Computing at Fermilab:

Looking toward the Future

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Fermilab 50th Anniversary Symposium and Users Meeting

June 8, 2017

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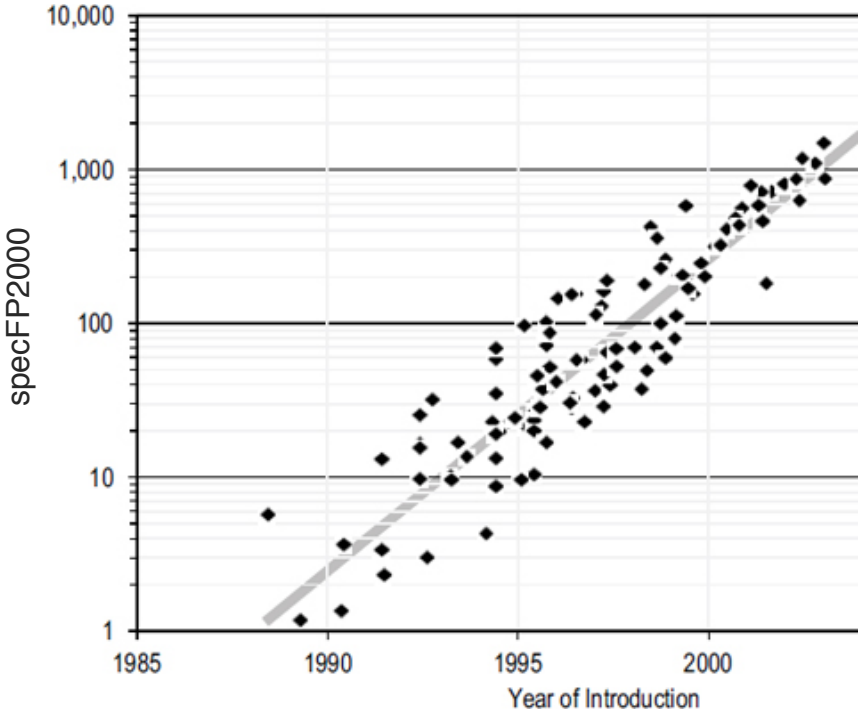
The Point of this Talk

- Computing in the good old days



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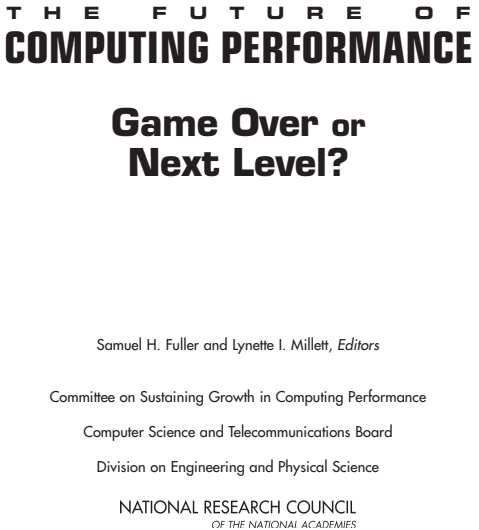

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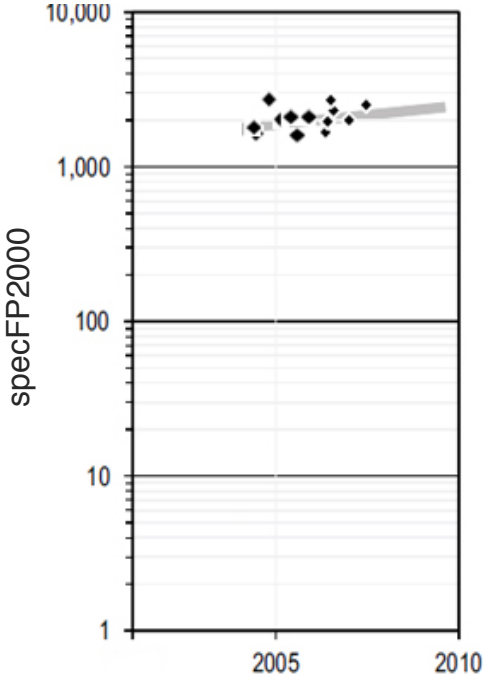
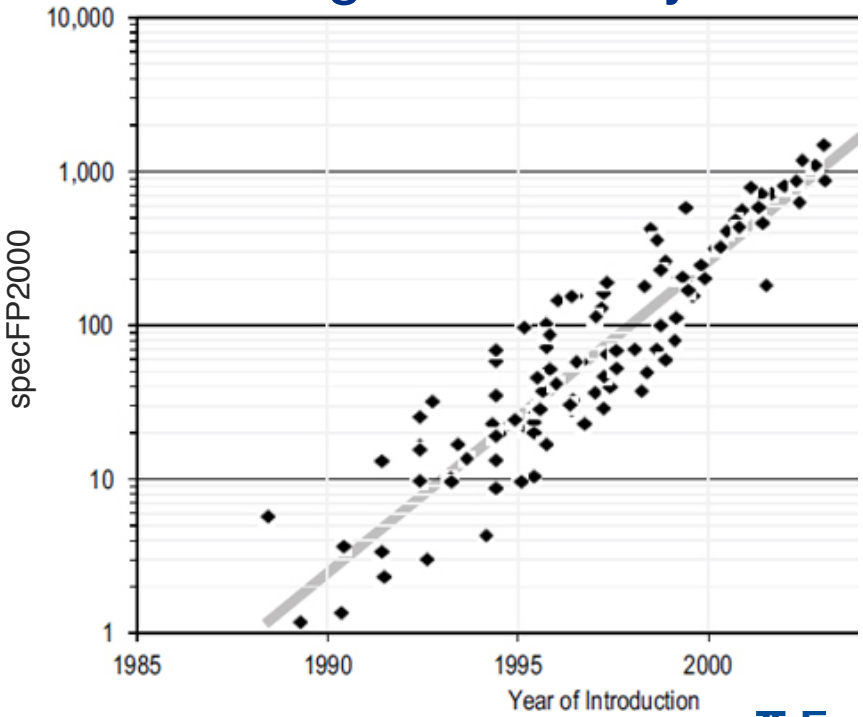
Things have changed already

