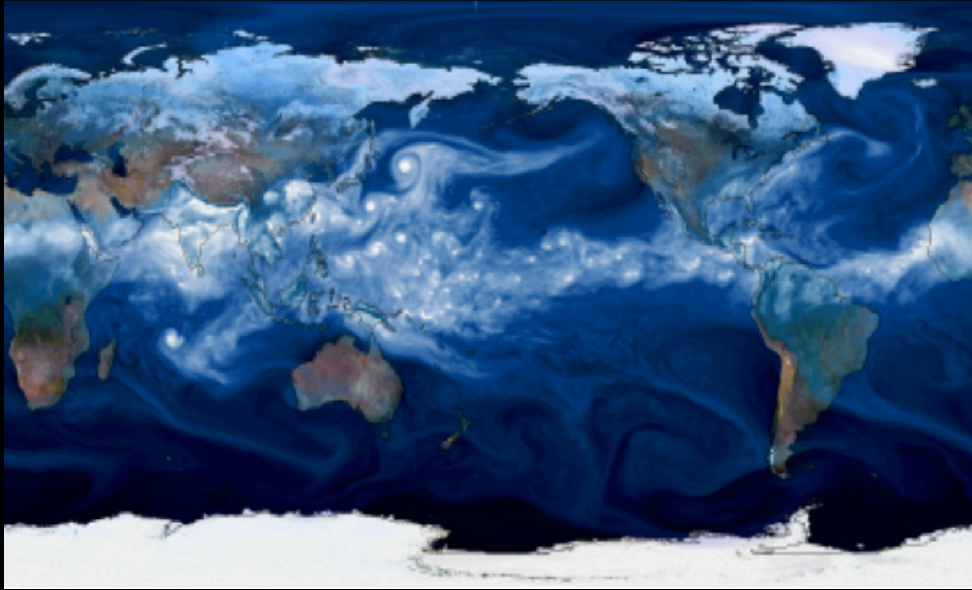
- **Simulation: Resolve clouds, identify tipping points, quantify confidence, quantify agriculture and economics**

- **Observation: Use environmental sensors and samples to refine models**

- **Analysis: Machine learning identifies extreme events; Reanalysis of 100+ years of weather to improve**

Breakthrough science will occur at the interface of observation and simulation

Environment and Climate
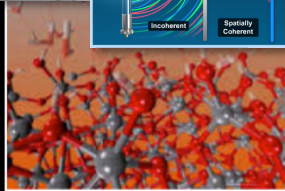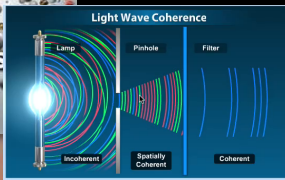
Cosmology

Materials and Chemistry

Subsurface science
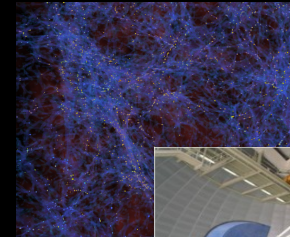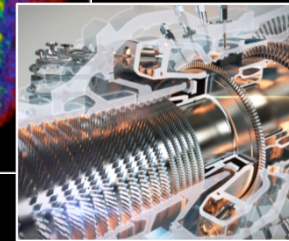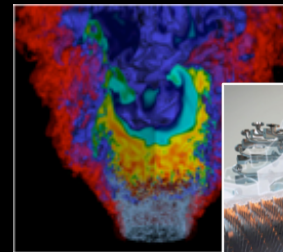
Combustion
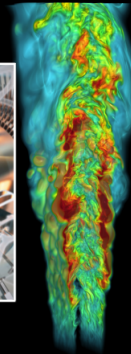
And it will need capable exascale systems, computer science, statistical machine learning and new mathematical models and algorithms

