30 Years of HPC from Gigaflops to Exaflops: No science left behind or thinning the herd?

Steve Plimpton
Sandia National Laboratories

2018 Salishan Conference on High-Speed Computing

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Impact of advancing HPC on particle simulations

- Many methods/models are $\sim$ **O(N)** cost in particle count
- Also scale as $\sim$ **O(N/P)** in parallel, for large enough N/P
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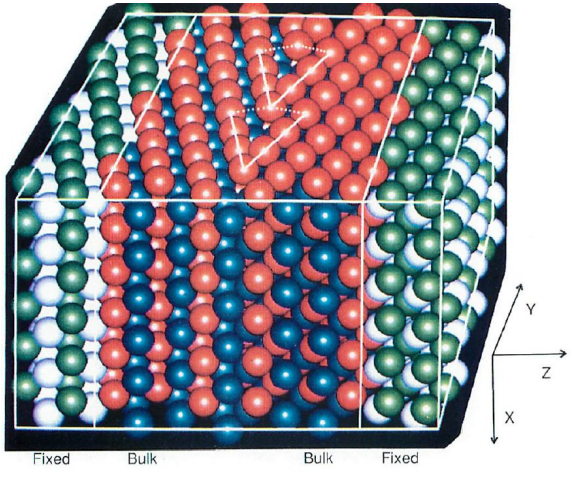

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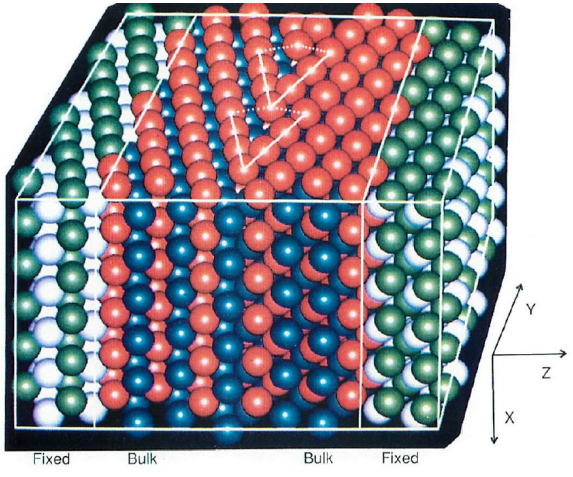

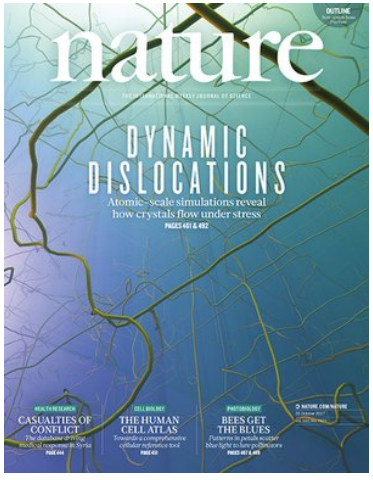

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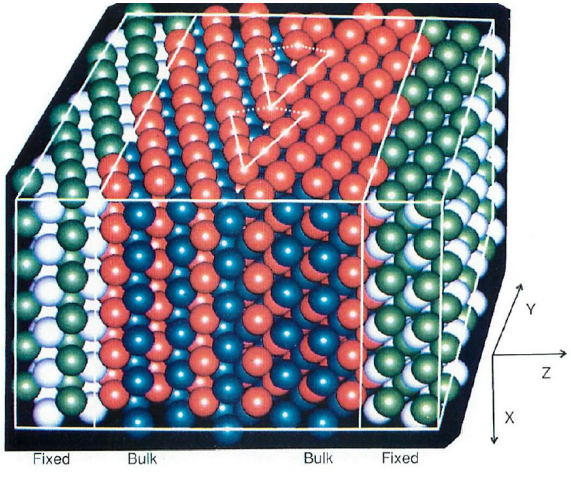