- Computing is changing for reasons based on both physics and economics

recent times



good old days



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Computing for High Energy Physics

Computing at Fermilab is Computing for HEP

- Historical perspective
  - B.C., VAXus Vulgaris, Unix Principium
- Where we are now
  - Linux Maximus
- Changes are beginning
  - Linux Nubes (Cloud Computing)
- Major changes are coming
  - Deus ex Machina (Exascale Computing)
- Qualitative changes are next
  - Terra Incognita (Quantum Computing)

I have given various epochs of HEP computing Latin(-ish) names to emphasize that change has happened before and will happen again

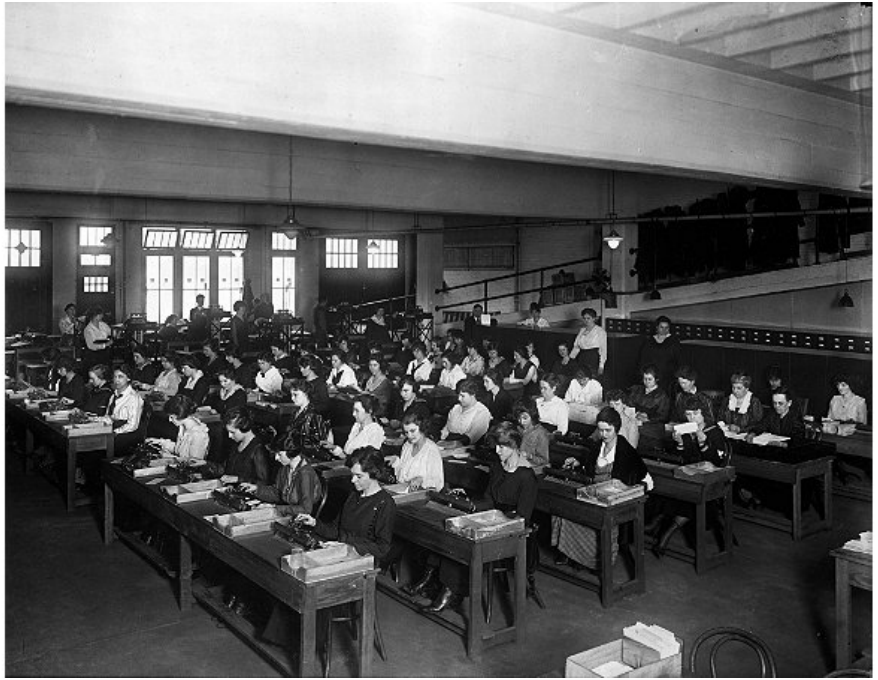
Epoch: B.C.

Before Computers

From an *Atlantic* article entitled

"Computing Power Used to Be Measured in 'Kilo-Girls'"

Presumably now we would use "Kilo-Grown Women."



Women at work tabulating during World War II (Shorpy)

