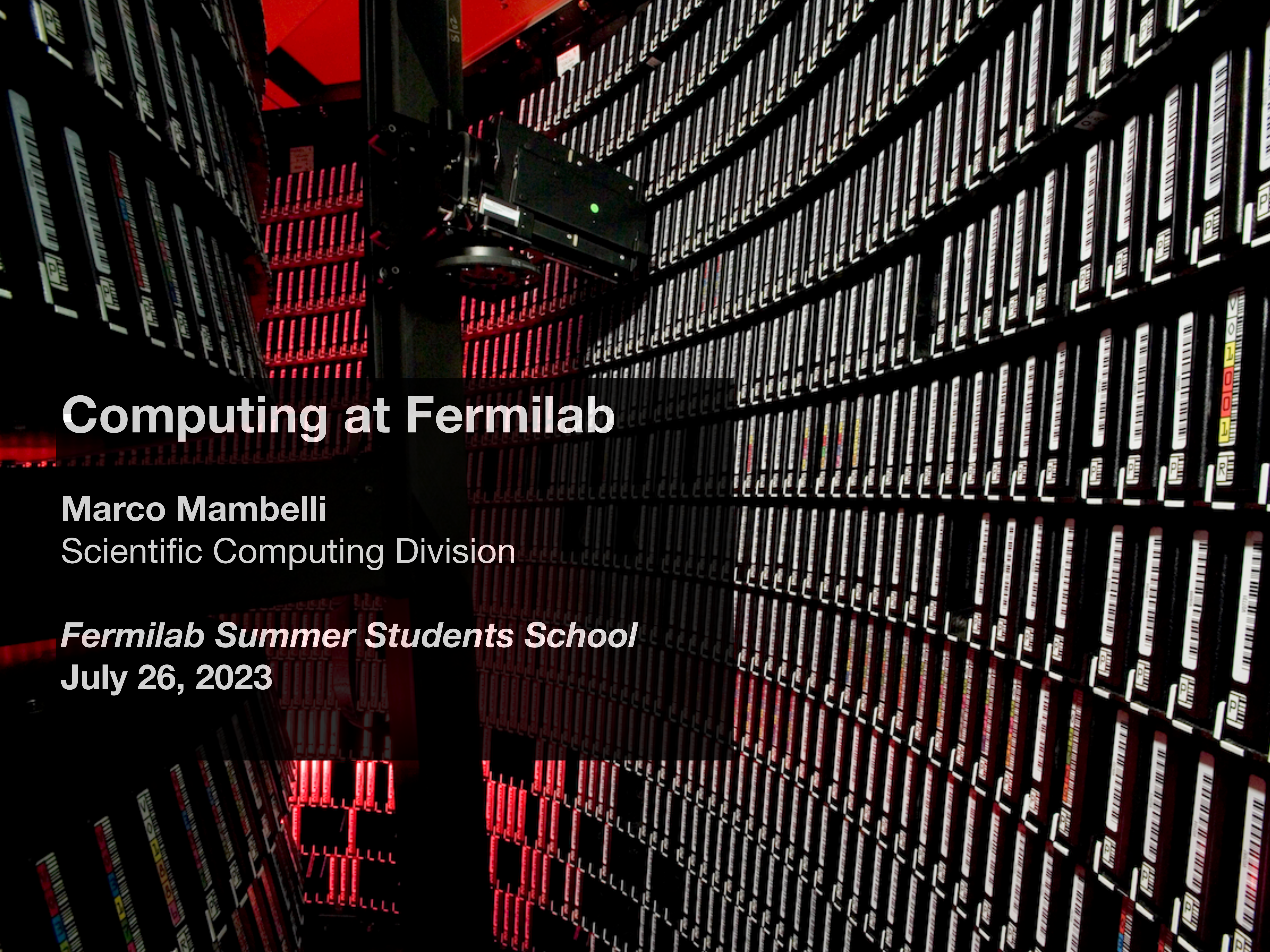
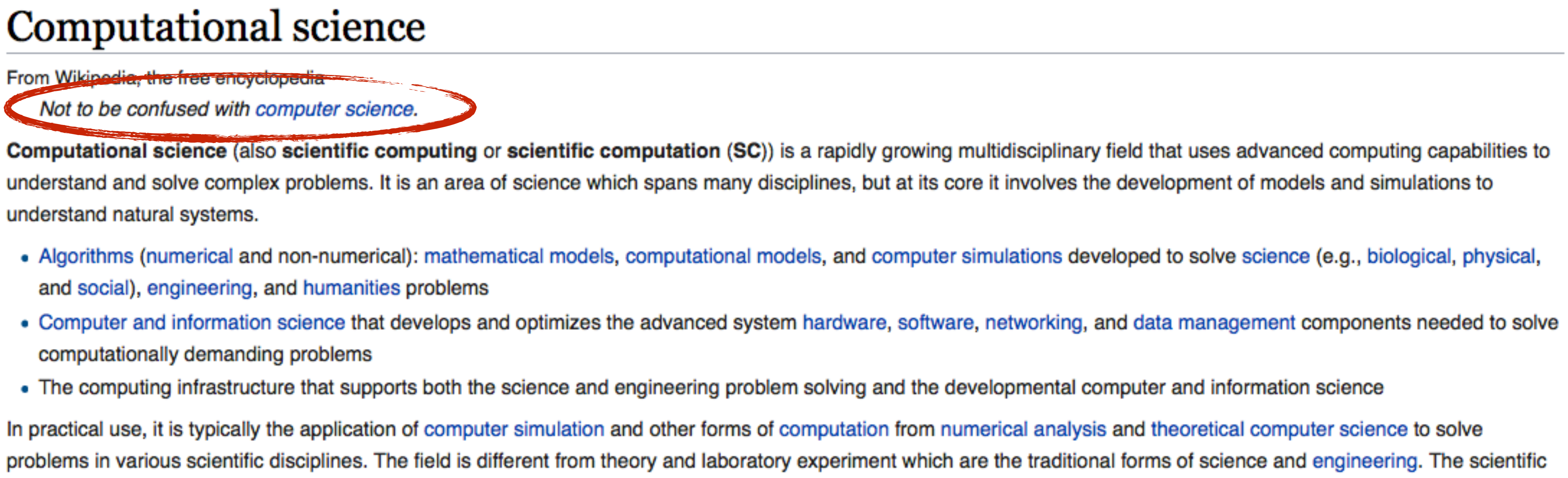


Computing at Fermilab

Marco Mambelli
Scientific Computing Division

Fermilab Summer Students School
July 26, 2023

What is scientific computing?



Computational science

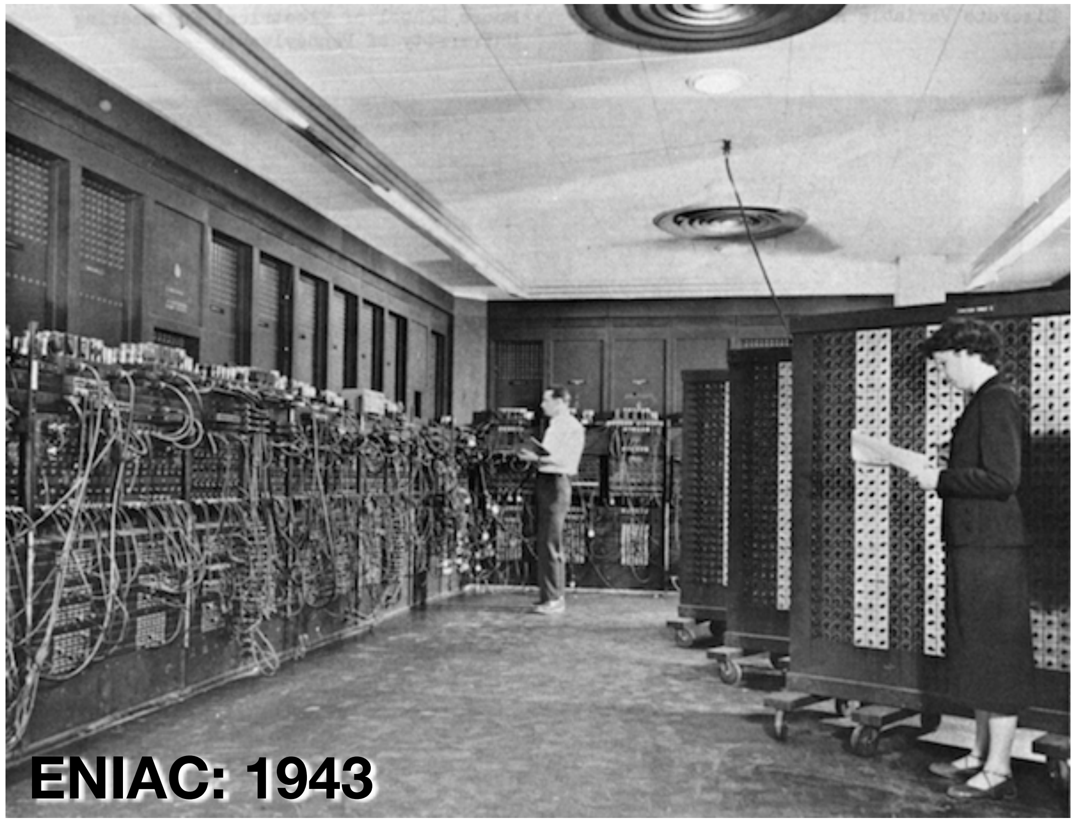
From Wikipedia, the free encyclopedia

Not to be confused with computer science.

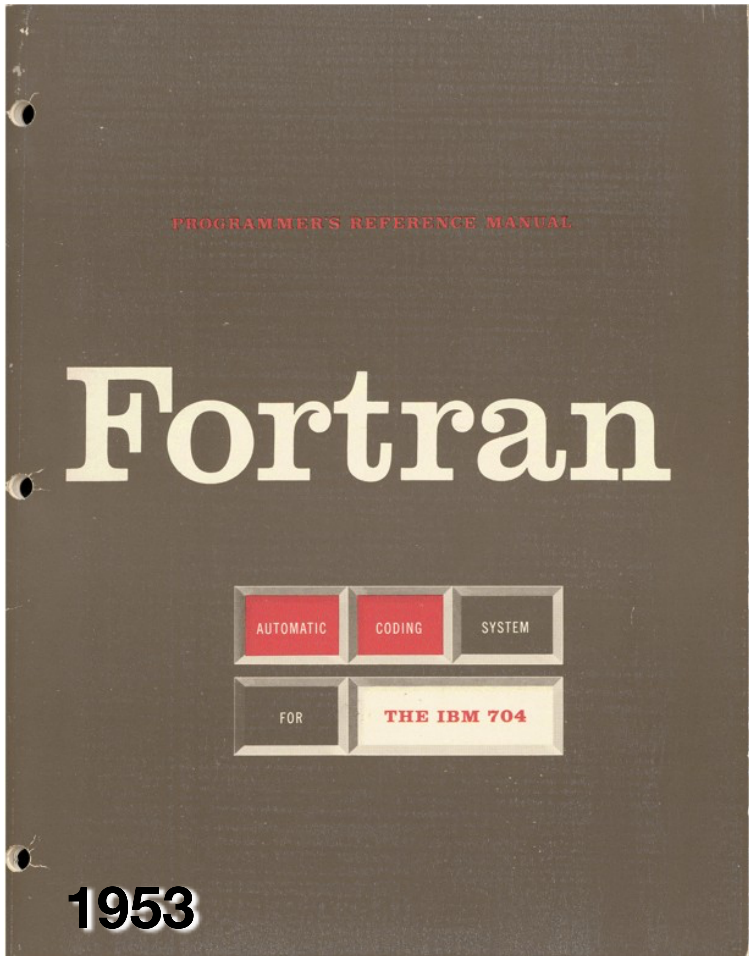
Computational science (also **scientific computing** or **scientific computation** (**SC**)) is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems. It is an area of science which spans many disciplines, but at its core it involves the development of models and simulations to understand natural systems.

- Algorithms (numerical and non-numerical): mathematical models, computational models, and computer simulations developed to solve science (e.g., biological, physical, and social), engineering, and humanities problems
- Computer and information science that develops and optimizes the advanced system hardware, software, networking, and data management components needed to solve computationally demanding problems
- The computing infrastructure that supports both the science and engineering problem solving and the developmental computer and information science

In practical use, it is typically the application of computer simulation and other forms of computation from numerical analysis and theoretical computer science to solve problems in various scientific disciplines. The field is different from theory and laboratory experiment which are the traditional forms of science and engineering. The scientific