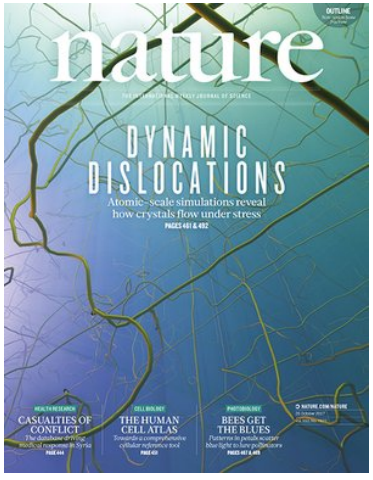

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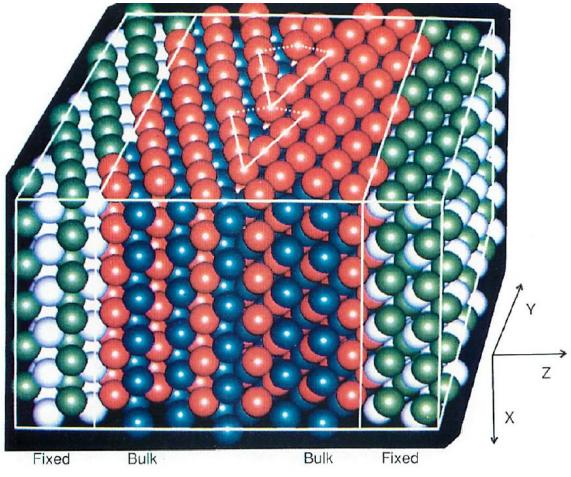

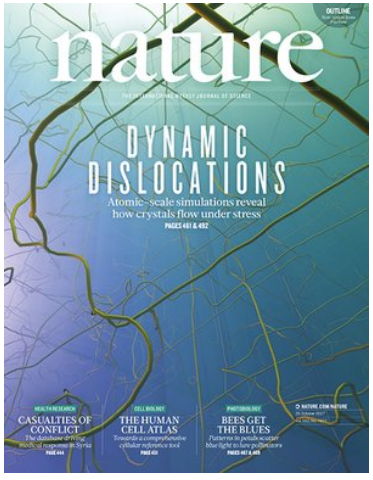

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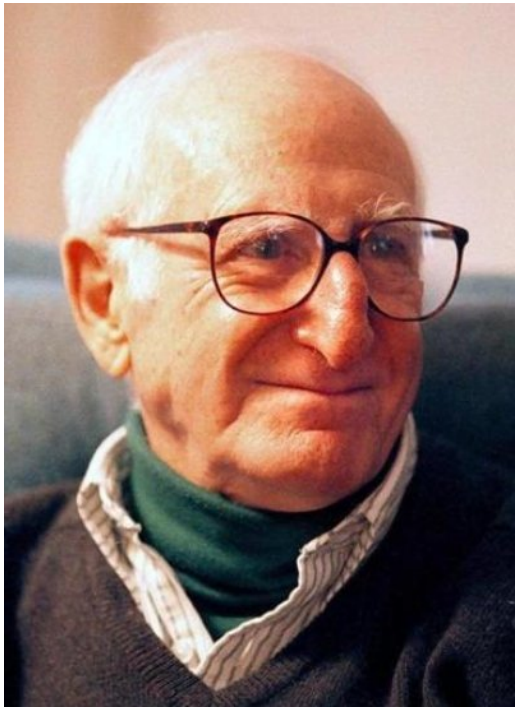
- Linpack: 1 BG/Q core / 1 Cray YMP proc = **41x** !!
- Cray YMP proc $\Rightarrow$ third of BG/Q Sequoia $\Rightarrow$ **21M** faster
- MD atom-steps/s $\Rightarrow$ **8.5M** faster