Challenge: Finding Scientific Data
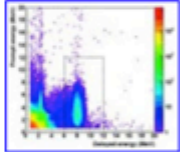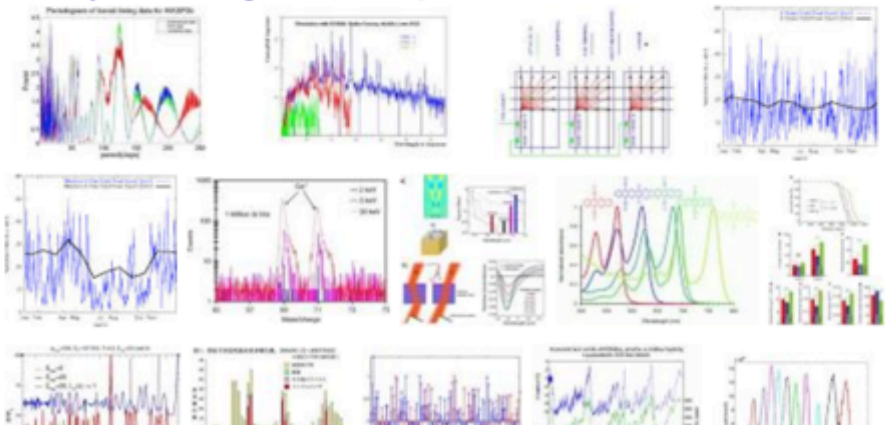
Challenge: Filtering, De-Noising and Curating Data
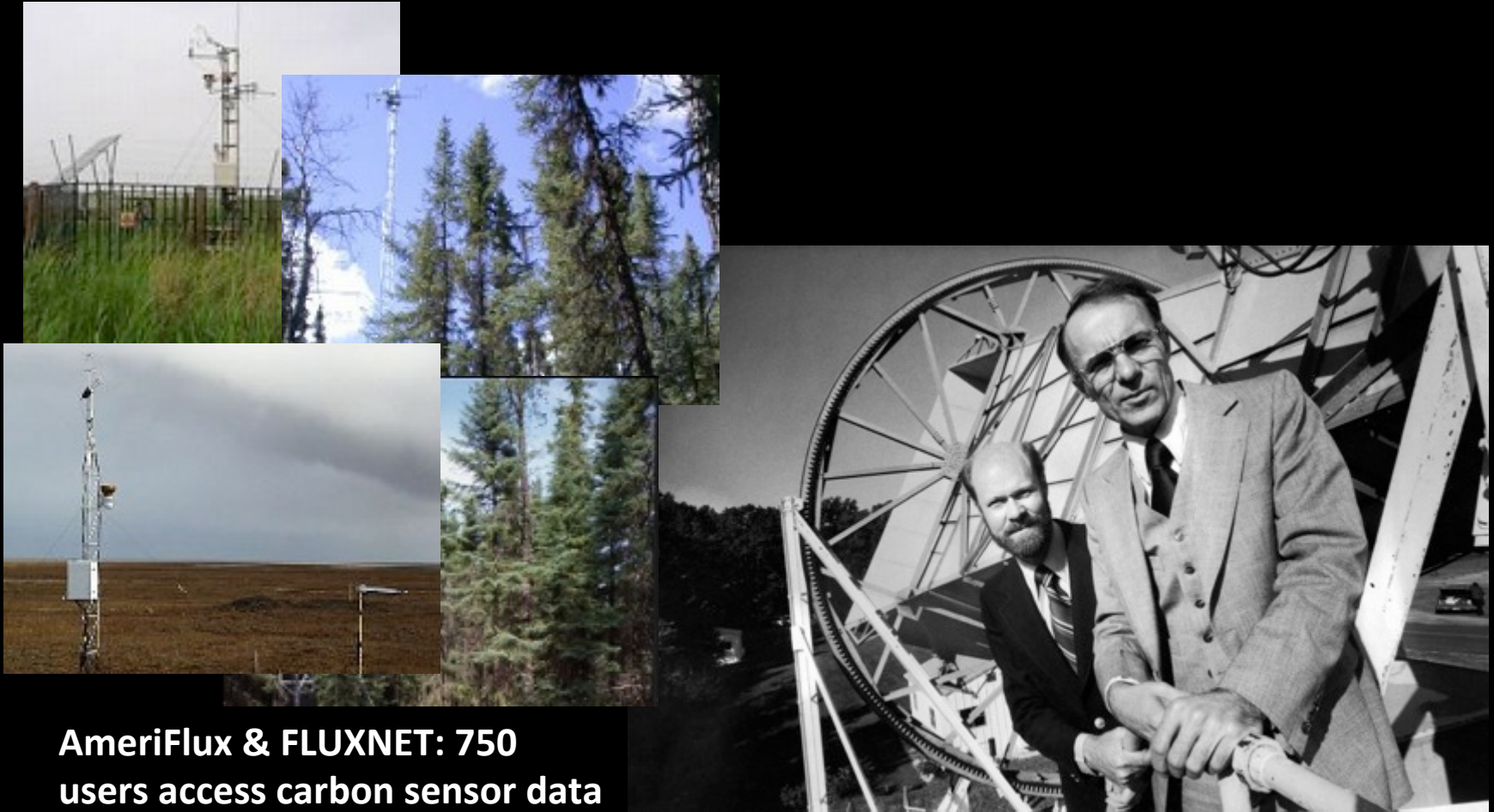
AmeriFlux & FLUXNET: 750 users access carbon sensor data from 960 carbon flux data years