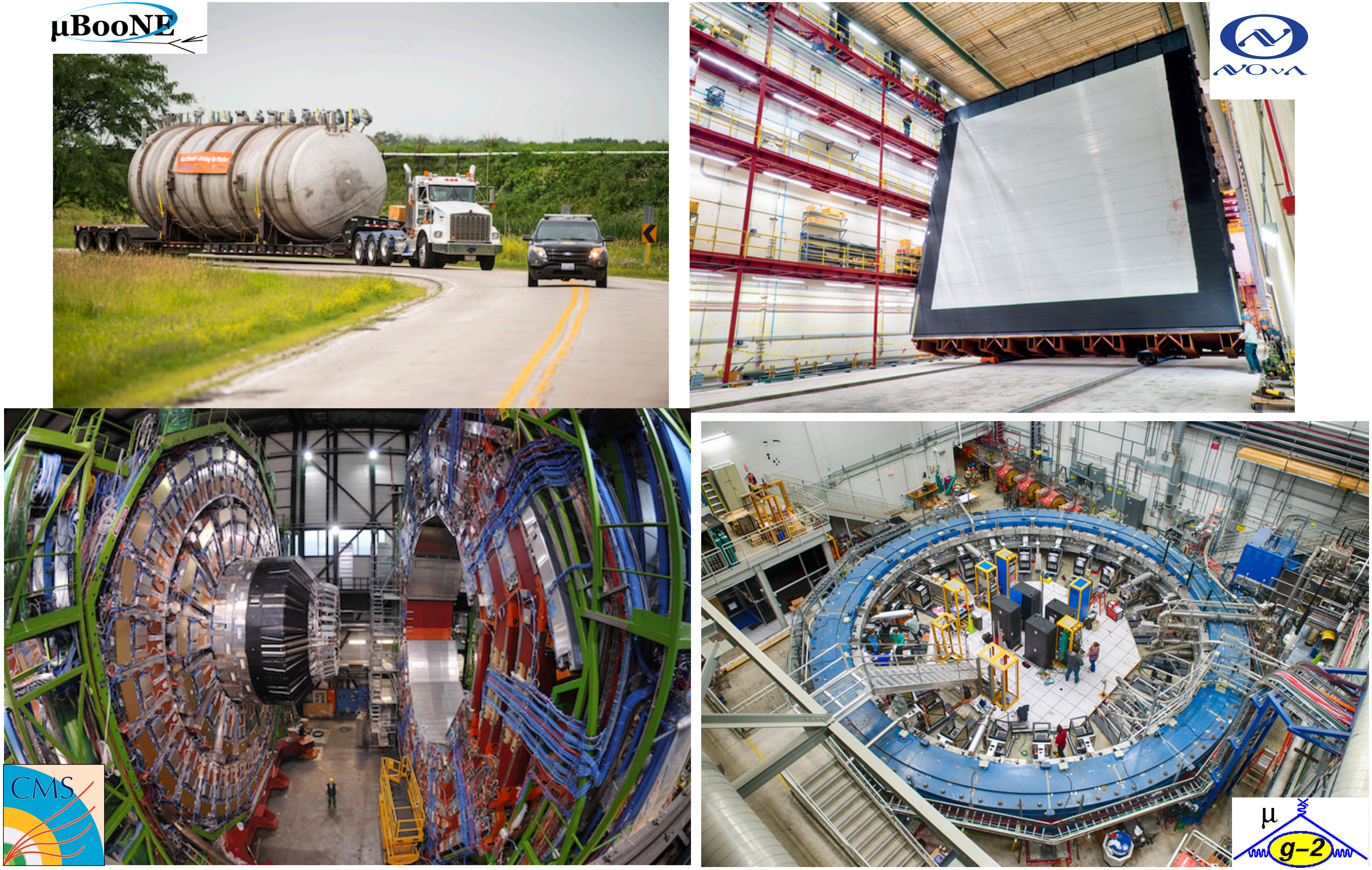


ENIAC: 1943

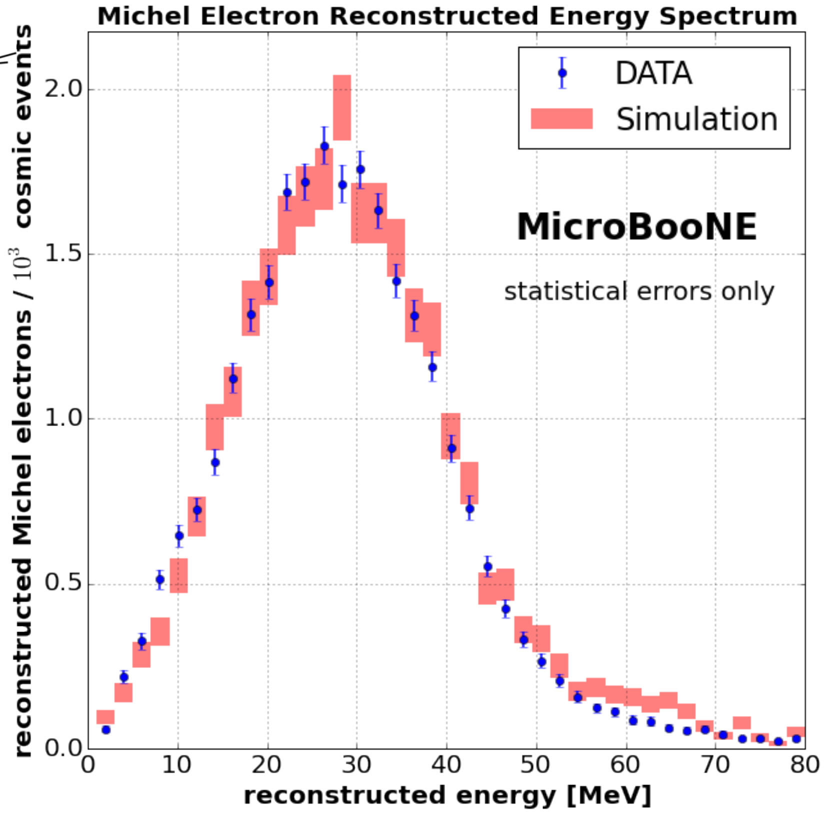


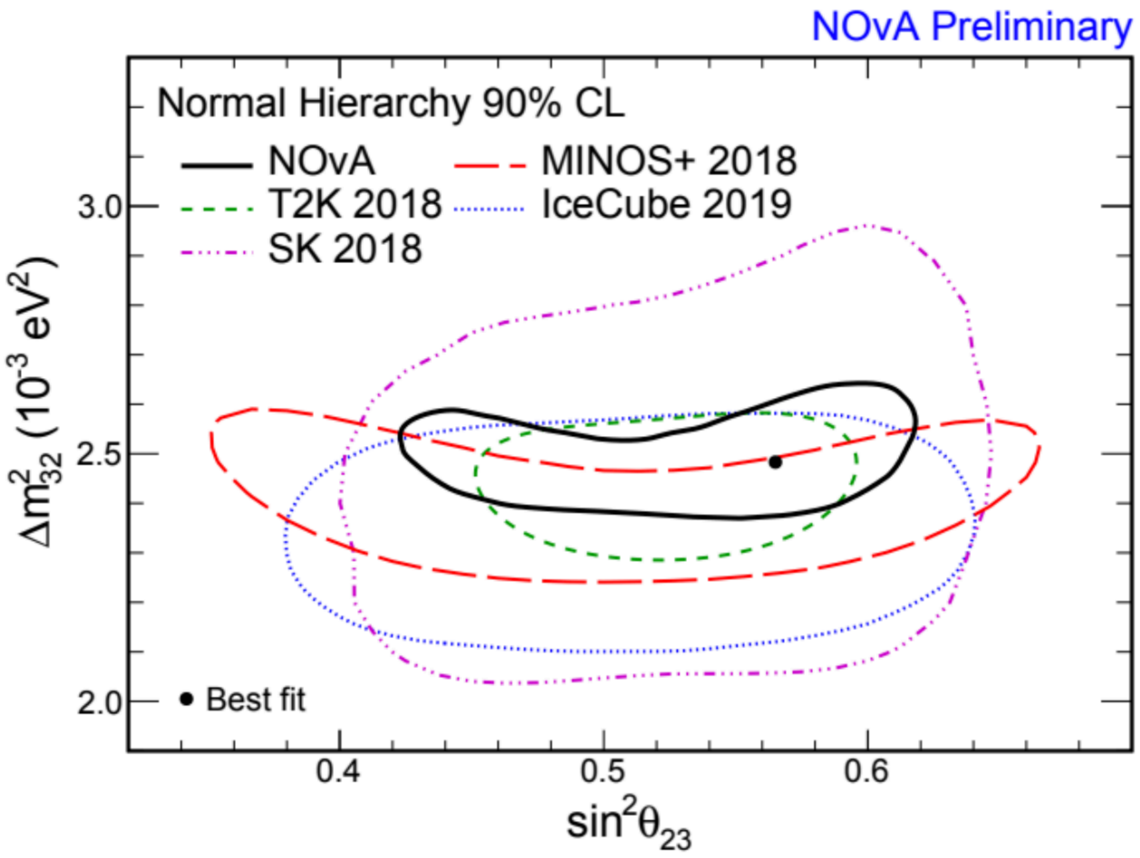
1953

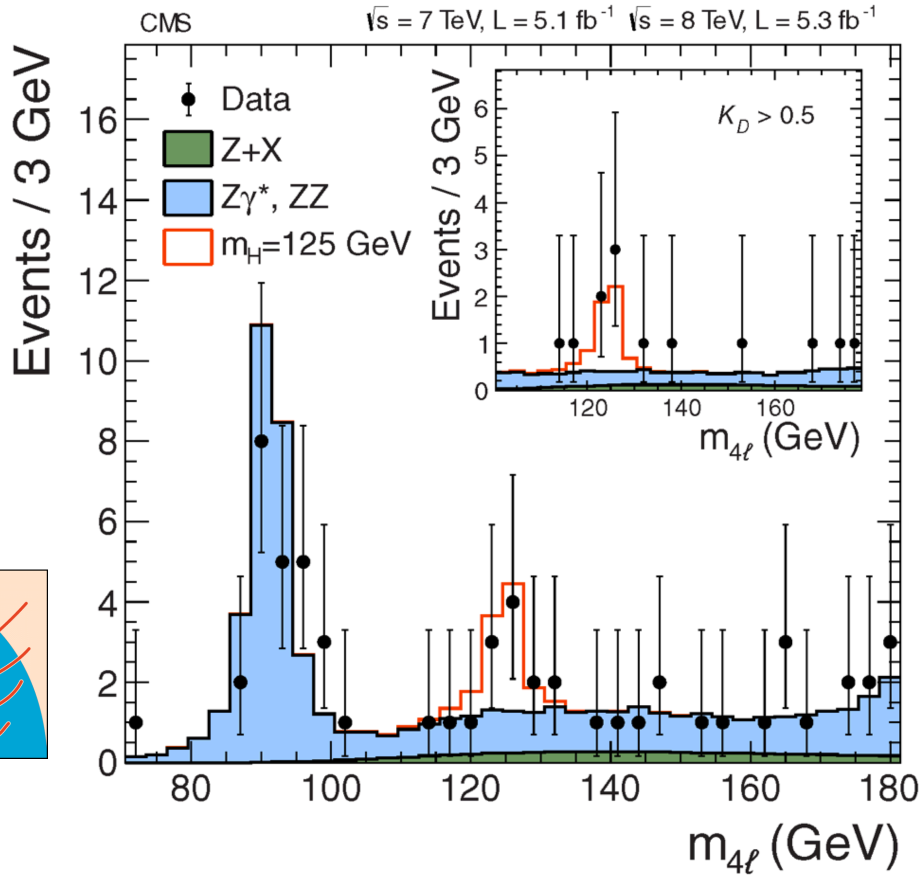
Scientific Computing in HEP: Getting from here…

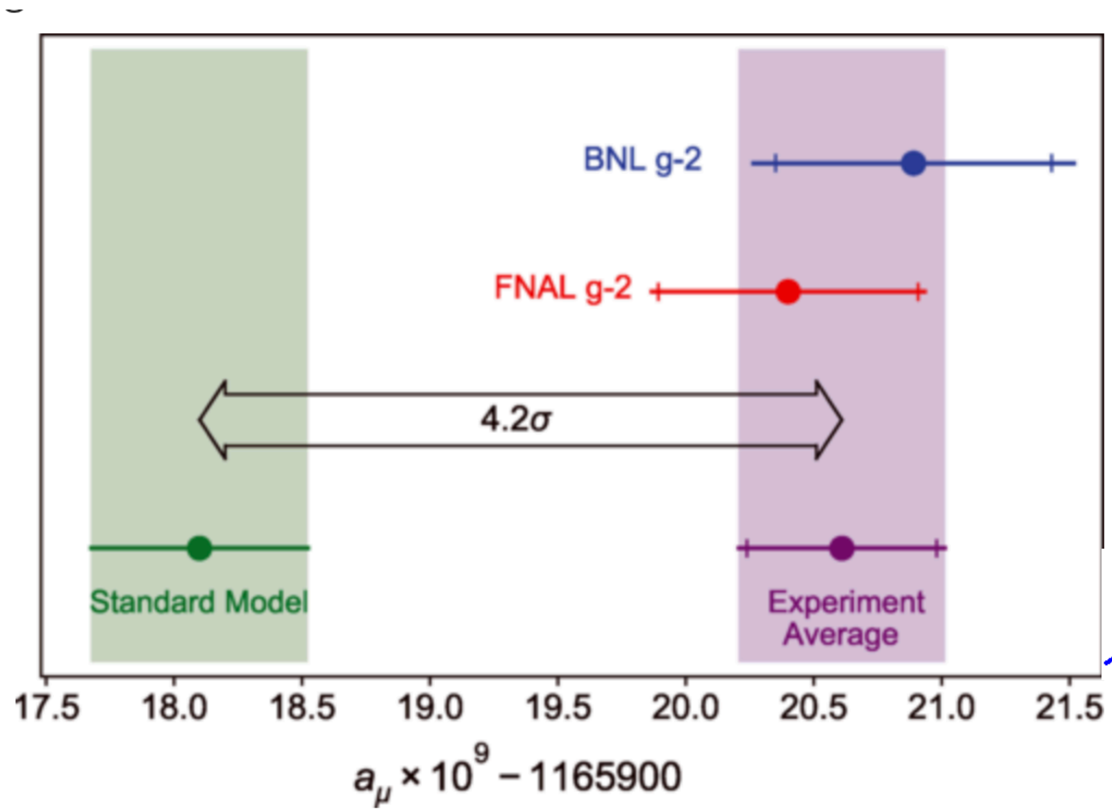


…to here


Michel Electron Reconstructed Energy Spectrum
DATA
Simulation
MicroBooNE
statistical errors only
reconstructed Michel electrons / 10^3 cosmic events
0.0
0.5
1.0
1.5
2.0
0
10
20
30
40
50
60
70
80
reconstructed energy [MeV]

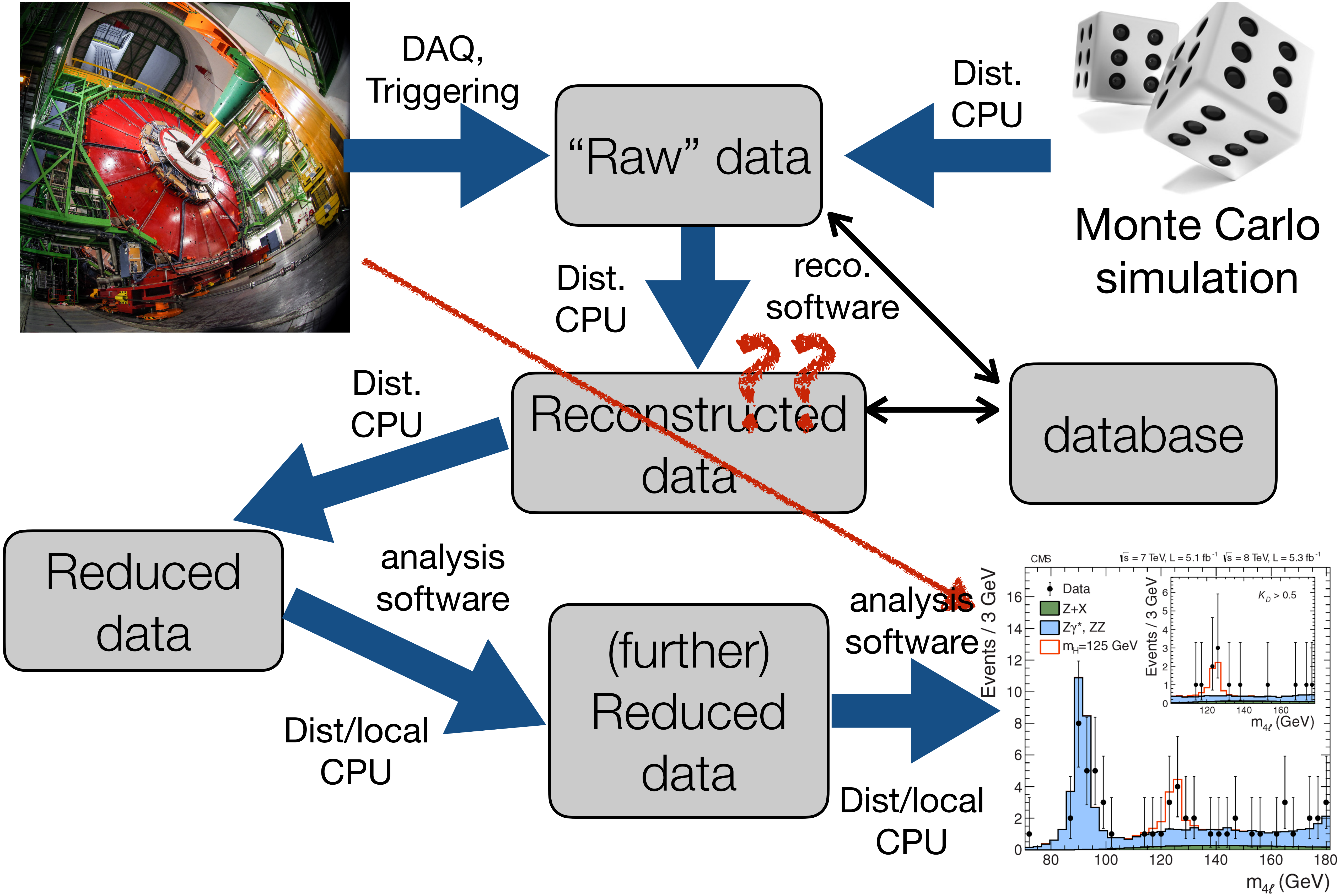

NOvA Preliminary
Normal Hierarchy 90% CL
NOvA
MINOS+ 2018
T2K 2018
IceCube 2019
SK 2018
Best fit
Δm^2_{32} (10^{-3} eV^2)
2.0
2.5
3.0
0.4
0.5
0.6
$\sin^2\theta_{23}$