Newspapers and ukuleles

Ben Bagdikian (1920-2016): Pulitzer prize journalist, professor



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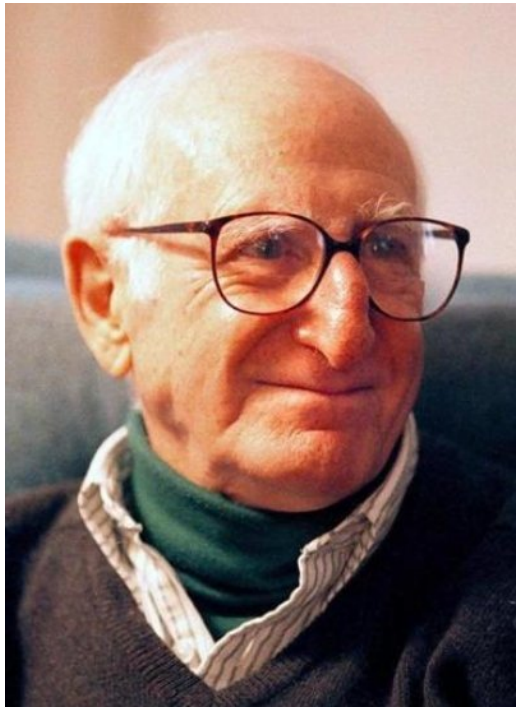

"Trying to be a first-rate reporter on the average American newspaper is like trying to play Bach's *St. Matthew's Passion* on a ukulele."

HPC and ukuleles

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average petascale (soon exascale) machine is like
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on a million ukuleles."

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  - current & future hardware is incredibly sophisticated
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  - current & future hardware is incredibly sophisticated
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  - google **Jake Shimabukuro**
- No one is doing **first-rate science** on petascale machines
  - Gordon Bell prizes at SC conference
  - INCITE allocations by DOE

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- These two realities have a cost:
  - may be optimal for flops, but is **sub-optimal for science**
  - lots of time/$$ not spent on science
  - leaving many apps and scientists on the sidelines
  - there **ain't that many** Jake Shimabukuros

What is Ukulele Syndrome?

Different than Ukulele Acquisition Syndrome (UAS)

- Google "ukulele syndrome", will find real thing called UAS

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- Many of you and your orgs have serious cases of HAS
- Sorry, there is **no known cure** for UAS or HAS

Five symptoms of Ukulele Syndrome

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- Write **allocation proposals** for computer time that:
  - jump thru hoops to show code can use 50%+ of the machine
  - run lots of small jobs (together) to boost machine usage

What is the impact on science, mission or otherwise?

- **Opportunity cost** for continually adapting apps to new machines
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- Deploying computers that are **hard to use and code for**:
  - shrinks the number of apps that can use it
  - we do less multiphysics, less multiscale
  - shrinks the pool of people that can program them
  - **casual HPC users** are not Jake Shimabukuros, but they are often **better scientists**
  - if make machines hard for them to code & use, we lose their science contributions

Why you might be singing the Ukulele Blues

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The Olde Timey Blues

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2016	Sunway TaihuLight (China)	93 Pflops	130	1500

Exascale blues

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- **Congratulations!** billion X speed-up in 30 years!

Commentary on the blues

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  - 1 core of YMP: 512 MB of memory, balance factor = 0.52
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- Bottom line: we're **selecting** for certain kinds of apps
  that can withstand these high imbalance ratios

But hey ... growing imbalance is good news for particles

- Particle apps:
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- But ...
  - particles don't represent **broad swath** of
    computational science, or majority of apps that need HPC
  - physics often isn't short-range
  - hard to reach long timescales with explicit timestepping

Coding apps for the bleeding-edge of HPC

- **Vectorize** for YMP (medium vector length)
- **Vectorize** for SIMD (deja vu, long vectors)
- **Vectorize** for CPU/KNL (deja deja vu, short vectors)
- Learn **MPI** (distributed memory)
- Add **OpenMP** directives (modest threading)
- Learn **CUDA** for GPUs (massive threading)
- Overlap comp and comm (hide latencies)
- Manage memory for CPUs (4 level caches and growing)
- Hybrid nodes (CPU + multiple GPUs)
- Make codes **fault tolerant** (what?)
- Convert to **asynchronous multi tasking** (really?)
- **MPI may vanish** (#@!% really??)