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Skipping ahead

I hope everyone saw Oliver Gutsche's excellent talk

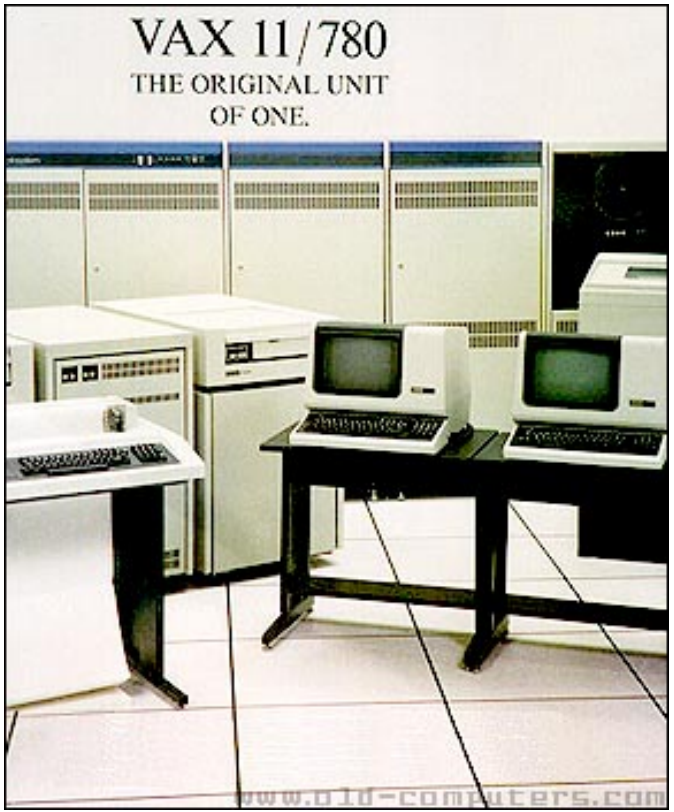
Computing Innovations

yesterday.

It covers the early days of HEP computing at Fermilab.

Epoch: VAXus Vulgaris

DEC VAX with the VMS operating system was the most popular HEP computing platform in the 80's.



Epoch: Unix Principium

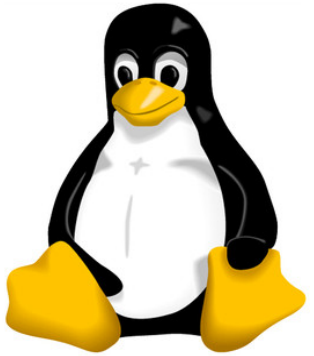
The 90's saw a transition to Unix-based computers

- Many people were skeptical that physicists could ever move from VMS to Unix.

- Nonetheless, Proprietary Unix workstations and large shared-memory machines came to dominate HEP.
  - *ca* lead in to Run II

Current Epoch: Linux Maximus

Since the early 2000's, HEP has been dominated by large clusters of x86-based Linux machines.



- Many people were skeptical that physicists could work without large shared-memory machines
- HEP was an early adopter of Linux clusters
  - We were among the world leaders in clusters!
    - … but we call them farms…
- Google, Amazon and others now have clusters that dwarf ours.

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Historical Perspective

- HEP has seen multiple computing epochs
- The current epoch, Linux Maximus, has lasted a long time
- We are no longer the world leaders in Linux clusters
- Each change in epoch has been meet with resistance
  - … but, ultimately, also led to success

Next:

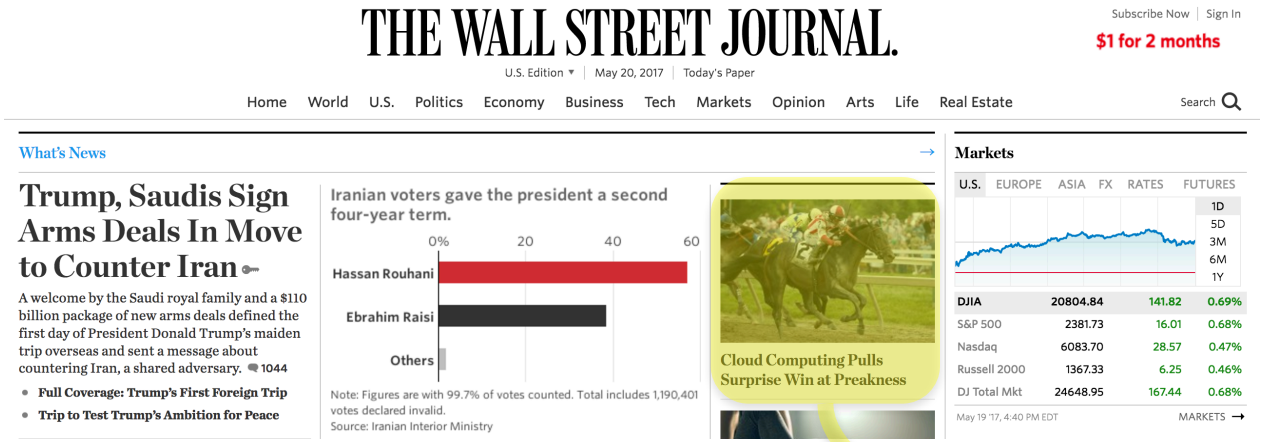
- Changes that are coming
  - and the developments driving them

P5 Recognizes the Need for Evolution

- Strategic Plan for U.S. Particle Physics (P5 Report)

  *Rapidly evolving computer architectures and increasing data volumes require effective **crosscutting solutions that are being developed in other science disciplines and in industry**. Mechanisms are needed for the continued maintenance and development of major software frameworks and tools for particle physics and long-term data and software preservation, as well as investments to **exploit next-generation hardware and computing models**.*

Changes are beginning: HEPCloud (Epoch: Linux Nubes)