CMS
$\sqrt{s}$ = 7 TeV, L = 5.1 fb^{-1} $\sqrt{s}$ = 8 TeV, L = 5.3 fb^{-1}
Data
Z+X
Zγ*, ZZ
m_H=125 GeV
Events / 3 GeV
0
2
4
6
8
10
12
14
16
80
100
120
140
160
180
$m_{4\ell}$ (GeV)
K_D > 0.5
Events / 3 GeV
0
1
2
3
4
5
6
120
140
160
$m_{4\ell}$ (GeV)


BNL g-2
FNAL g-2
4.2σ
Standard Model
Experiment Average
17.5
18.0
18.5
19.0
19.5
20.0
20.5
21.0
21.5
$a_\mu \times 10^9 - 1165900$

Software

The process



DAQ, Triggering

"Raw" data

Dist. CPU

Monte Carlo simulation

Dist. CPU

reco. software

??

Reconstructed data

database

Dist. CPU

Reduced data

analysis software

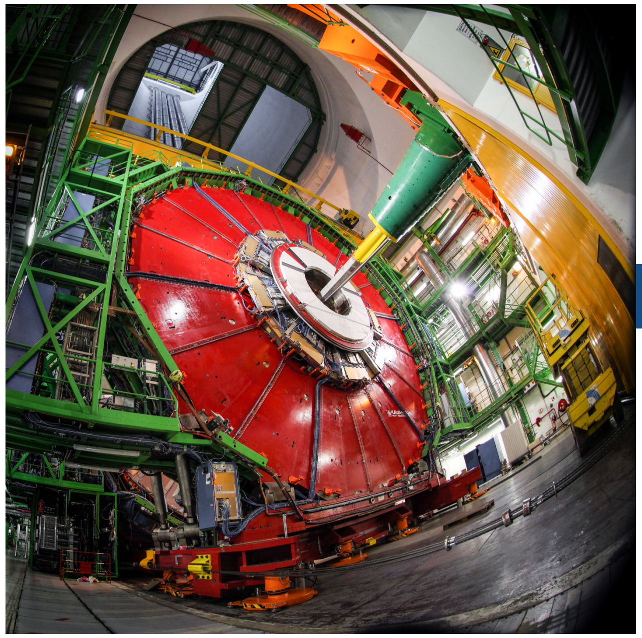
(further) Reduced data

analysis software

Dist/local CPU

Dist/local CPU

Reconstruction



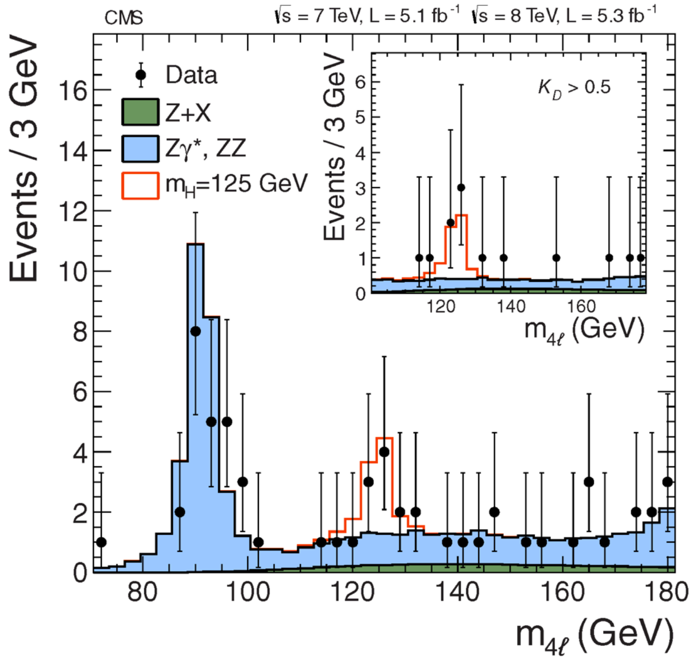
"Raw" data

Monte Carlo simulation

Reconstructed data

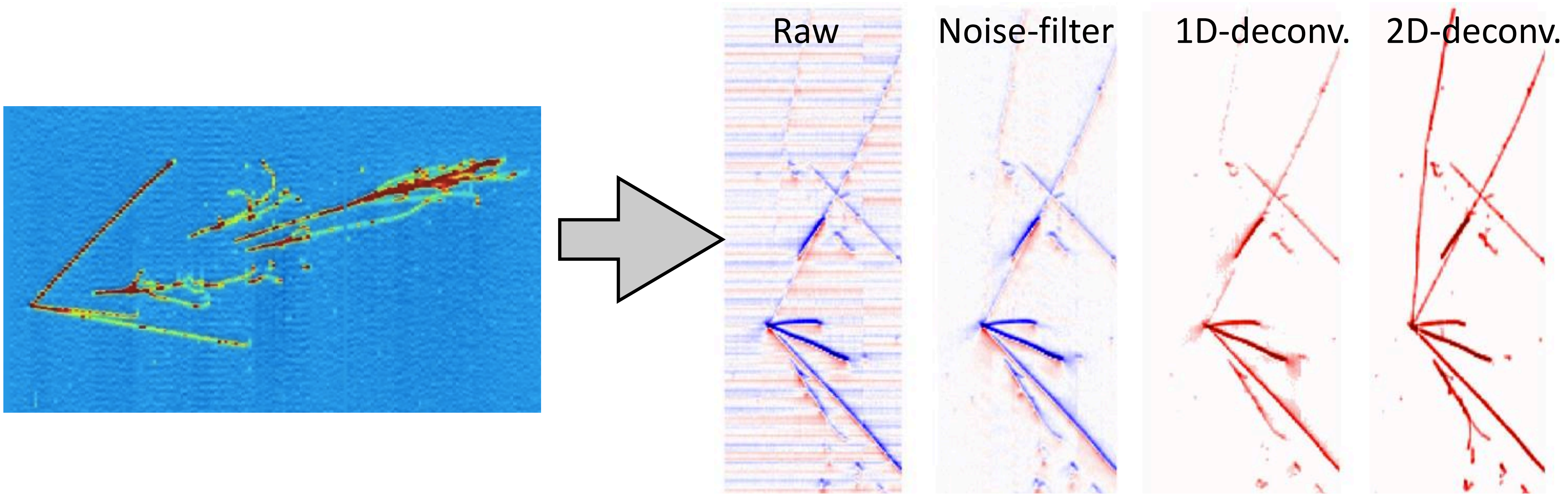
Reduced data

(further) Reduced data

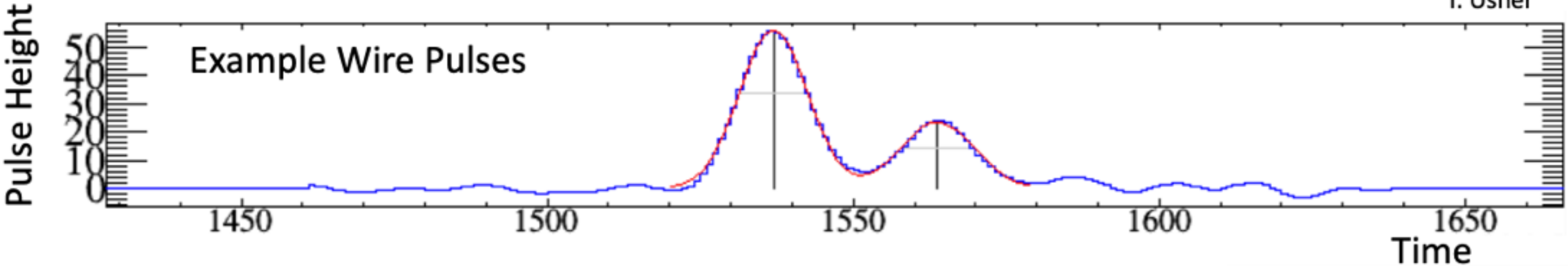


Reconstruction: LArSoft (MicroBooNE)

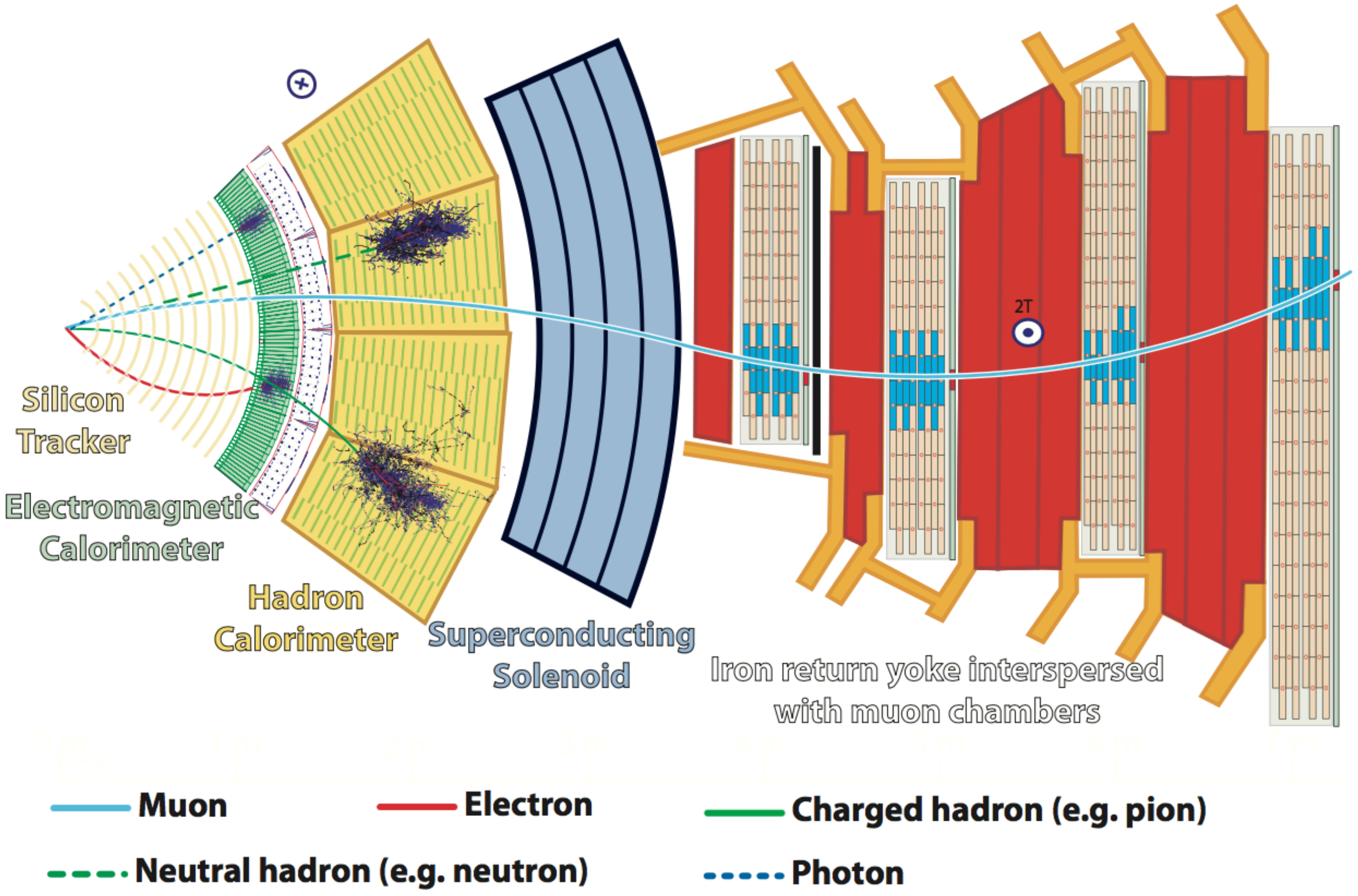
- **LArSoft**, developed at Fermilab, is a common code base for LAr neutrino detectors
  - Used by MicroBooNE, SBND, ICARUS, DUNE
  - Includes tools for both reconstruction and data analysis