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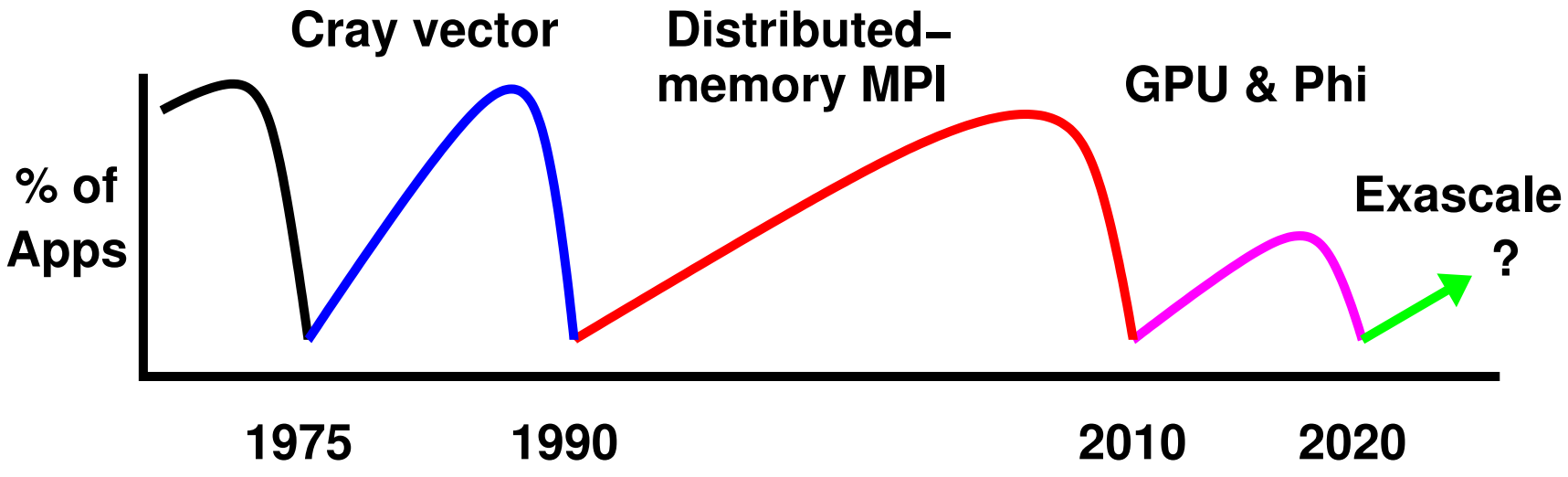
- App developers: this is a ton of not-so-useful **work**
- Scientists: this is a **barrier to the science** I want to do

Qualitative history of apps on evolving HPC platforms

X-axis = paradigm shifts in HPC node hardware
Y-axis = percentage of scientific apps that adapt



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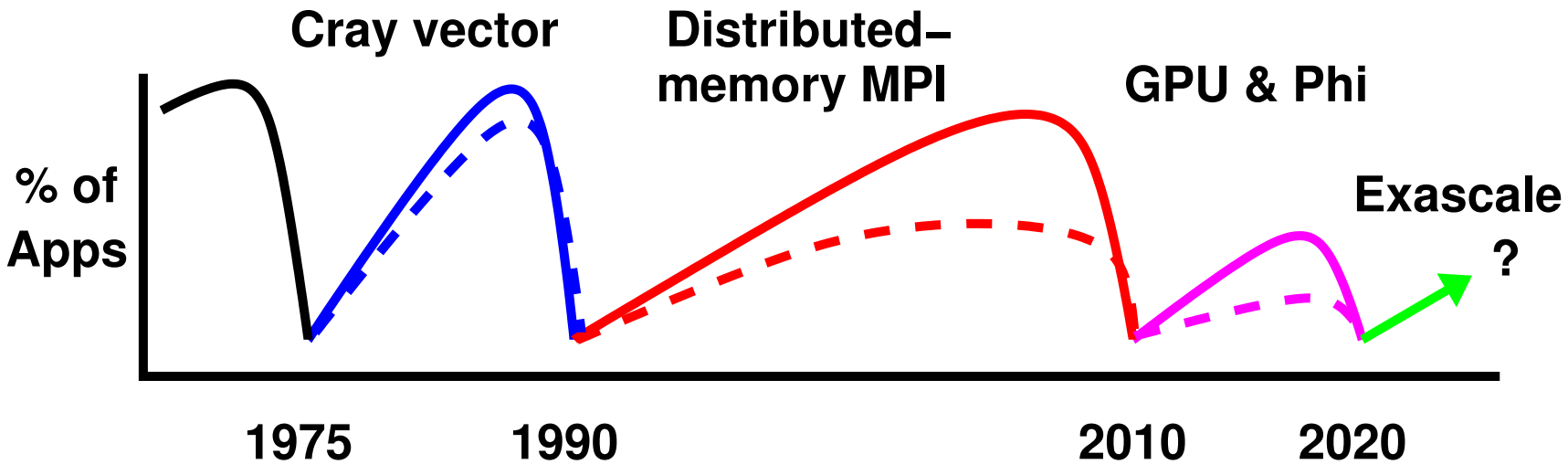