Cloud computing is everywhere now

Cloud Computing Pulls Surprise Win at Preakness

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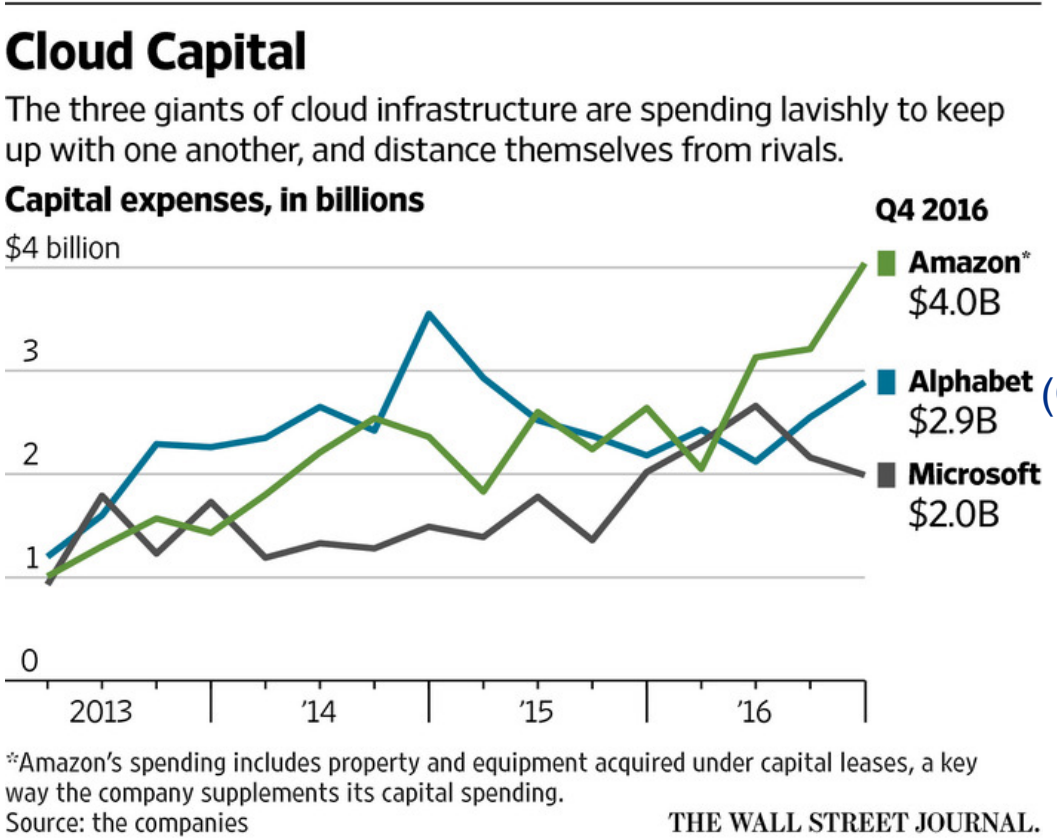
Industrial Clouds Dwarf HEP Clusters



(Google)

Most cloud content courtesy Burt Holzman

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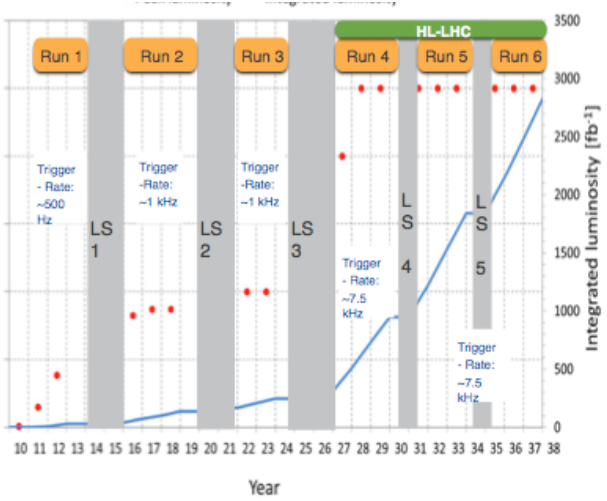
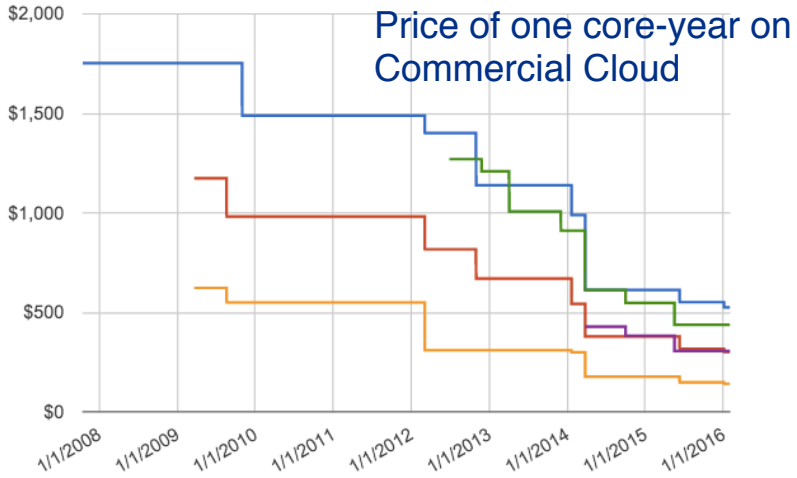
Computing Needs are Growing, Clouds are Getting Cheaper