Arno Penzias and Robert Wilson discover Cosmic Microwave Background in 1965

The Black Swans of Computing with 1990s Technology
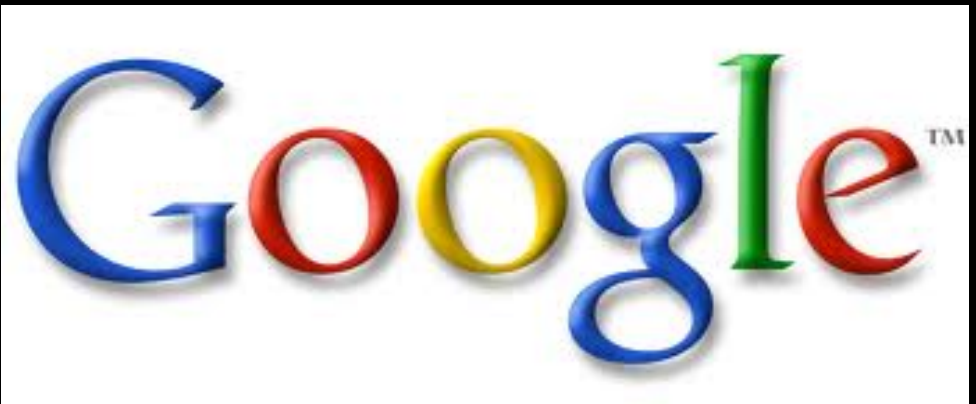
Part II

- **Science is poised for transformation**
- **Computing performance growth is slowing**

Computing Performance Stalls
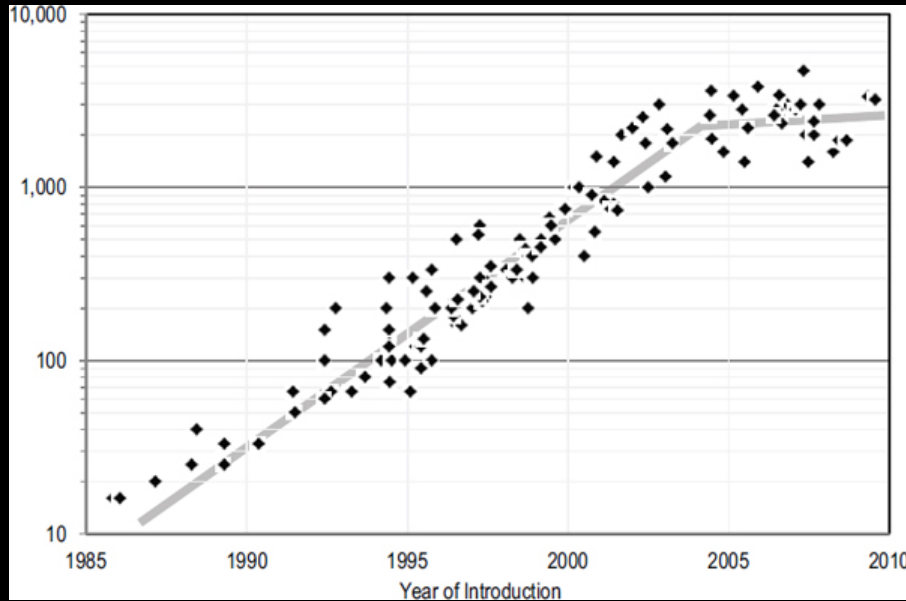
2004: End of clock speed scaling
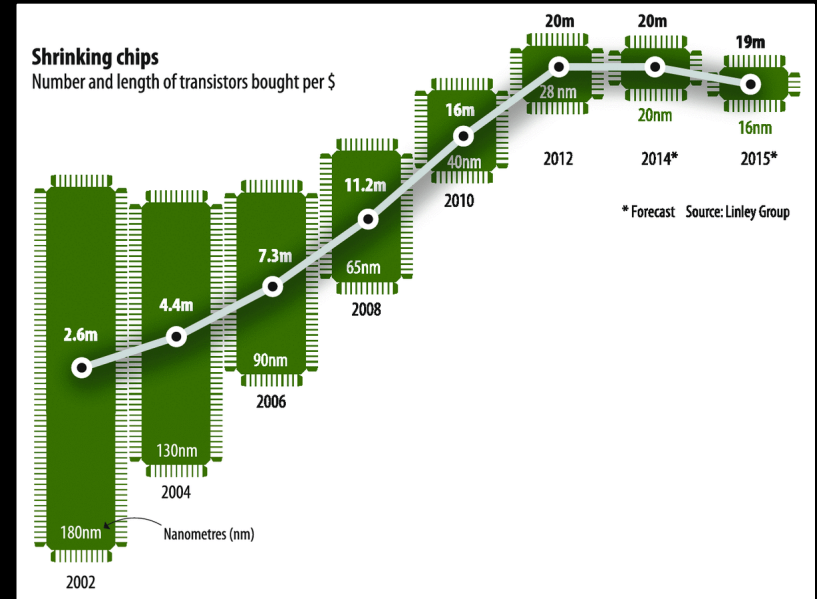
202?: End of transistor density scaling