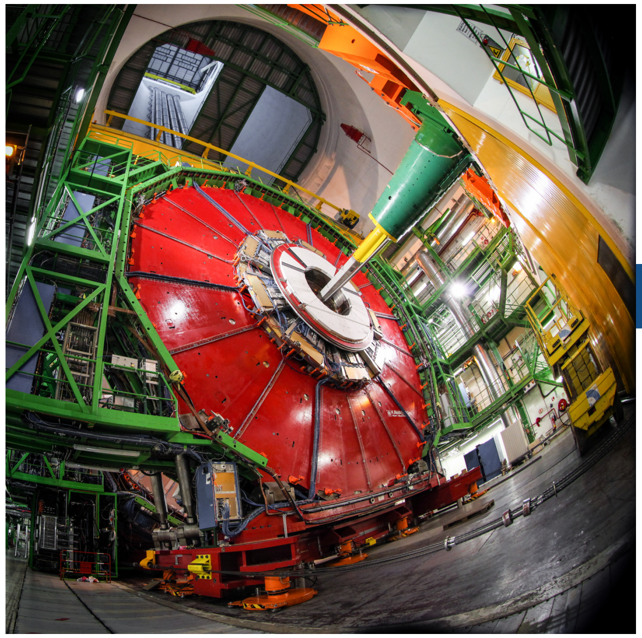
T. Usher



Reconstruction: CMS



Simulation



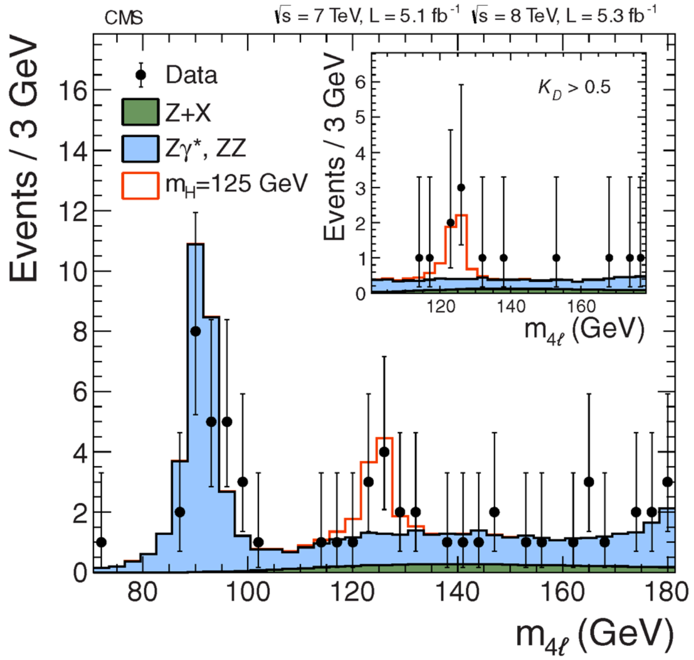
“Raw” data

Monte Carlo simulation

Reconstructed data

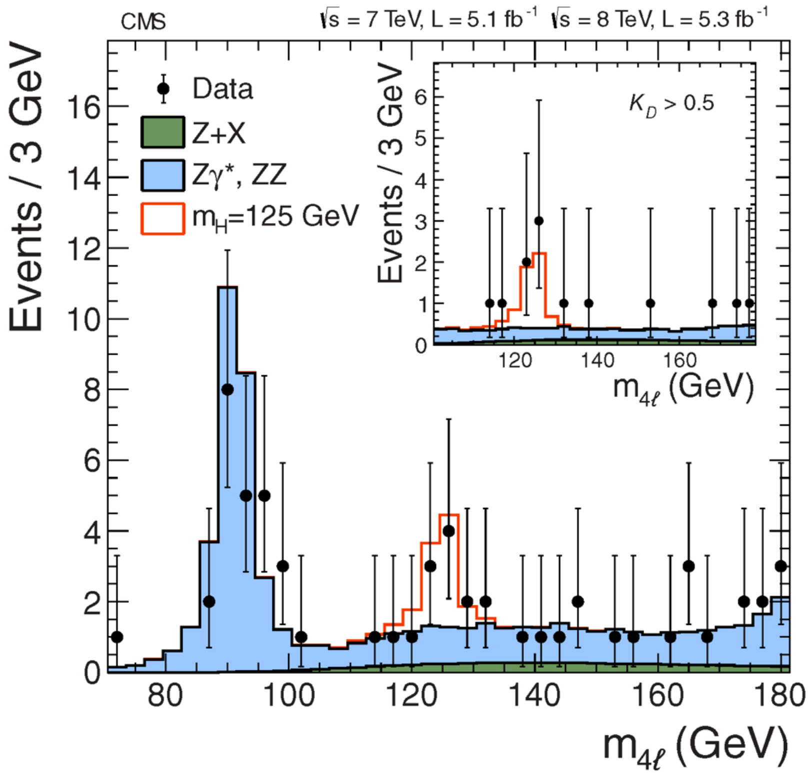
Reduced data

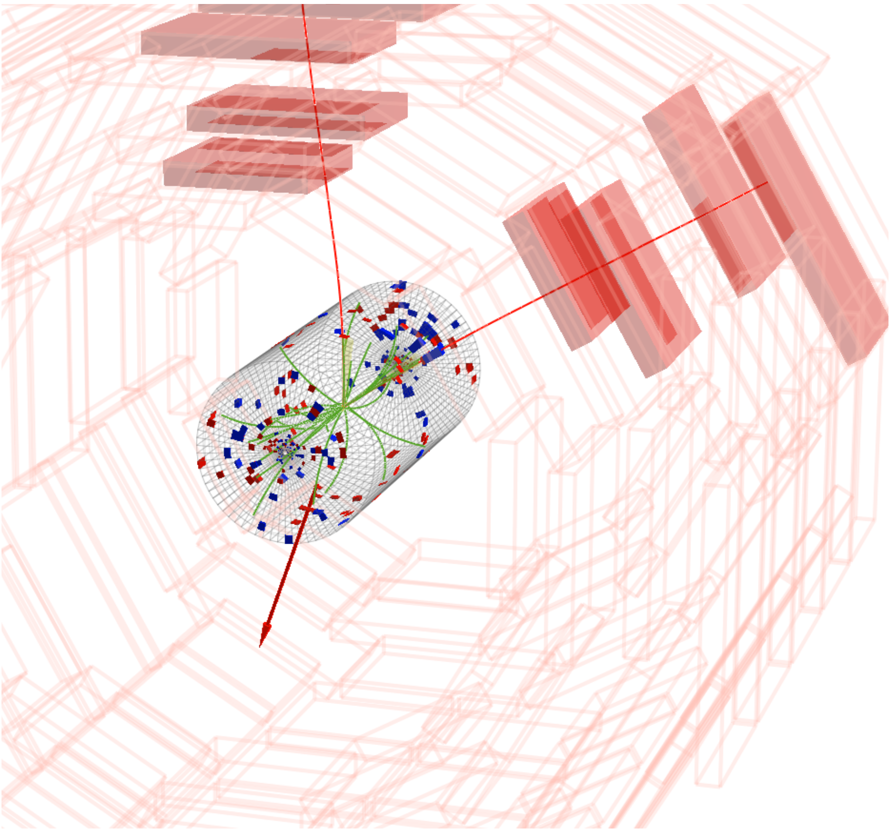
(further) Reduced data



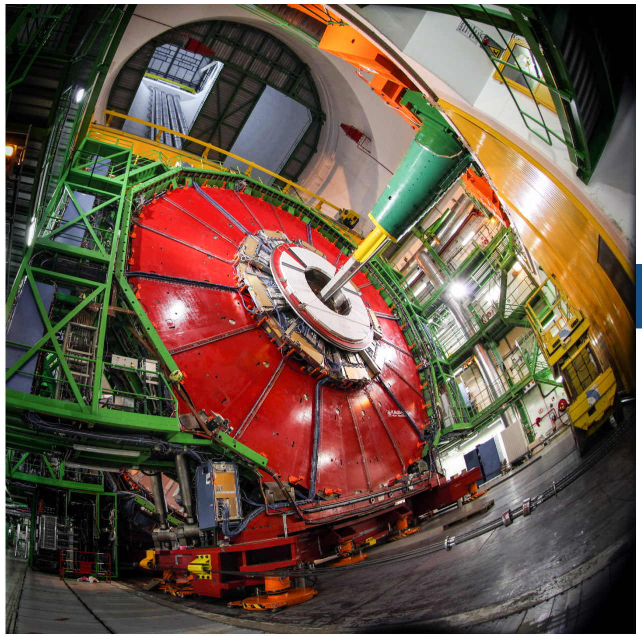
Simulation

- **Simulated events** are crucial to science at HEP experiments
  - Rely on **Monte Carlo Simulation** to produce these events
- **Event generators** simulate the underlying particle interaction of interest
- Resulting interaction event is then fed to a **detector simulator**
  - Consider the **material** and **geometry** of every part of the detector
  - Simulate how particles from interaction and decay would propagate
  - Most detector simulations use **GEANT**
    - Also used in nuclear and accelerator physics as well as medical and space science





Analysis



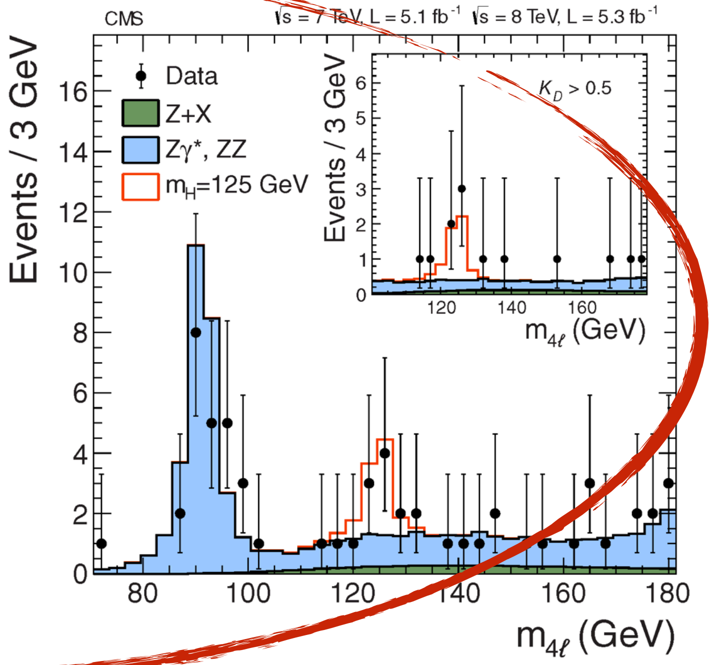
“Raw” data

Monte Carlo
simulation

Reconstructed
data

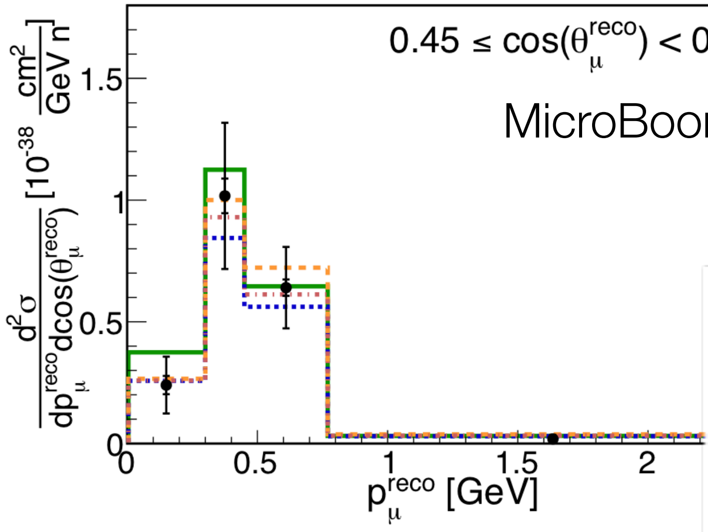
Reduced
data

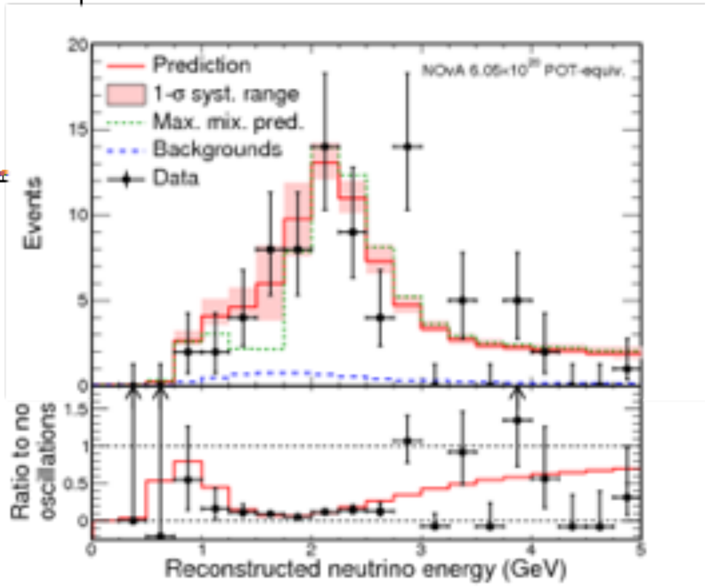
(further)
Reduced
data

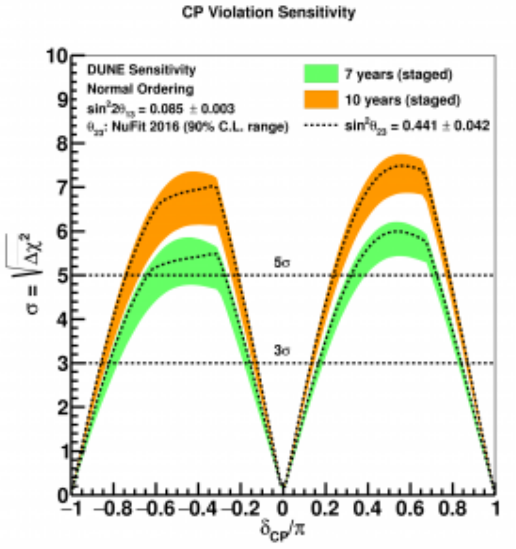


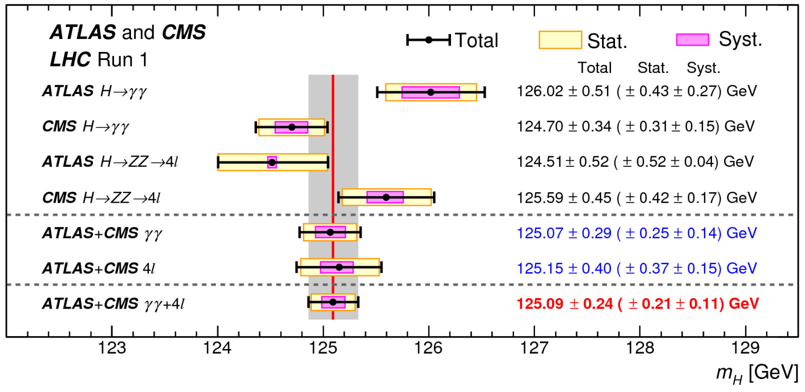
Analysis

- Getting from data events of interest to plots, tables, and numbers
  - This is the computing step nearly all HEP experimentalists are familiar with
- Common tools are needed
  - Mathematical functions
  - Statistical analysis
  - Plotting/histogramming
- Nearly all HEP experiments use the **ROOT** framework
  - Developed by CERN and Fermilab
  - **C++** (object oriented)
  - Couples with code written in other languages (e.g. Python)
  - https://pos.sissa.it/093/002/pdf