- High Energy Physics computing needs will be 10-100x current capacity
  - Two new programs coming online (DUNE, High-Luminosity LHC), while new physics search programs (Mu2e) will be operating



- Scale of industry at or above R&D
  - Commercial clouds offering increased **value** for decreased **cost** compared to the past



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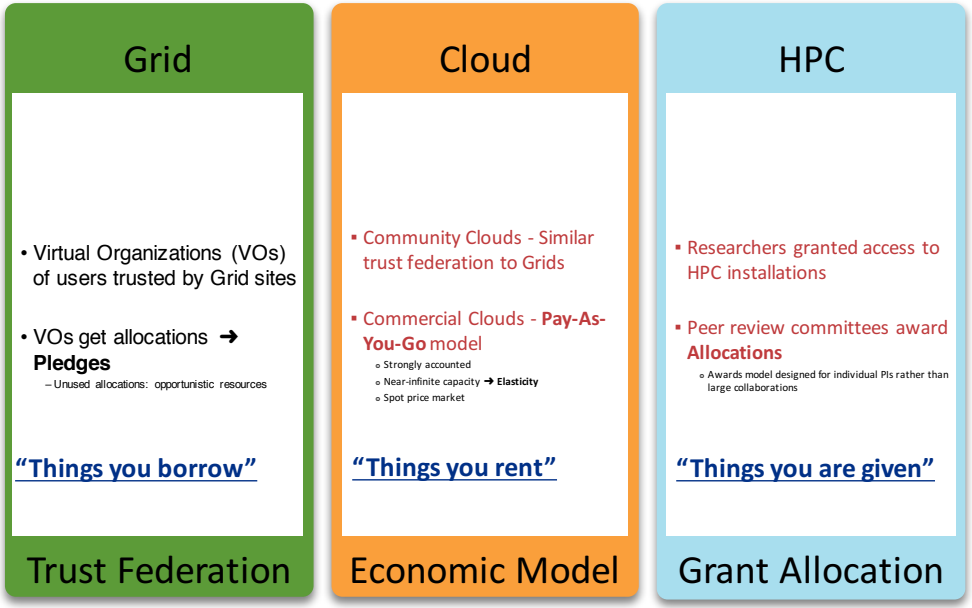
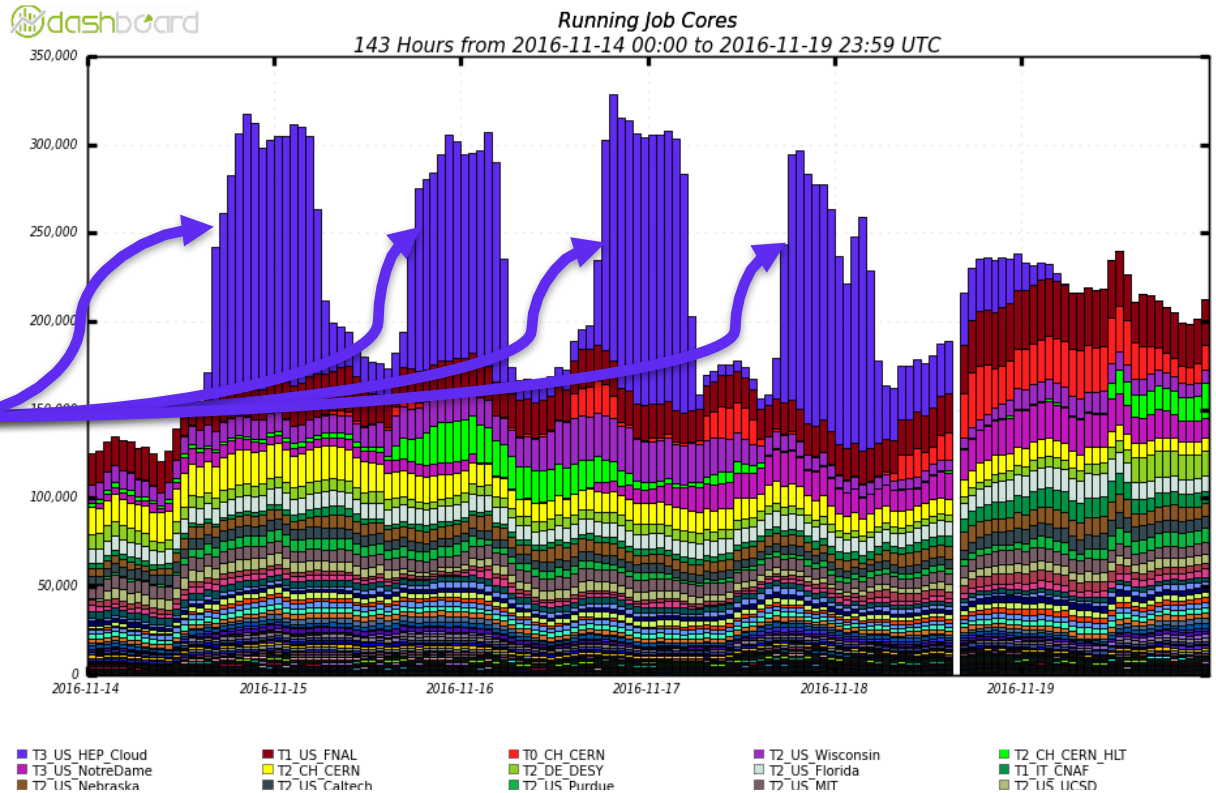
HEPCloud: the Evolved Facility