We need an end game for Moore's Law and a new game after that

A Generic 2020+ Node Architecture

Memory Stacks on Package
Low Capacity, High Bandwidth, Software Control?

Lightweight Cores
(tiny, simple, massively parallel)
Throughput-Optimized

Bulky Cores
Latency Optimized

DRAM

DRAM

DRAM

DRAM

NVRAM: Burst Buffers / rack-local storage (software control)

Part III

- Science is poised for transformation
- Computing performance growth is slowing
- **How more productive tools can help**

(What productivity means to me)

The right machine for the problem
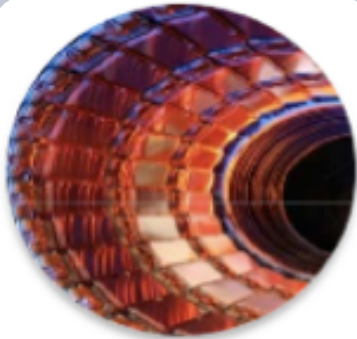
Massive Independent Jobs for Analysis and Simulations	Nearest Neighbor Simulations	All-to-All Simulations	Random access, large data Analysis
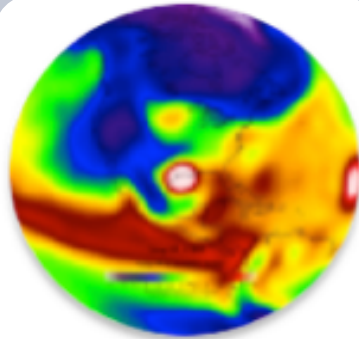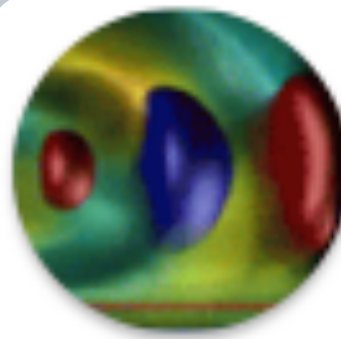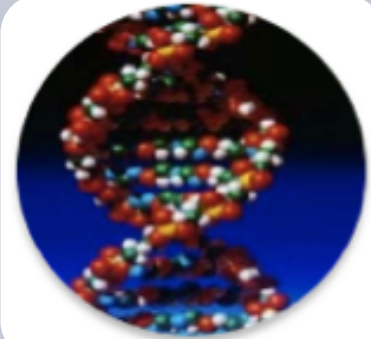
Applications often fit in multiple categories

The right systems software for the problem

Cloud Computing
Map-Reduce w/ Resilience
Flexible software stack
On-demand scheduling
Price ≠ Cost