Y-axis = percentage of apps that adapt
and run efficiently on full machine

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sex for the students,
athletics for the alumni, and
parking for the faculty."

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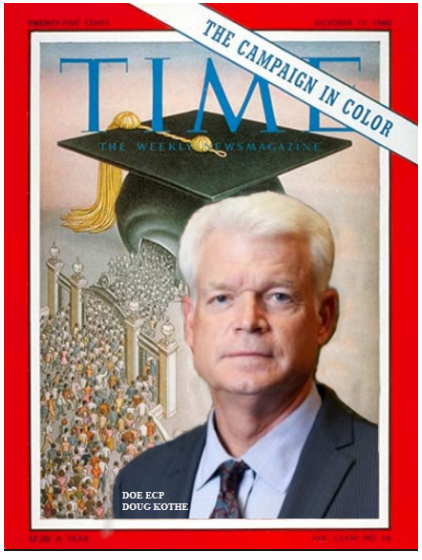

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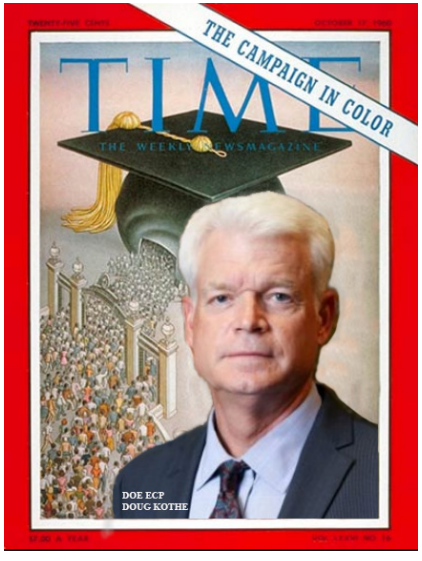

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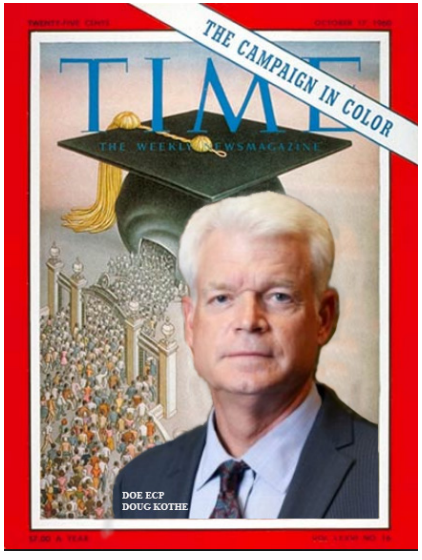

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- Funders (students): flops are sexy, grab the headlines

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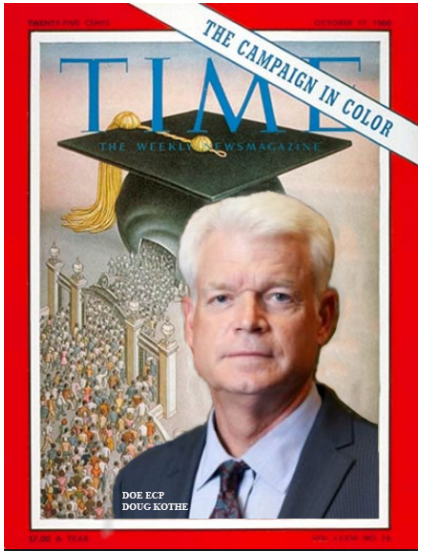

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Thinking outside-the-box for branding ...