- HEPCloud provides a unified interface to grid, cloud and HPC resources
- Pilot project to explore feasibility, capability of HEPCloud
  - Goal of moving into production during FY18



HEPCloud: Doubling CMS compute capacity

HEPCloud in purple



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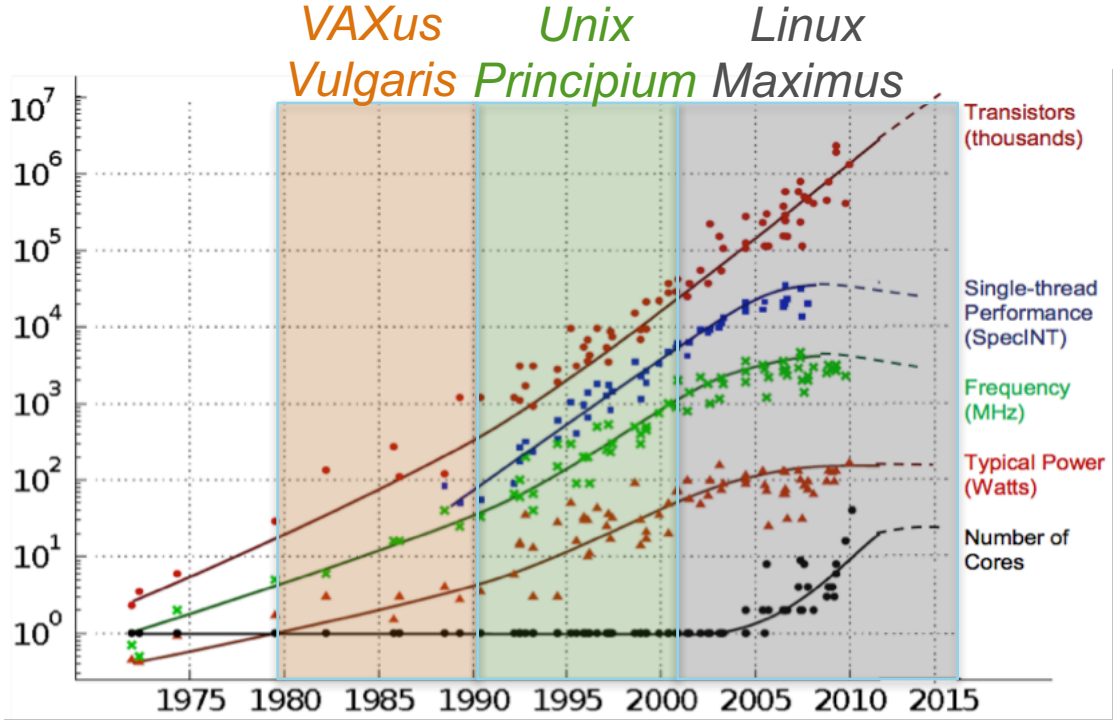
Hardware Trends are Changing



"Data Processing in Exascale-Class Computing Systems", Chuck Moore, AMD Corporate Fellow and CTO of Technology Group, presented at the 2011 Salishan Conference on High-speed Computing, Original data collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten, dotted line extrapolations by C. Moore

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Coming Epoch: Deus Ex Machina (Exascale Computing)

President Obama, July 29, 2015:

EXECUTIVE ORDER

CREATING A NATIONAL STRATEGIC COMPUTING INITIATIVE

By the authority vested in me as President by the Constitution and the laws of the United States of America, and to maximize benefits of high-performance computing (HPC) research, development, and deployment, it is hereby ordered as follows:

…

Sec. 2. Objectives. Executive departments, agencies, and offices (agencies) participating in the NSCI shall pursue five strategic objectives:

1. **Accelerating delivery of a capable exascale computing system that integrates hardware and software capability to deliver approximately 100 times the performance of current 10 petaflop systems across a range of applications representing government needs.**

…

Exascale Computing Challenges (Epoch: Deus Ex Machina)