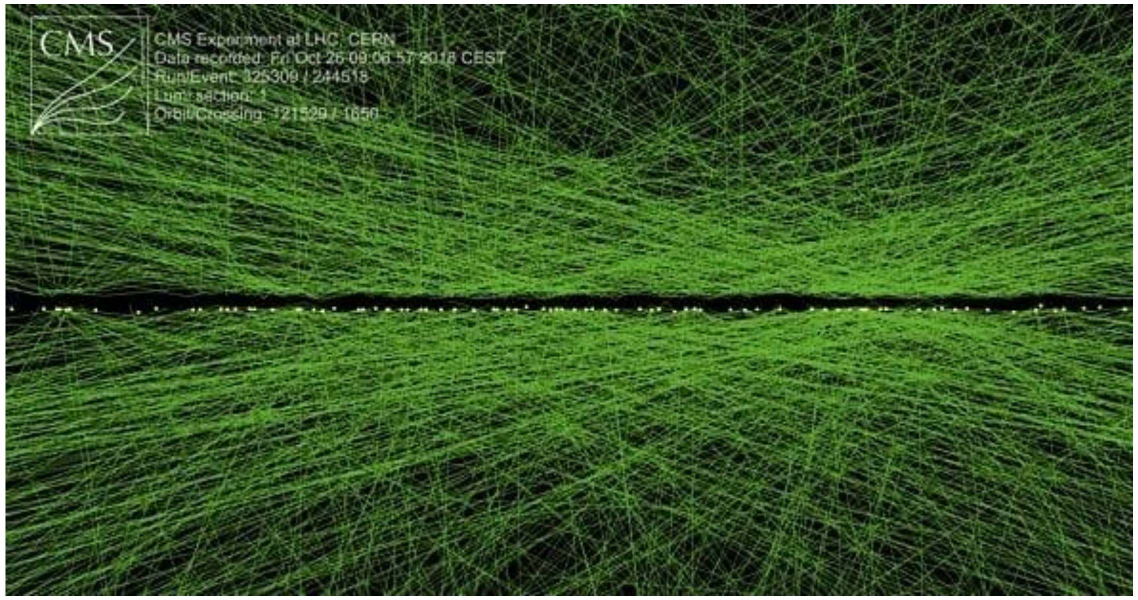


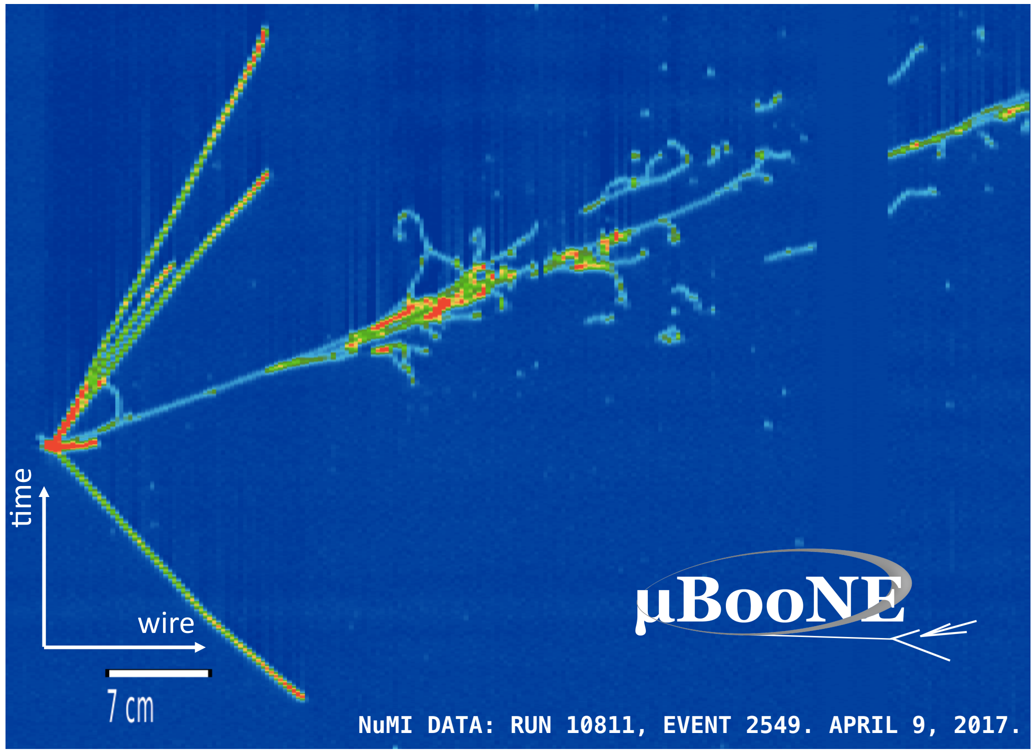


Hardware (CPUs, Storage and Networks)

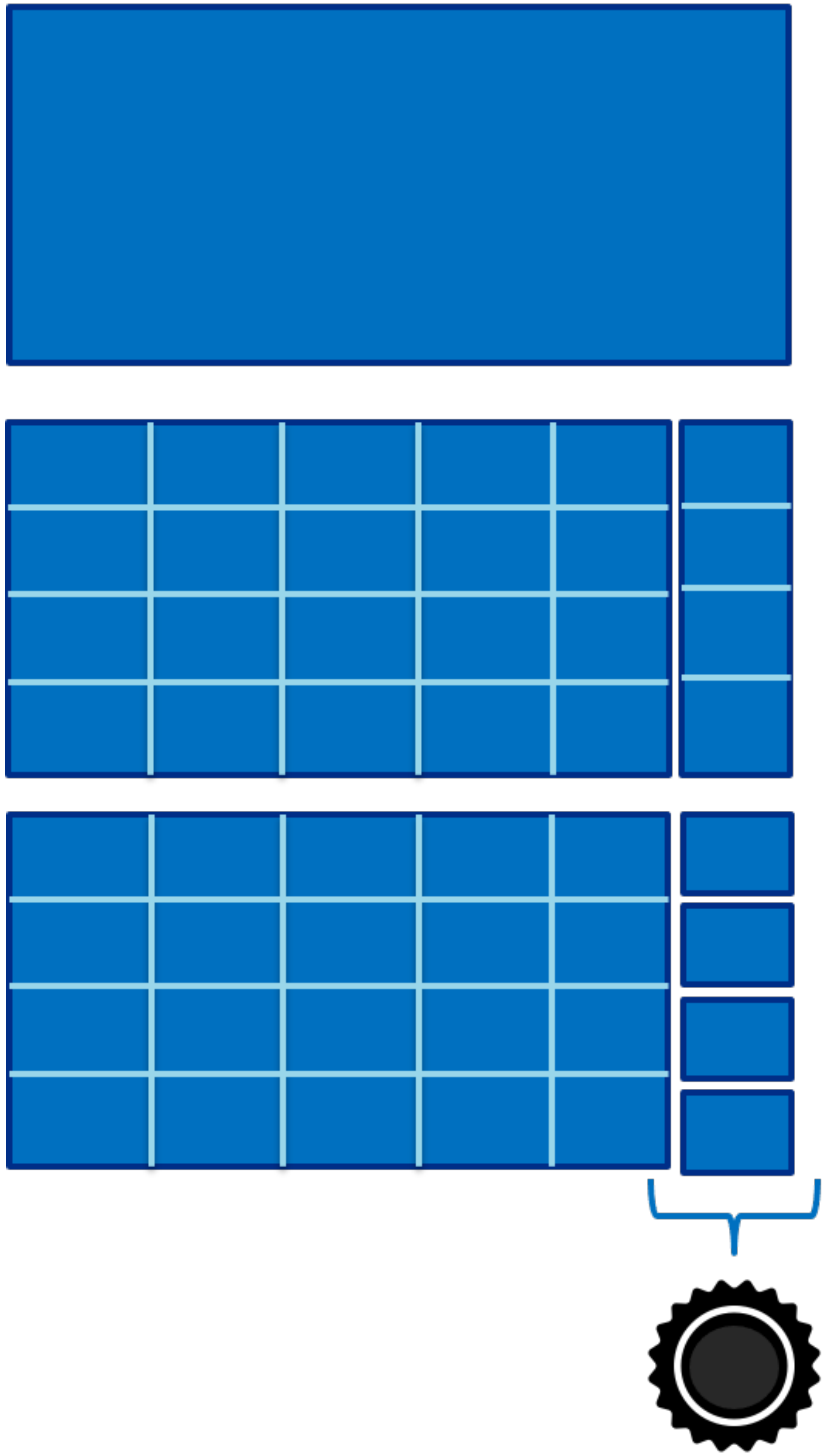
CPU

- **Reconstruction** and **simulation** of events are biggest CPU drivers
- Such computing is **“pleasantly parallel”**
    - Processing one event is completely independent of processing any other
    - Relatively short processing times but **many events** and **growing complexity**
- **CMS -** typical collider experiment
    - ~30 s/event (~30x more in a decade!)
    - ~billions events (simulated+collision)/month
- **MicroBooNE -** liquid Argon (LAr) neutrino experiment
    - ~1-2 min/event
    - ~million events (simulated+beam)/month
    - 1 event in DUNE will have ~50x more channels (!)





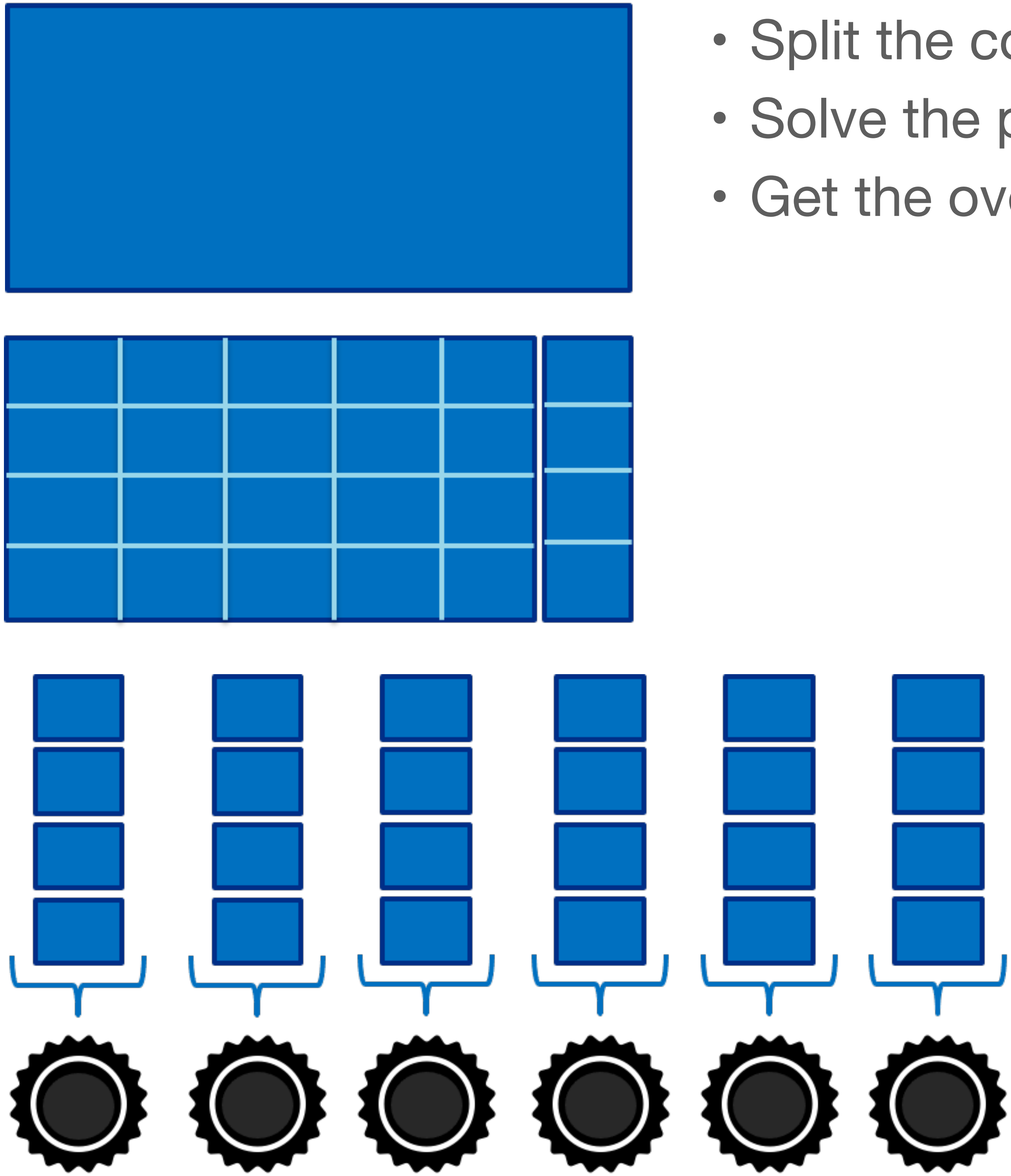
Divide et Impera



- Split the complex problem
- Solve the parts (jobs)
- Get the overall solution

Divide et Impera

- Split the complex problem
- Solve the parts (jobs)
- Get the overall solution

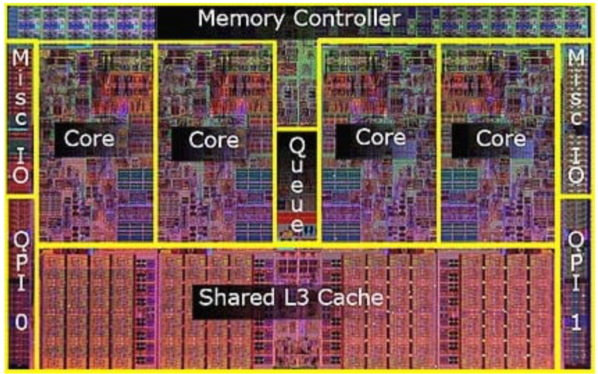


Get it fast!