High Performance Computing
General programming
High speed networks
Co-scheduling large jobs
Algorithms and libraries
Performance expertise
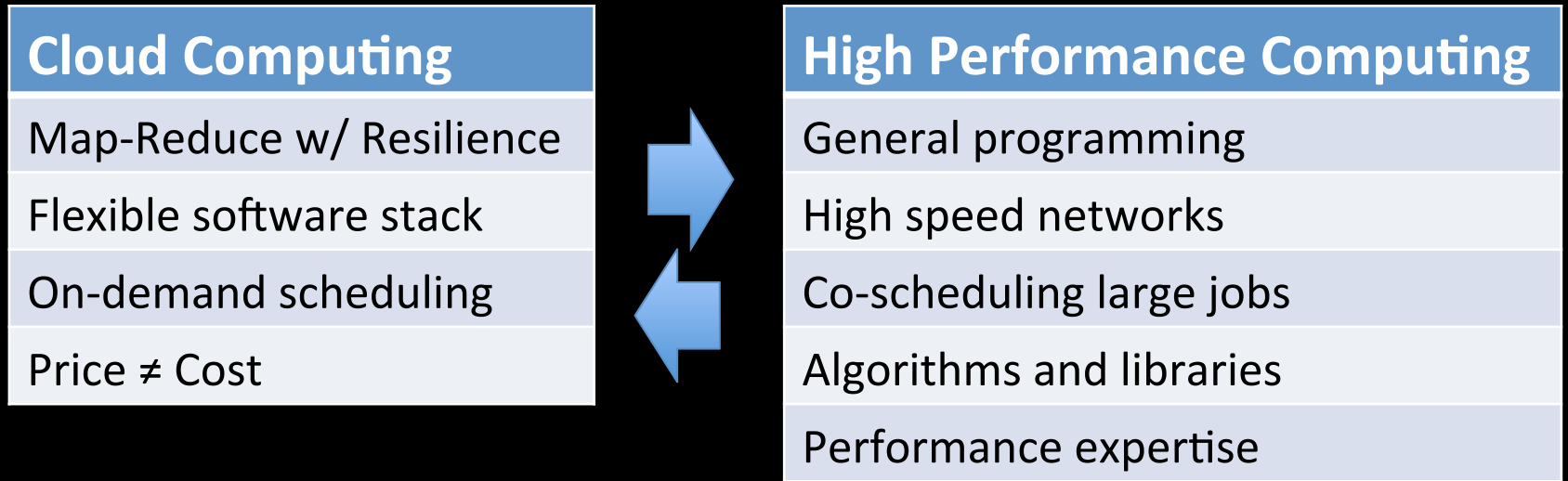
Ideas and technologies have transferred in both directions

Ultimately, cloud computing is business model not a technology

A convenient programming model for the problem

De Novo Genome assembly for the environment and health
"Scaffolding" step on shared memory
- Human: 44 hours to 20 secs
- Wheat: "doesn't run" to 32 secs
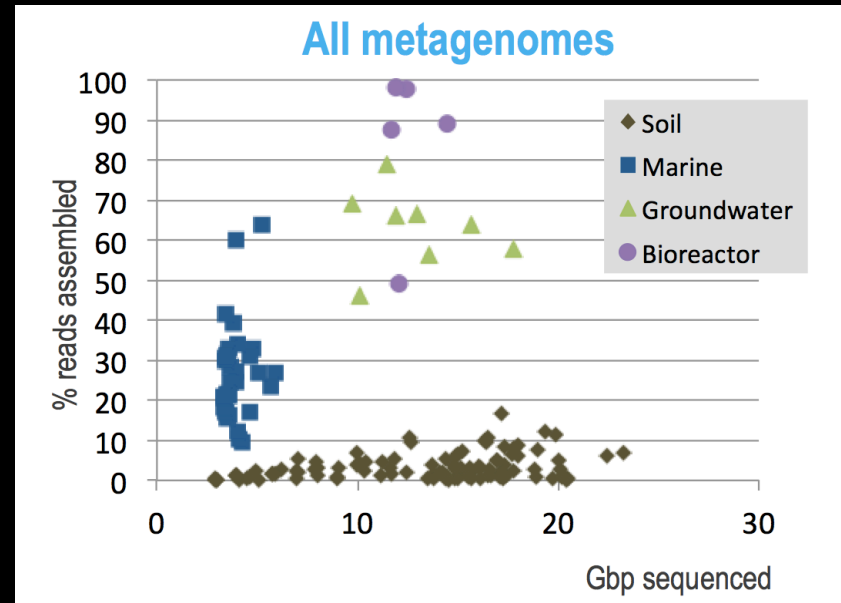
All 2015 human sequences could have been assembled on 10% of annual NERSC resources; metagenomes are much harder

A programming model (UPC) that encourages the right algorithmic thinking (hash tables, atomics,…)

A Network that Makes Location Irrelevant

Technology, policy, and social challenges across:

- Networks and countries
- Facilities
- Universities (Science DMZ)
- Systems (SDN)

ESnet Goal: Scientific progress **completely unconstrained by the location** of people, instruments, computational resources, or data.