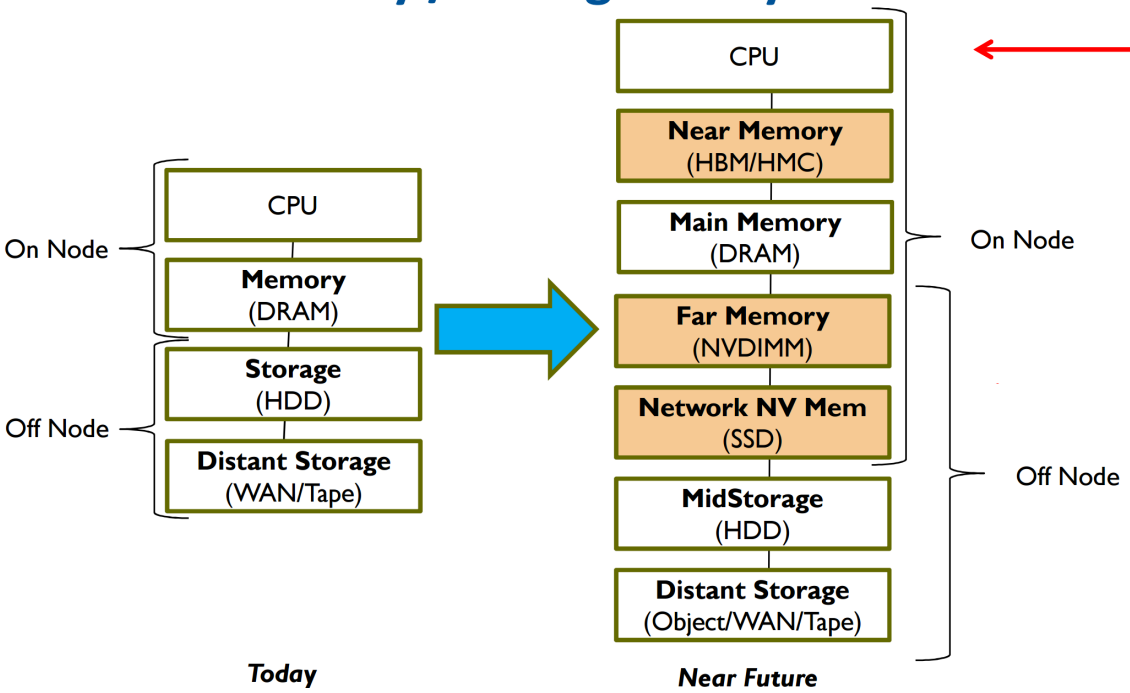
http://science.energy.gov/ascr/research/scidac/exascale-challenges/

- Power. Power, power, power.
  - Naively scaling current supercomputers to exascale would require a dedicated nuclear power plant to operate.
    - ALCF's Mira: 4 MW, 0.01 exaflop
    - "The target is 20-40 MW in 2020 for 1 exaflop"
- *Many* more threads. Less memory and performance per thread.
- Memory bandwidth
  - "Memory bandwidth is not expected to scale with floating-point performance."
- I/O
  - "The I/O system at all levels – chip to memory, memory to I/O node, I/O node to disk—will be much harder to manage, as I/O bandwidth is unlikely to keep pace with machine speed."

Exascale I/O Challenges

https://hpcuserforum.com/presentations/paris-munich/CRAY.HPCUserForumOctoberParis%202015CRAY.pdf

Trends in the Memory / Storage Subsystem



CRAY + accelerators

Memory bandwidth and I/O are difficult to scale. Need to combine available technologies to achieve reasonable scaling.

What Comes After Exascale?

"Post-Moore Computing"

Quantum Computing is the leading contender

Quantum Computing (Epoch: Terra Incognita)

- What is exciting about Quantum Computing?
  (Generically, **Quantum Information Science, QIS**)
- Early example: factoring large numbers
  - Taken from LA-UR-97-4986 "Cryptography, Quantum Computation and Trapped Ions," Richard J. Hughes (1997)

Size of modulus (bits)	1,024	2,048	4,096
Factoring time in 1997	10^7 years	$3x10^{17}$ years	$2x10^{31}$ years
Factoring time in 2006	10^5 years	$5x10^{15}$ years	$3x10^{29}$ years
Factoring time in 2015	2,500 years	$7x10^{13}$ years	$4x10^{27}$ years
Factoring time in 2024	38 years	10^{12} years	$7x10^{25}$ years
Factoring time in 2033	7 months	$2x10^{10}$ years	10^{24} years
Factoring time in 2042	3 days	$3x10^8$ years	$2x10^{22}$ years

Table 2: Projected future factoring times using the GNFS for various moduli using 1,000 workstations.

Size of modulus (bits)	512	1,024	2,048	4,096
Quantum memory (qubits)	2,564	5,124	10,244	20,484
Number of quantum gates	$3x10^9$	$3x10^{10}$	$2x10^{11}$	$2x10^{12}$
Quantum factoring time	33 seconds	4.5 minutes	36 minutes	4.8 hours

Table 3: Quantum factoring times of various moduli on a hypothetical 100-MHz QC.

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HEPAP Meeting (earlier this week!)

- https://science.energy.gov/hep/hepap/meetings/201706/
- Jim Siegrist:
  - **QIS identified as a national (interagency) and Office of Science priority**
  - **HEP QIS emphasis (both near-term and long-term) is on:**
    - P5 science drivers – exploiting entanglement and QIS technology
    - New computational and foundational techniques via QIS
    - Advancing the national QIS enterprise
- Glen Crawford:
  - **Increased funding in FY18 Request for Computational Physics will support new Quantum Information Science (QIS) and advanced computing initiatives**
    - QIS is Administration and SC priority which provided additional funds to HEP ($15M) in late stages of FY18 budget development
    - HEP to work with ASCR and other SC offices to develop R&D plan that takes advantage of particular HEP capabilities (e.g., theory, SRF cavities, sensor development)