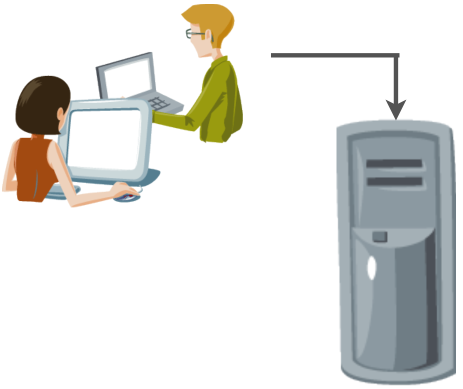
High Throughput Computing (HTC)

Divide et Impera: 1 Billion Events

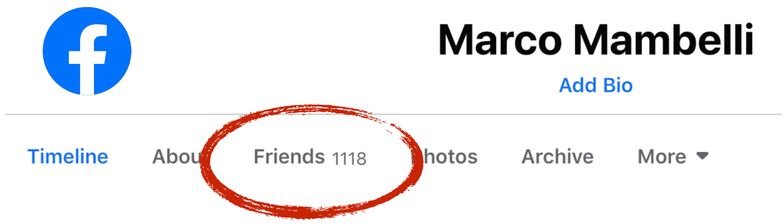
- Use one computer for the CMS events?
  - CPU: Central Processing Unit (typically whole chip)
    - Between 2 and 64 individual cores
    - Each core can process one instruction at a time

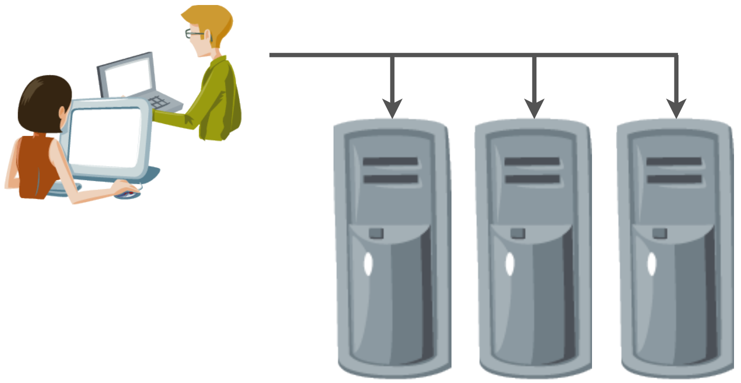


30s/8 cores*1B events ~120 years



- Use your friends' computers as well
  - To get 1B events in one month, we require **1,440 8-core computers**
    - We are almost there with the friends!
  - Your **software and data** would need to get to each of those computers
  - You'd need to **collect output** from each
  - And you'd need **user accounts** on all of them

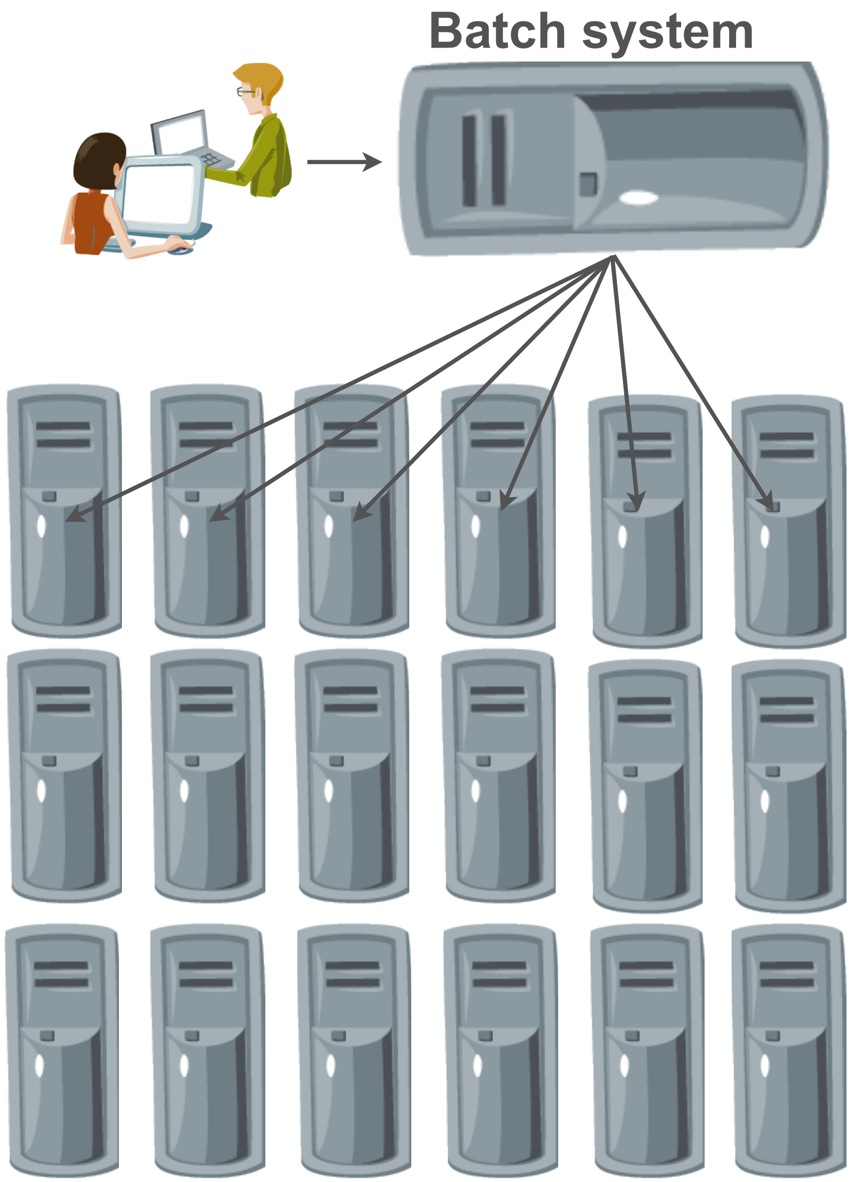




- Need to find an easier way to get from one computer to many!

Divide et Impera: batch systems

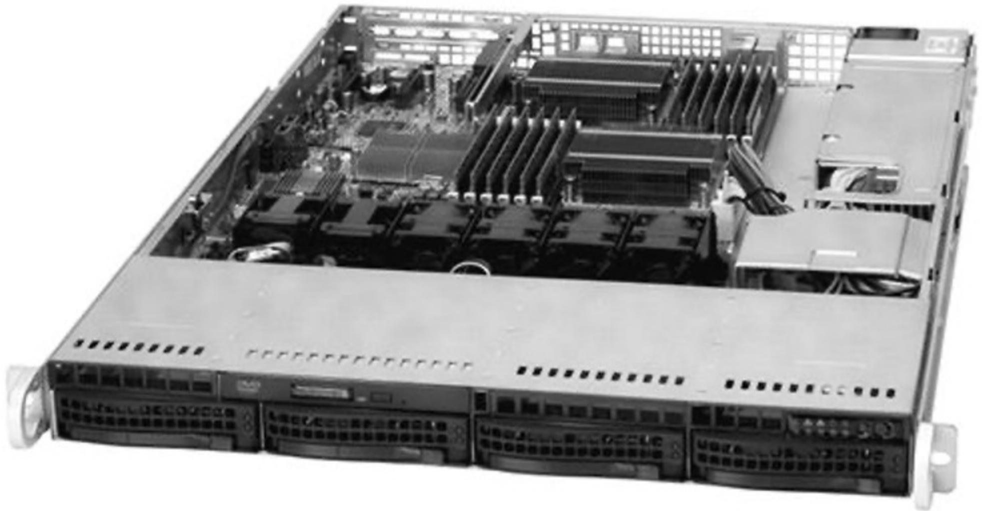
- Batch systems
  - Single entry point (queue for many users)
  - Jobs to any available slot
  - **Output** from each job handled in the same way
  - Batch system can handle user authentication on each individual computer



Some batch systems at Fermilab:
Fermigrid (~20k CPU cores)
US CMS Tier1 (~20k CPU cores)
CMS LPC (~5k CPU cores)

30s/20,000 cores*1B events ~17 days

Inside a Data Center: Computing Racks



Rack-mounted units "pizza boxes"
dual multi-core processors, large amount of memory, system and small local disk
Newest units with 64-core processors, 256 GB of memory, 100 Gb/s network
All running Linux!

Hot and Cold rows
Limited by power and cooling
GCC has a power capacity of ~ 2.5 Megawatts

The Two Fermilab Data Centers

Feynman Computing Center (FCC)

Two “logical” data centers (FCC2, FCC3)
High Availability, each has own generator / UPS system
Each a “corner” of a redundant network

GRID Computing Center (GCC)

Two “logical” data centers:

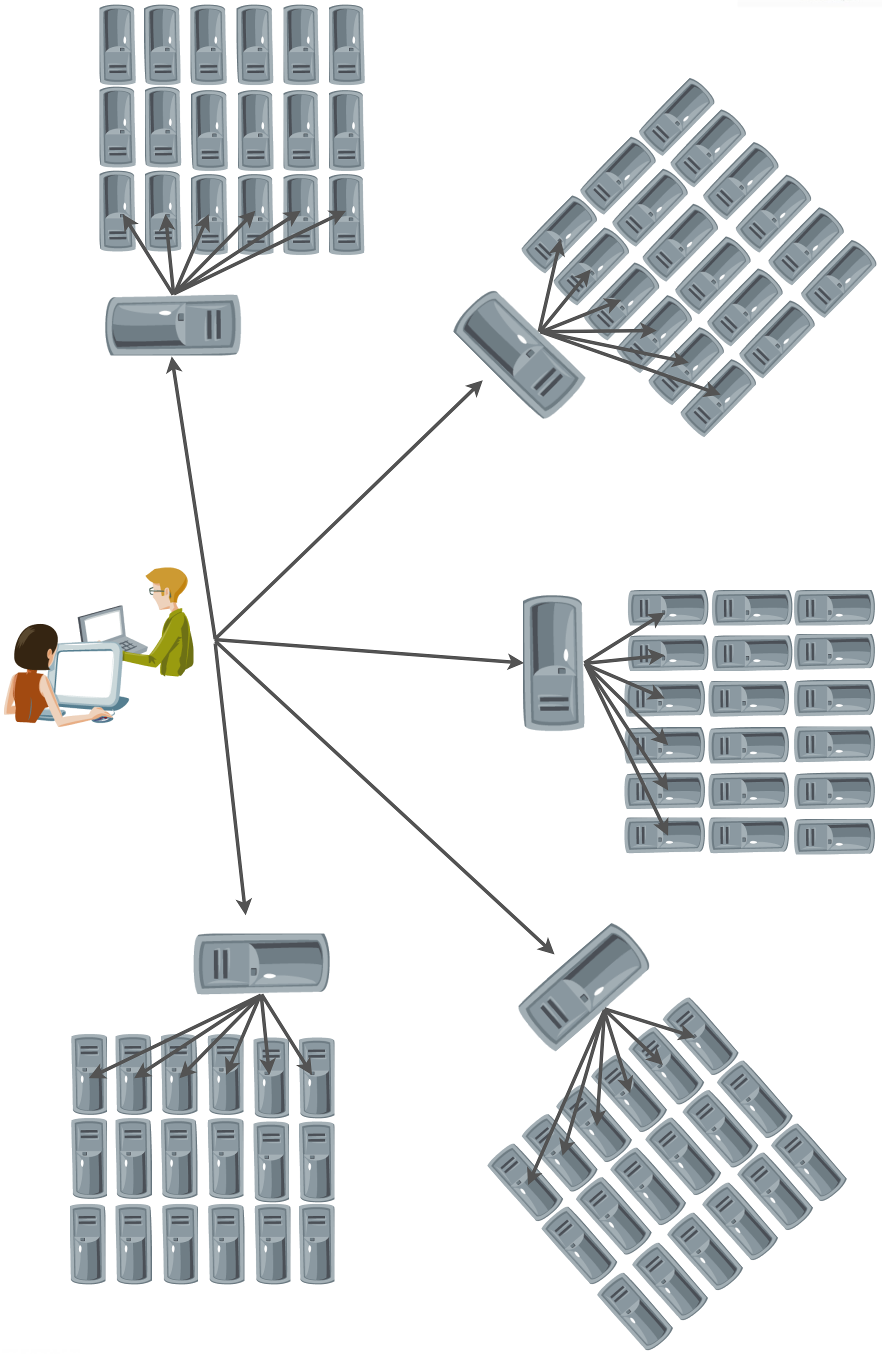
- Room A, Tape Room, Network Room A
- Rooms B, C, Network Room B

“Lights out” facility, with UPS systems, only good for minutes
Each a “corner” of a redundant network

Divide et Impera: the Grid

- Many batch systems accessible from one point: a computing **grid**
    - **grid sites** (batch systems) from universities and labs across the world into one grid
    - **Distributed high-throughput computing** (DHTC)
- Analogy: utility grids

- Delegated and Federated Trust Model
    - Use **tokens** (JWT) or **grid certificates** (x509) and **Virtual Organization** (VO)
    - A certificate is an encrypted “signature” that verifies you belong to an organization (e.g., a collaboration like NOvA)
    - Each site decides which VOs to trust



Open Science Grid

NORDUGRID

Grid Solution for Wide Area Computing and Data Handling

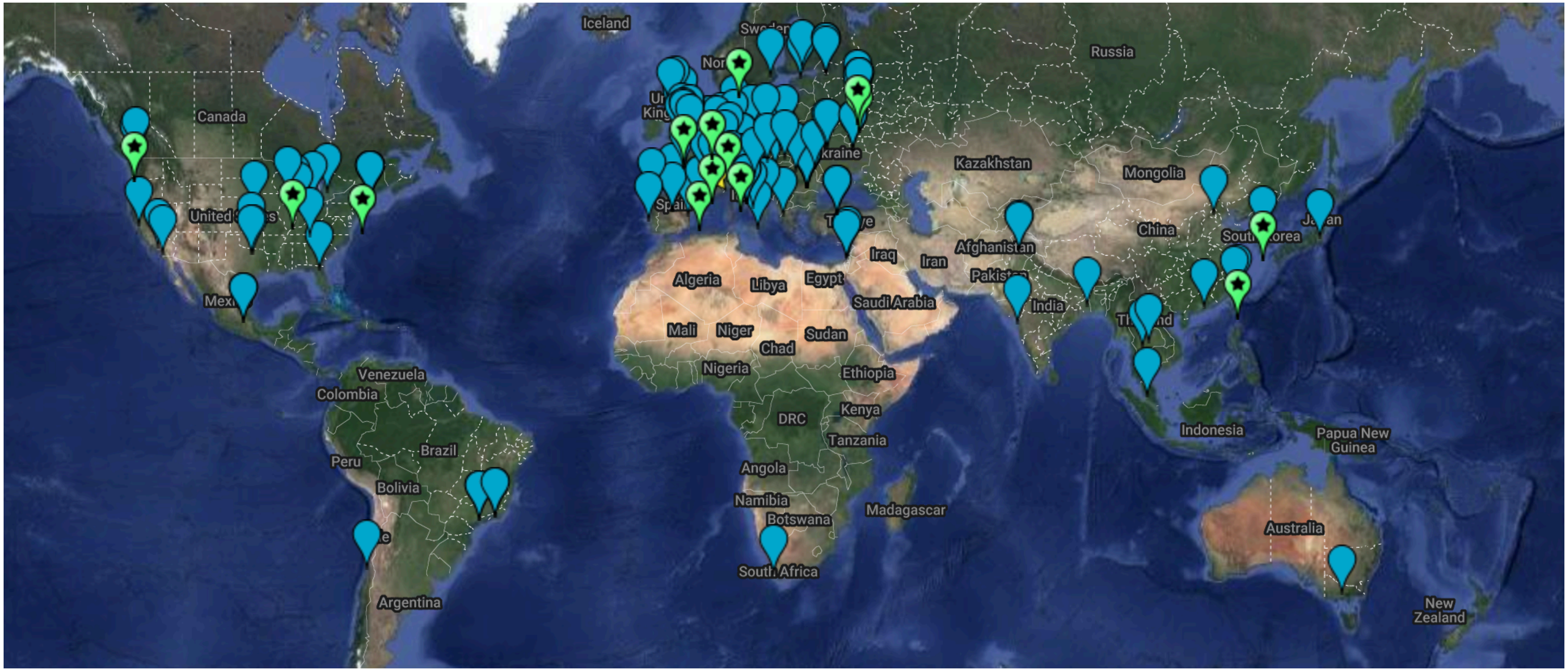
WLCG

Worldwide LHC Computing Grid

Overlapping grids

Overlapping grids

World LHC Computing Grid



200+ sites, 2M+ CPU cores

Divide et Impera: the Cloud

- And when you still don't have enough, then you can rent it
  - **Commercial Clouds** like AWS (Amazon), GCE (Google) and Azure (Microsoft) can rent you a seemly endless amount of computing power
  - **Elastic computing:** expands at will