Use scientific libraries and frameworks

- *Encapsulate the best algorithms*
- *Hide machine details*
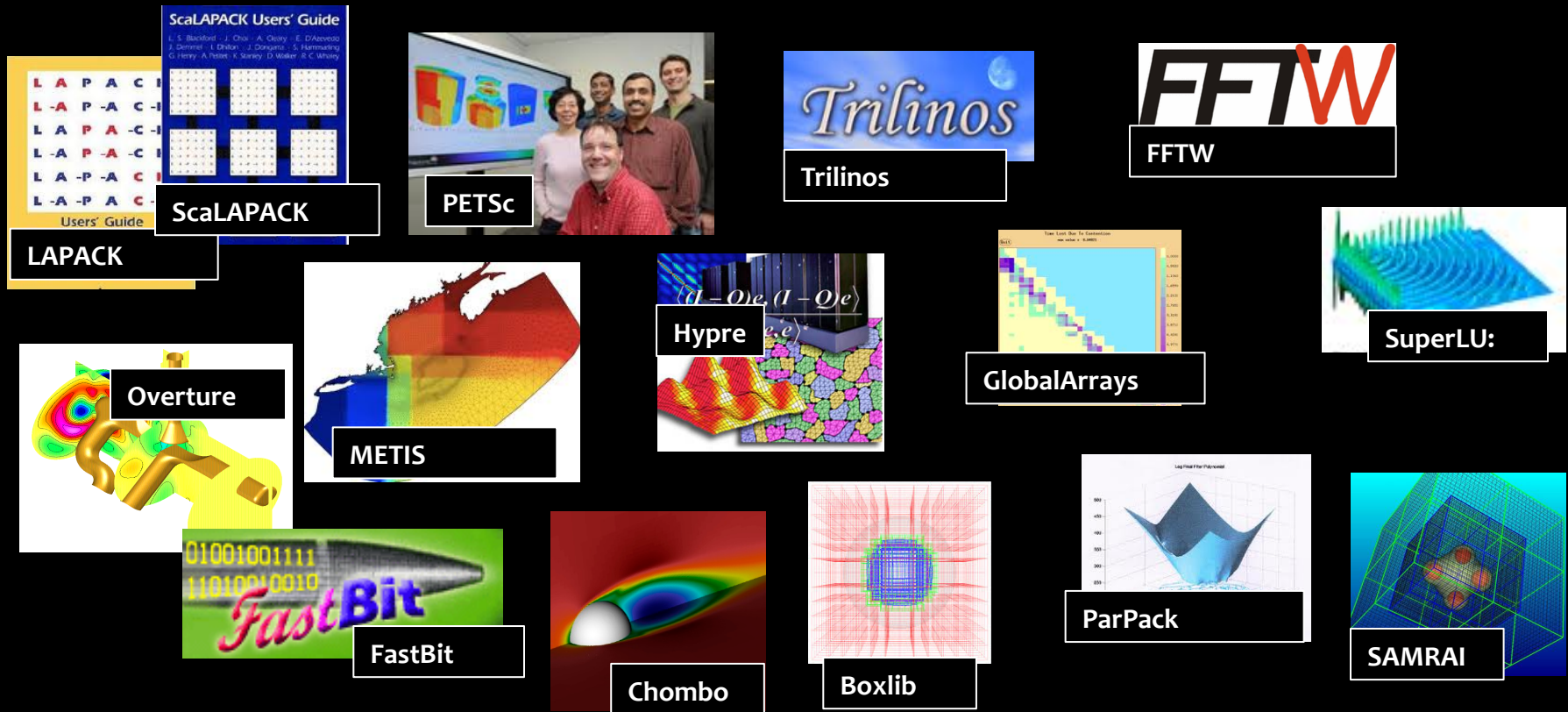
Enabled by portable programming models like MPI