What is Needed for (HEP) Quantum Computing

- Hardware
  - No non-trivial (more than a few qubits) quantum computers currently exist!
    - Quantum computers expected to start rival existing supercomputers around 50 qubits
    - Google and IBM are promising 50-qubit quantum computers later this year
      - Just the beginning…
- Software (quantum algorithms)
  - Existing supercomputers are massively parallel
    - Most current HEP applications are trivially parallel
  - Existing quantum algorithms are for large, coupled problems

- I call it “Terra Incognita” for a reason

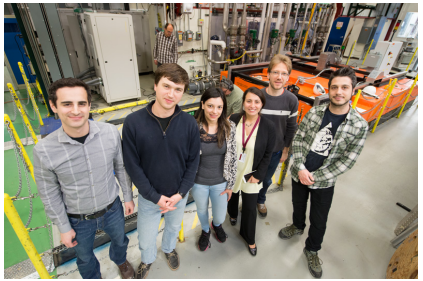
Fermilab Quantum Hardware Initiatives

- Quantum sensors
  - Adapting quantum devices for use as quantum sensors for particle physics experiments such as direct dark matter detection

- Superconducting technologies
  - Some quantum computers use superconducting cavities similar to those we develop for accelerators.

- Quantum networks
  - We have agreed to host a quantum network on site in collaboration with Caltech and AT&T

Quantum sensors for axion search LDRD by Aaron Chou, Andrew Sonnenschein, and Dan Bowring



Fermilab SRF group is in a R&D collaboration with U. Chicago and Argonne

Quantum networks visit with John Donovan of AT&T

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Quantum Algorithms for HEP

- Quantum algorithms are very different from today's HEP software

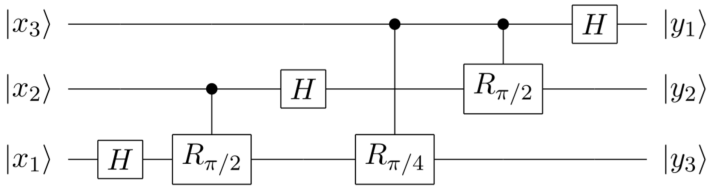
```
void transform(complex<double>* f, int N) //
{
  ordina(f, N);
  complex<double> *W;
  W = (complex<double> *)malloc(N / 2 * sizeof(complex<double>));
  W[1] = polar(1., -2. * M_PI / N);
  W[0] = 1;
  for(int i = 2; i < N / 2; i++)
    W[i] = pow(W[1], i);
  int n = 1;
  int a = N / 2;
  for(int j = 0; j < log2(N); j++) {
    for(int i = 0; i < N; i++) {
      if(!(i & n)) {
        complex<double> temp = f[i];
        complex<double> Temp = W[(i * a) % (n * a)] * f[i + n];
        f[i] = temp + Temp;
        f[i + n] = temp - Temp;
      }
    }
    n *= 2;
    a = a / 2;
  }
}

void FFT(complex<double>* f, int N, double d)
{
  transform(f, N);
  for(int i = 0; i < N; i++)
    f[i] *= d; //multiplying by step
}
```

Fast Fourier Transform in C++

The 3-qubit quantum Fourier transform is the following operation:

$$|x_1, x_2, x_3\rangle \mapsto \frac{1}{\sqrt{2^3}} \left(|0\rangle + e^{2\pi i\,[0.x_3]}|1\rangle\right) \otimes \left(|0\rangle + e^{2\pi i\,[0.x_2 x_3]}|1\rangle\right) \otimes \left(|0\rangle + e^{2\pi i\,[0.x_1 x_2 x_3]}|1\rangle\right).$$

This quantum circuit implements the quantum Fourier transform on the quantum state $|x_1, x_2, x_3\rangle$.



The quantum gates used in the circuit above are the Hadamard gate and the controlled phase gate R_θ.

3-qubit Quantum Fourier Transform

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Fermilab Quantum Algorithm Initiatives

- Finding good matches for quantum computers in HEP is challenging
  - Ultimately, quantum computers will probably allow us to solve problems we are not currently even attempting
- Quantum Field Theory applications are promising
  - Preliminary work from Jordan, Lee and Preskill
  - Lattice QCD?
  - Just getting started
- Partial Differential Equations
  - Major supercomputing topic
  - Used in accelerator modeling
  - Also getting started
- Optimization Problems
  - Possible uses in HEP analyses
- ???
  - Creativity needed
    - This means you!

Conclusions

- HEP Computing is changing for reasons based on both physics and economics
  - Computing properties have ceased to improve in the way they were improving (physics!)
  - HEP data continues to grow (physics!)
  - HEP large-scale computing is no longer large on the commercial scale (economics!)
  - DOE is launching the largest supercomputing effort ever, the Exascale Program (physics and economics!!)
    - HEP computing is small compared to the entire Exascale Program (economics!)
  - The next stage beyond exascale will be very different (physics!)
    - Quantum Computing (QIS) is the leading contender for the way forward

- Fermilab Computing is working to anticipate these changes with
  - HEPCloud
  - multithreading efforts (and beyond) for advanced architectures, including exascale,
  - and the beginnings of a QIS effort