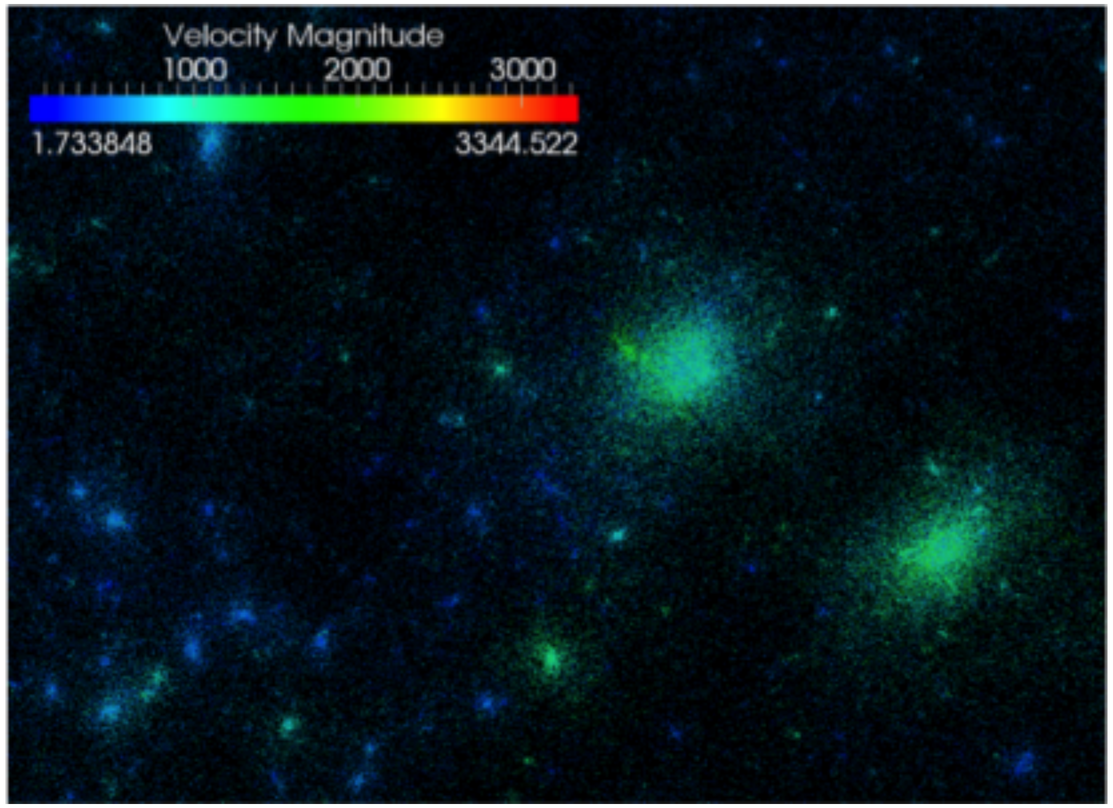
- Problem: irregular use pattern
- Solution: **burst-out** by **renting** resources on the Cloud for peak usage

- More expensive than local resources
- Difficult to justify non-capital expenditures

High Performance Computing

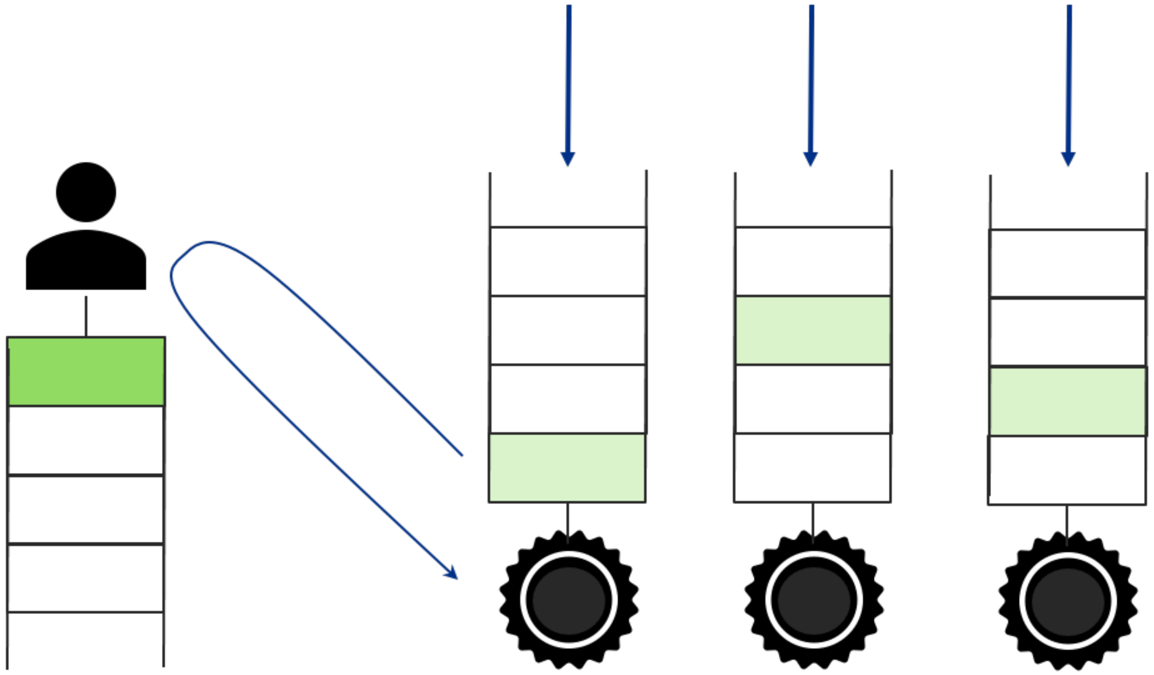
- Much scientific computing outside of experimental HEP is not "pleasantly parallel"
- Better platform: **High Performance Computing** (HPC)
  - Batch systems where individual computers are **interconnected** via high-speed links
  - Large HPC systems are often called "supercomputers"
- Fermilab has 5 HPC clusters
  - Total of 18.5k CPU cores
  - Used for Lattice QCD calculations, accelerator modeling, large-scale astrophysical simulations and testing
- Used also for event processing by splitting it into pieces

Aurora@Argonne: 20k CPUs 60k GPUs, 10PB memory, 2 DP exaflops

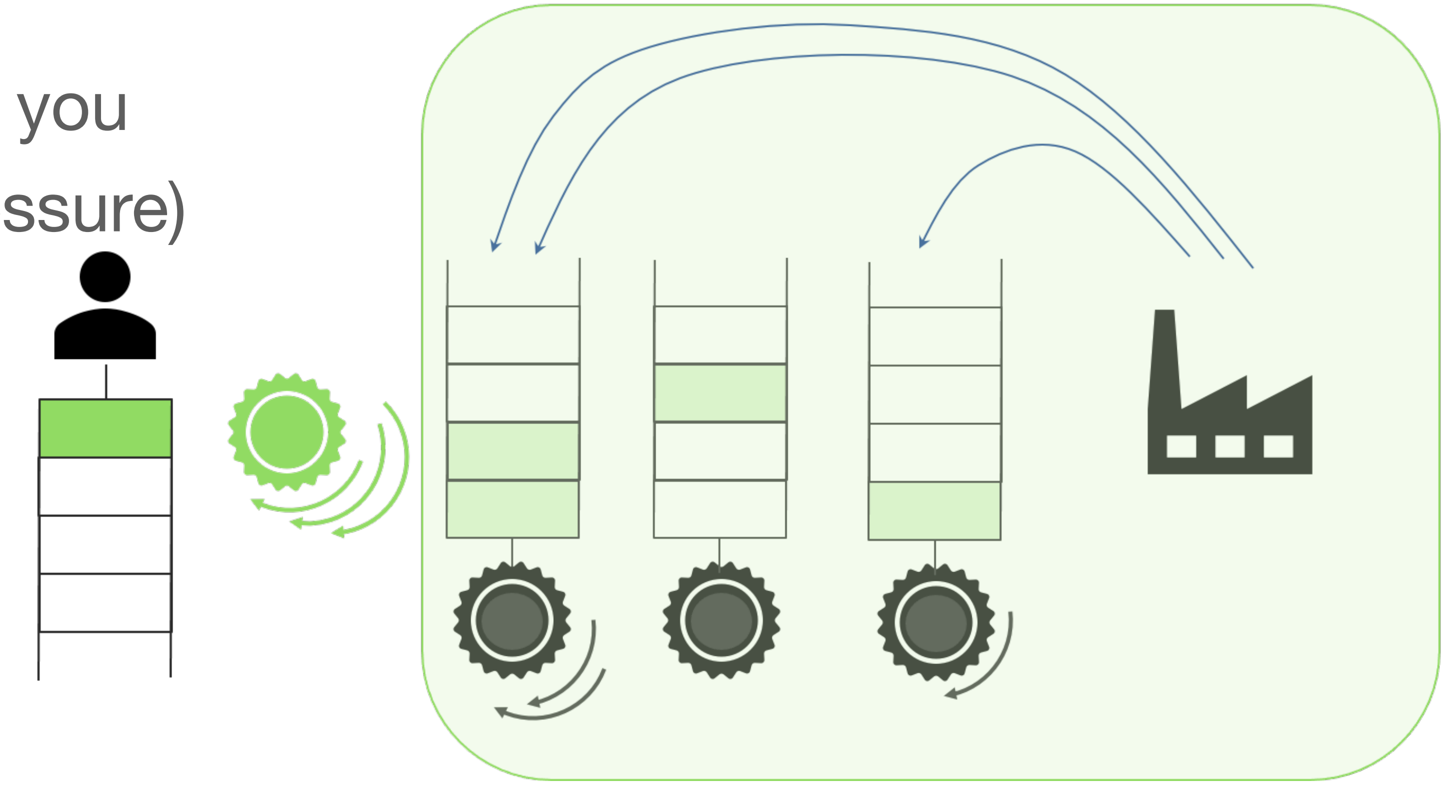


Simplify access: Pilot jobs

- Late binding
- Separation of tasks
  - Pilot jobs
    - Test
    - Set up
    - Wait in the queue
  - User jobs
    - Science

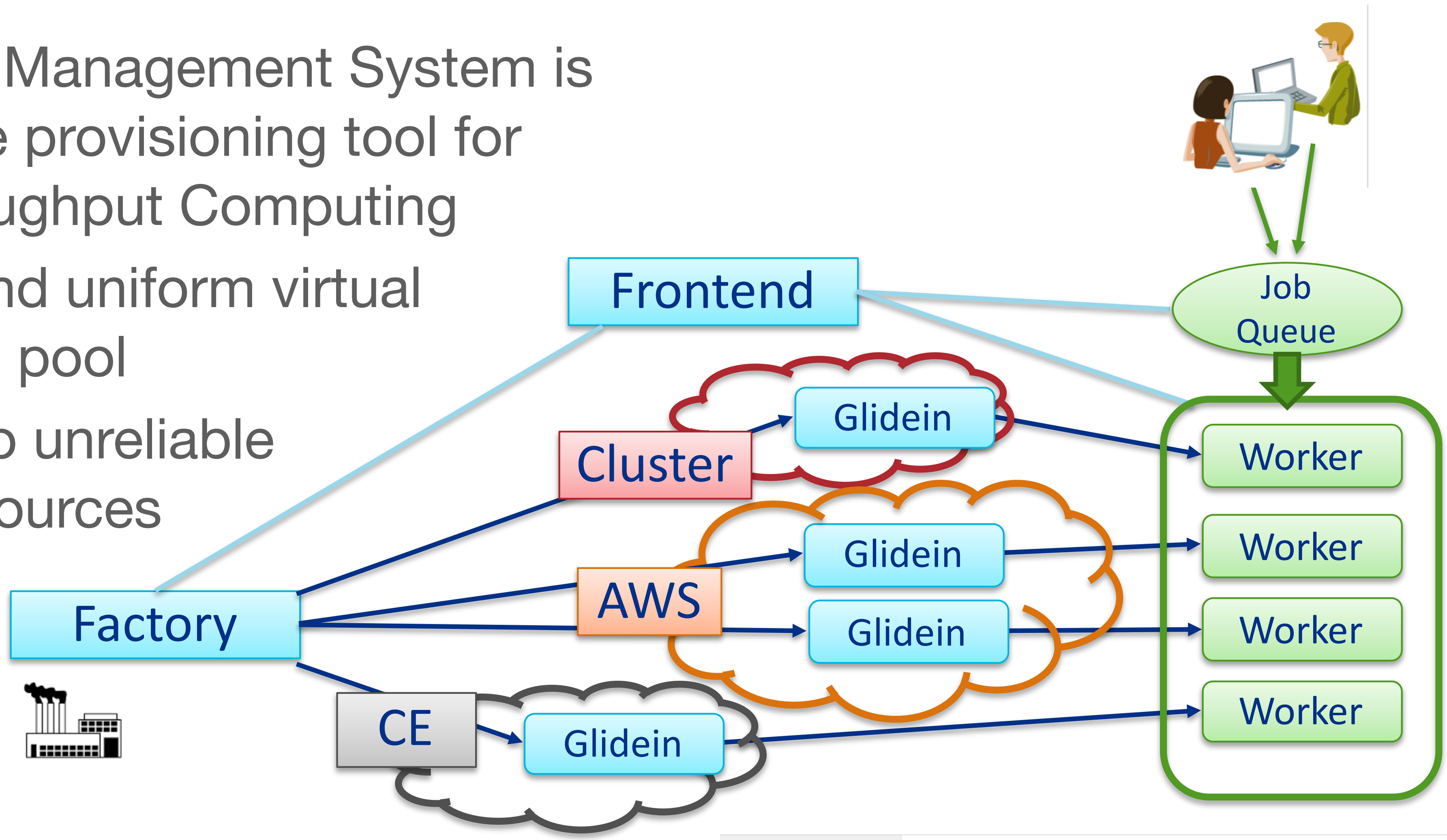


- A Factory will submit pilot jobs for you
  - Use resources as available (pressure)
  - Separation of knowledge