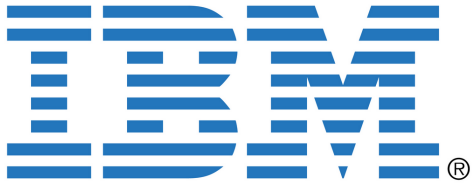
Introducing the new

Chick-fil-A® IBM® NVIDIA®

Summit supercomputer at ORNL

California version of branding ...

Introducing the new



Sierra supercomputer at LLNL

"A new way to get **high** (flop rates)"

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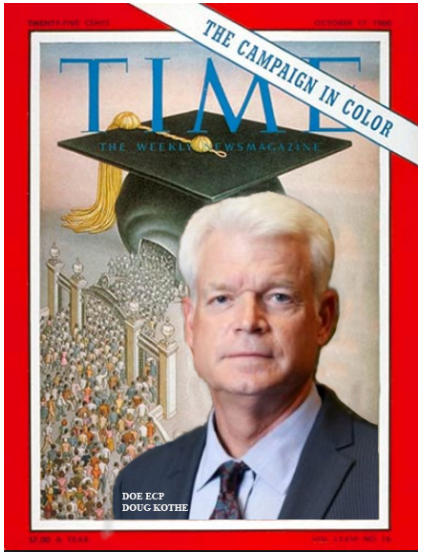

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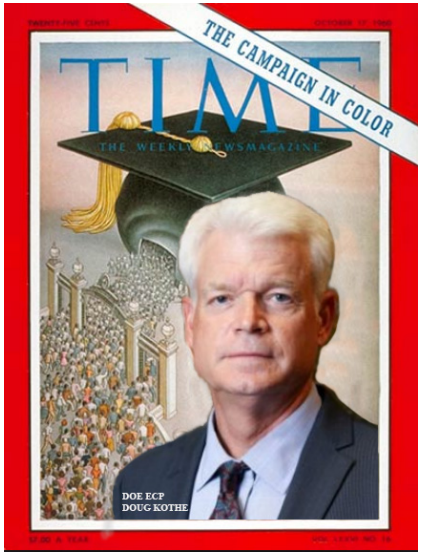

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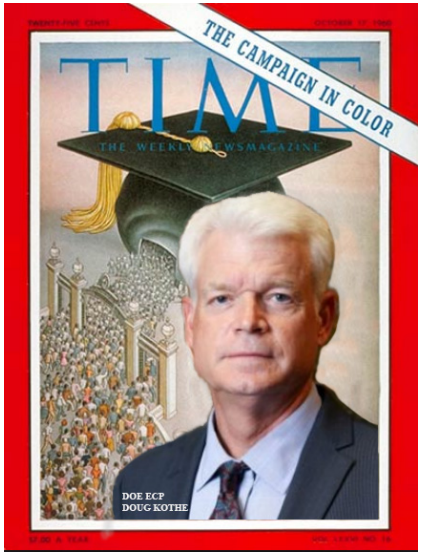

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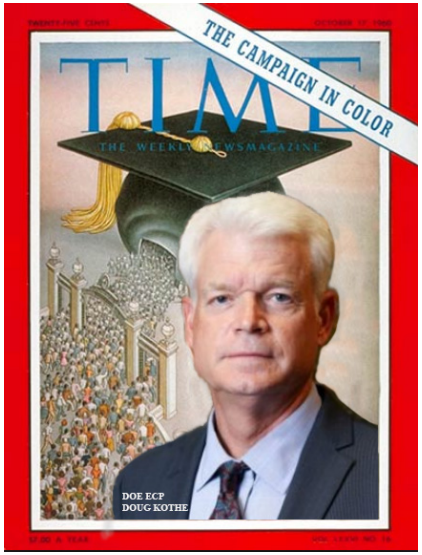