The right libraries for the problem

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

The right algorithms, models and methods
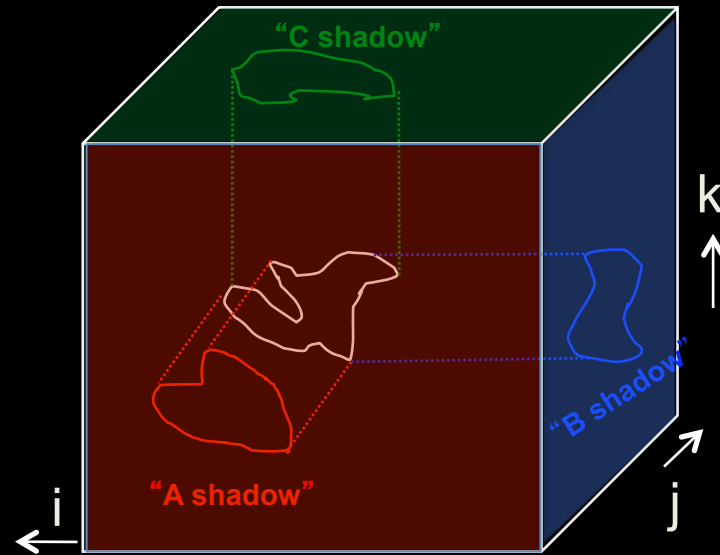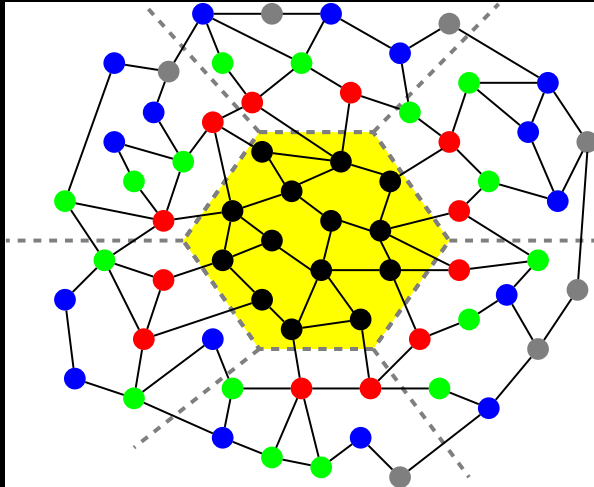
Optimize for data movement as first-class concern

- Change numerical methods (e.g., high order)
- Design algorithms that minimize data movement

High level programming abstractions

Where is Performance Portability?

- **Multiple generations of GPUs, Xeon Phi, …**
  - Not performance portable across systems

- **How do applications address this problem?**

#ifdef

Approach 1: Use of libraries, templates and preprocessors

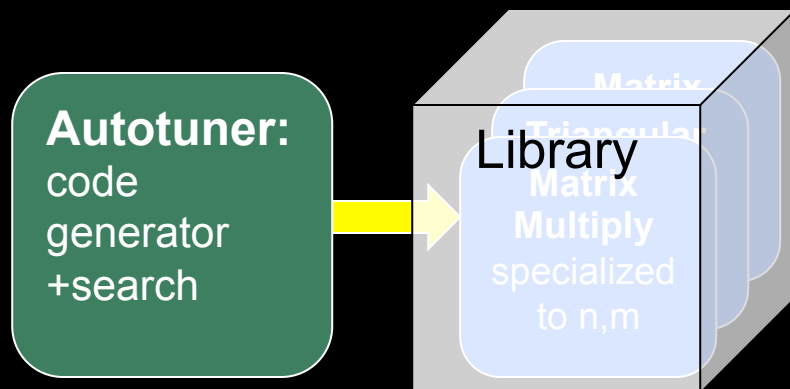Approach 2: OpenMP4 absorbs necessary accelerator features (likely), but code still diverges

Approach 3: Architectures converge "enough" by 2023, perhaps with co-design help

Write code generators and autotuners

What code generators do we have?

Autotuner:
code generator
+search

Library

Matrix Multiply specialized to n,m

Dense Linear Algebra	**Atlas**
Spectral Algorithms	**FFTW, Spiral**
Particle	**TCE**
Sparse Linear Algebra	**OSKI**
Structured grids	**TBD**
Unstructured Grids	
Monte Carlo	

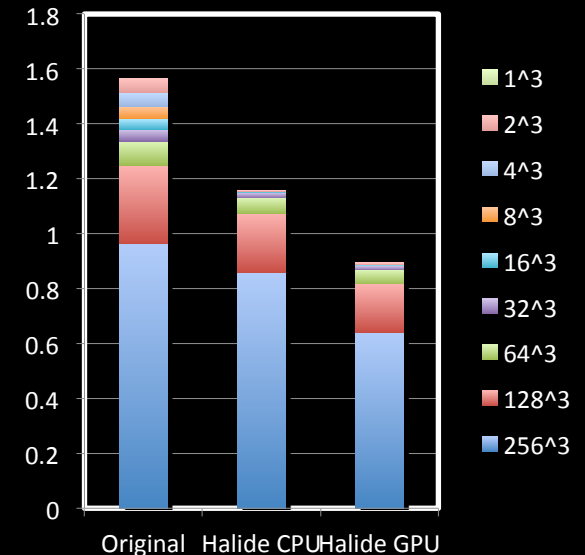Two unsolved compiler problems
- Dependence analysis
- Optimization selection

Develop and influence languages and compilers

Rose compiler input

Halide DSL has 10+ developers and 50+ users in industry
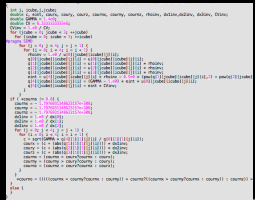
Rose compiler output