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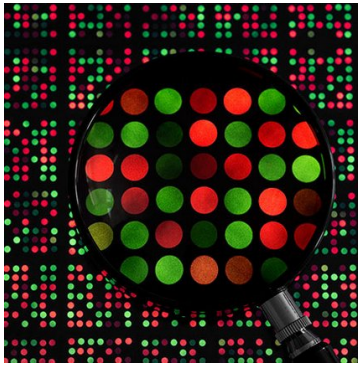
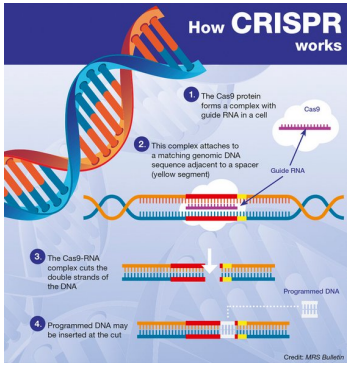
- Can you make all 3 happy?
- Maybe at a rich university, but not with a supercomputer
- Because the 3 constituencies have **competing interests**

Cell biology

- PCR (1983) = polymerase chain reaction, DNA replication
- Microarray chips (1995) = parallel gene expression (millions)
- DNA sequencing (2001) = \$10K/Mb $\Rightarrow$, few \$0.01/Mb
- CRISPR (2012) = genome editing in living cells





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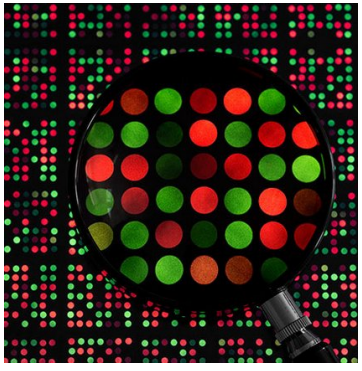

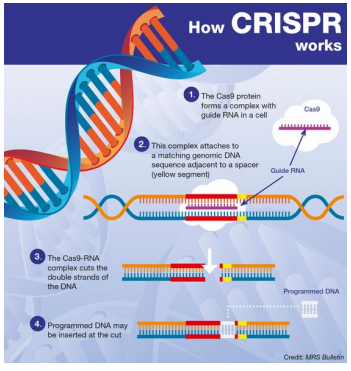

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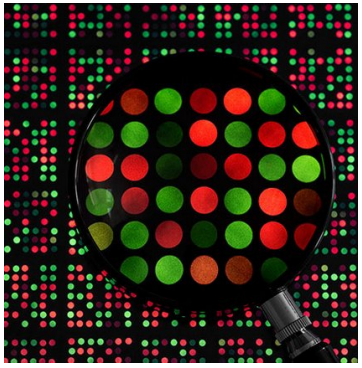
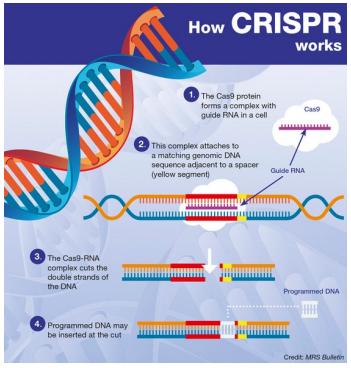
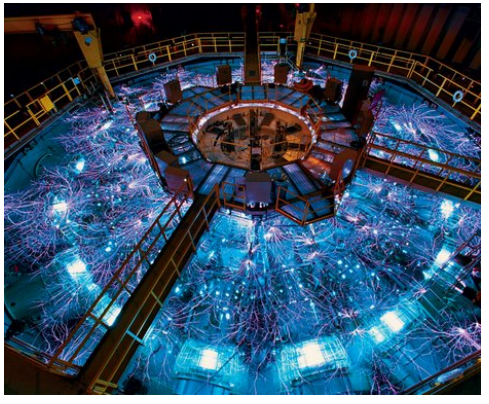




- All these technologies rapidly became **ubiquitous**
- Any lab, any grad student can use them
- Don't need add-on experts to write an NIH proposal
- Could we aspire to that **ease-of-use** for HPC machines?

User facilities with billion $ instruments

- Hubble telescope (NASA/ESA),
  SNS (ORNL), Z-machine (Sandia)



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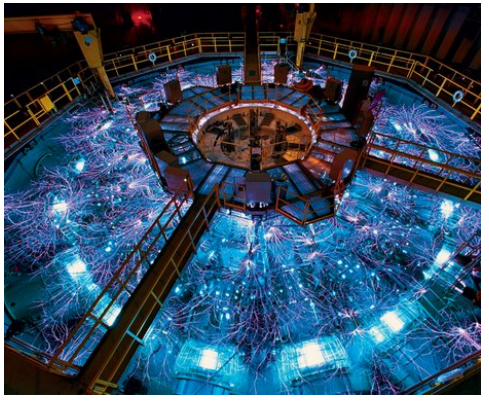

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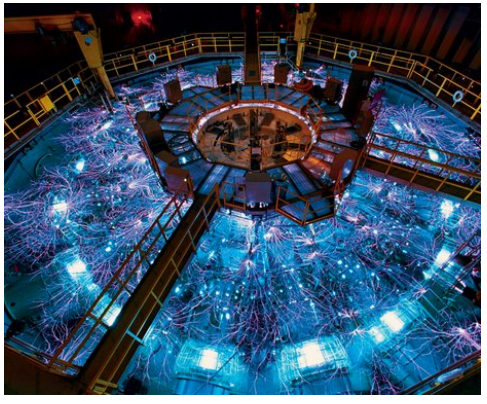

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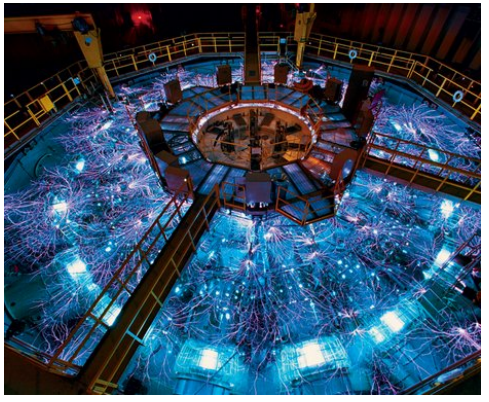

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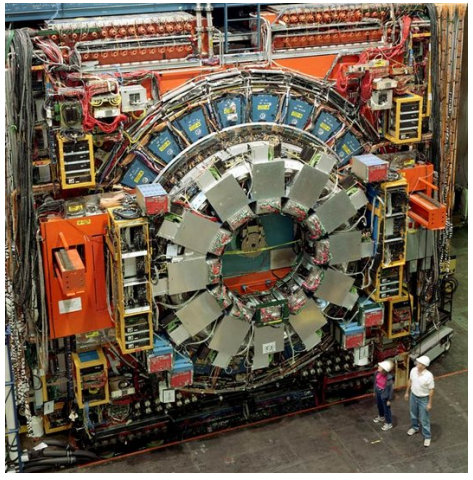
- What if 20x new HPC machine just gave all users 20x more?

High-energy particle physics

- CERN, FermiLab, etc



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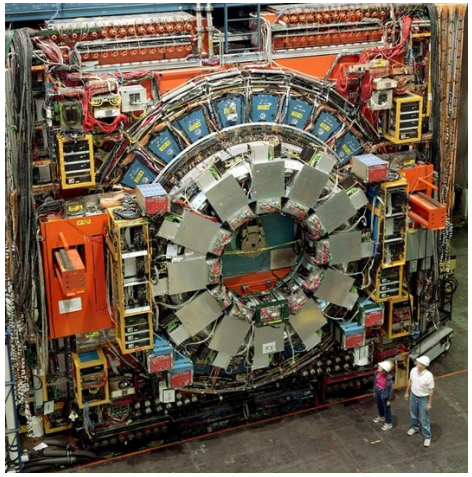

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- **Is HPC more like** cell bio, user facilities, or HE physics?

No silver bullet solutions ...

- Can we create easy-to-use machines & software
  for the 99% of **mere-mortal computational scientists**
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David Parnas: "**Complexity is not a goal**. *I don't want to be remembered as an engineer of complex systems.*"