■	1^3
■	2^3
■	4^3
■	8^3
■	16^3
■	32^3
■	64^3
■	128^3
■	256^3

Original   Halide CPU   Halide GPU

Productivity will be key to dealing with complexity
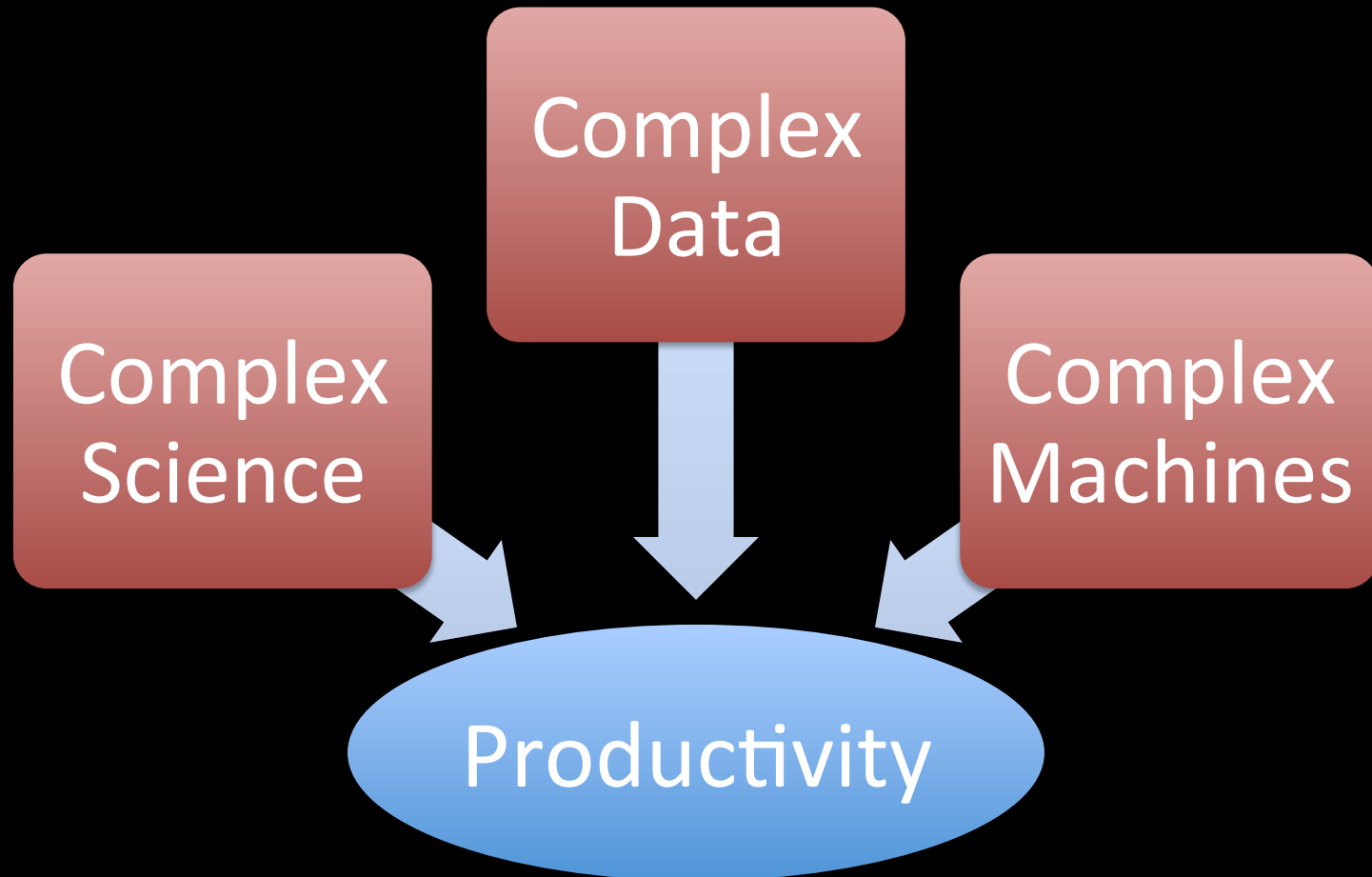
Conclusions

NSCI is not:

- limited to the high end

- about integrating enough chips to reach exaflop

It is about:

- The cost of computing

- Power requirements, size, and speed of computers

- Solving real problems that require more computing