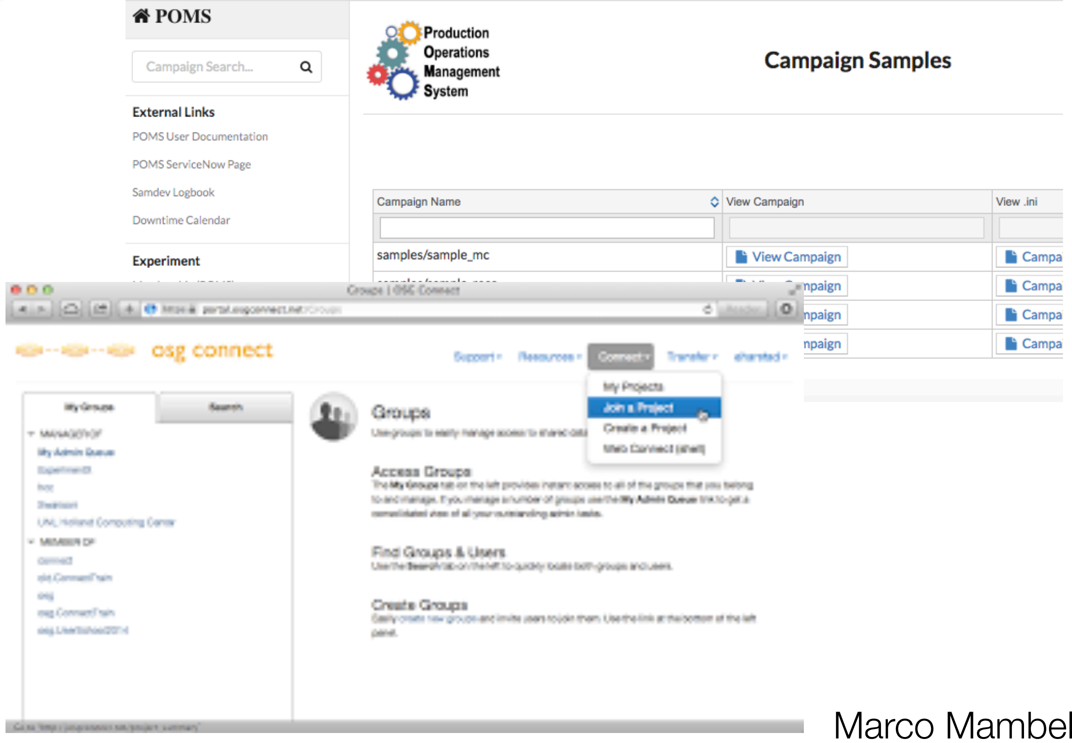


Putting it all together: GlideinWMS

- The Glidein Workload Management System is a pilot based resource provisioning tool for Distributed High Throughput Computing
  - Provides reliable and uniform virtual clusters, the global pool
  - Submits Glideins to unreliable heterogeneous resources



- Knows "how to talk" to all the different systems
- Multiple Frontends and Factories work together to provide High Availability
- Used by: CMS, DUNE, FIFE, OSG, (POMS, Jobsub, OSG-Connect)



Production Operations Management System

Campaign Samples

External Links

POMS User Documentation

POMS ServiceNow Page

Samdev Logbook

Downtime Calendar

Experiment

Campaign Name	View Campaign	View .ini
samples/sample_mc	View Campaign	Campa

Groups

Access Groups

Find Groups & Users

Create Groups

HEPCloud

- Making it all possible from one place: **HEPCloud**
- **Unified interface** to Grid, Cloud, and HPC resources
- Currently used mainly to run CMS workflows on NERSC supercomputers
- Optimized bidding for AWS spot pricing
- Better handling of heterogeneous resources (GPUs, QPUs)
- In 2021 doubled CMS Tier 1 capacity using NERSC and other facilities, 160M CoreHrs
- Simulated 1 billion events in 48 hours

Grid

- Virtual Organizations (VOs) of users trusted by Grid sites
- VOs get allocations ➜ **Pledges**
  - Unused allocations: opportunistic resources

“Things you borrow”

Trust Federation

Cloud

- Community Clouds - Similar trust federation to Grids
- Commercial Clouds - **Pay-As-You-Go** model
  - Strongly accounted
  - Near-infinite capacity ➜ **Elasticity**
  - Spot price market

“Things you rent”

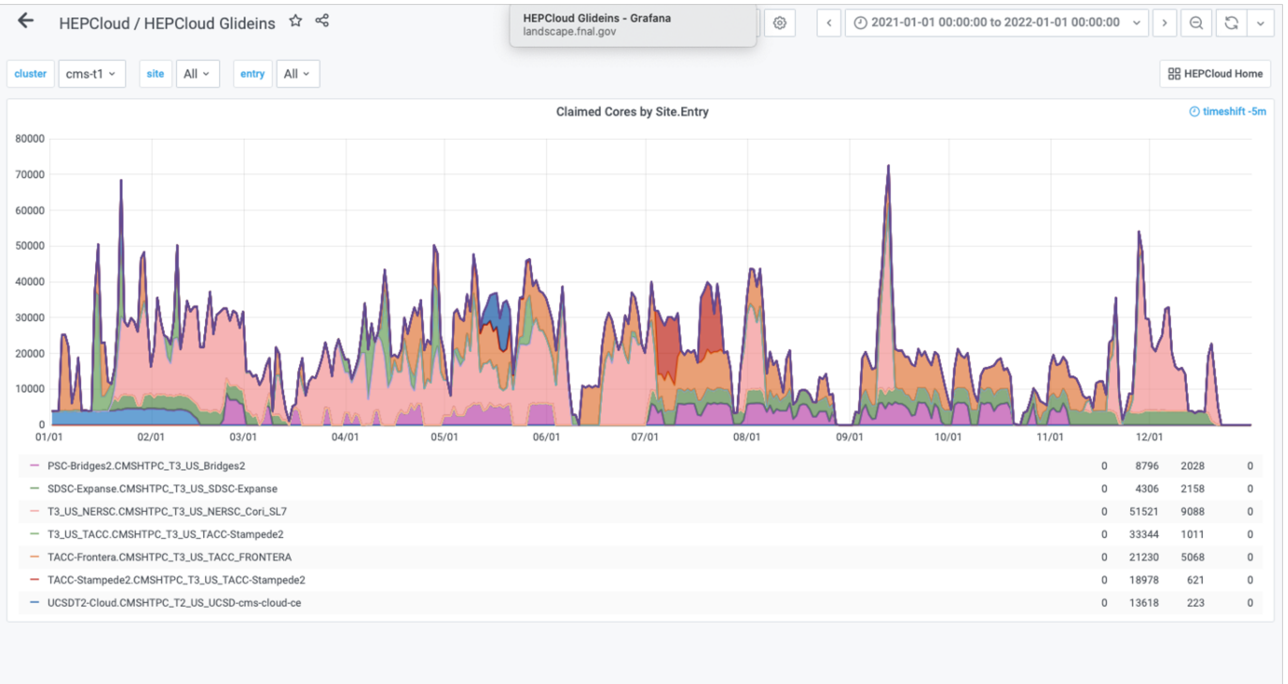
Economic Model

HPC

- Researchers granted access to HPC installations
- Peer review committees award **Allocations**
  - Awards model designed for individual PIs rather than large collaborations

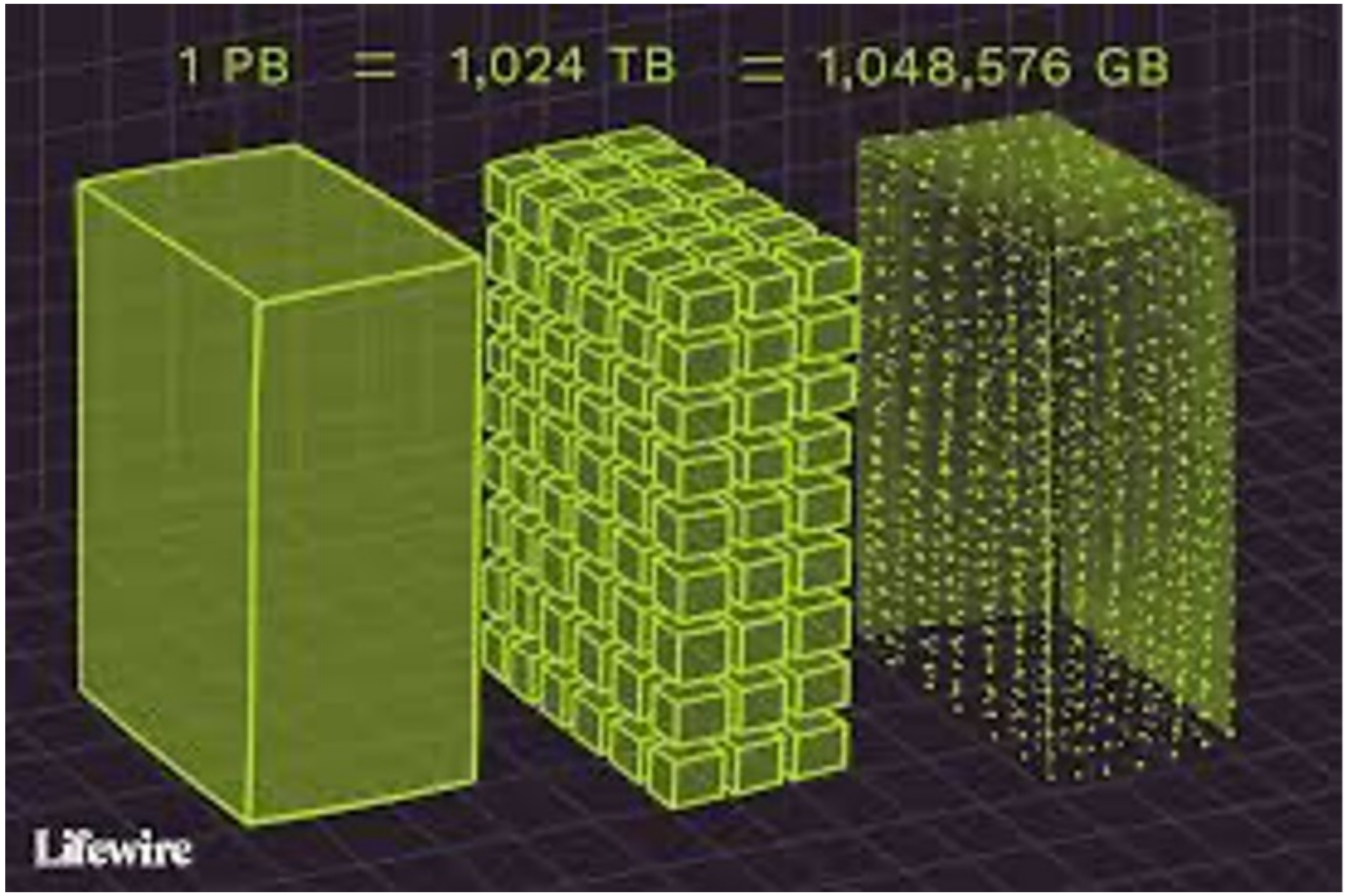
“Things you are given”

Grant Allocation

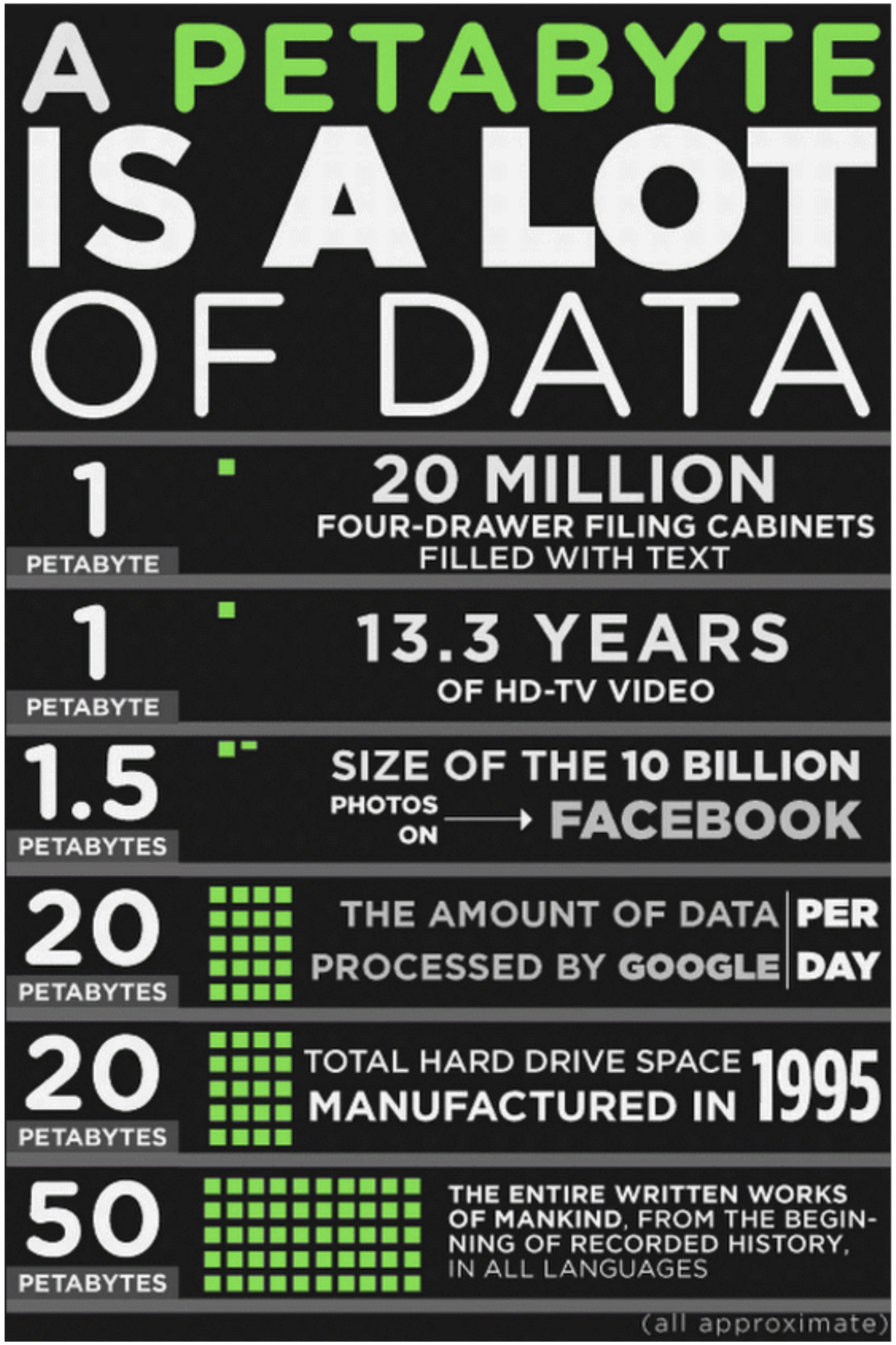


PSC-Bridges2.CMSHTPC_T3_US_Bridges2	0	8796	2028	0
SDSC-Expanse.CMSHTPC_T3_US_SDSC-Expanse	0	4306	2158	0
T3_US_NERSC.CMSHTPC_T3_US_NERSC_Cori_SL7	0	51521	9088	0
T3_US_TACC.CMSHTPC_T3_US_TACC-Stampede2	0	33344	1011	0
TACC-Frontera.CMSHTPC_T3_US_TACC_FRONTERA	0	21230	5068	0
TACC-Stampede2.CMSHTPC_T3_US_TACC-Stampede2	0	18978	621	0
UCSDT2-Cloud.CMSHTPC_T2_US_UCSD-cms-cloud-ce	0	13618	223	0

Storage: understanding units



It would take over 20 YEARS TO TWEET 150 PB if everyone in the world tweeted once per day.



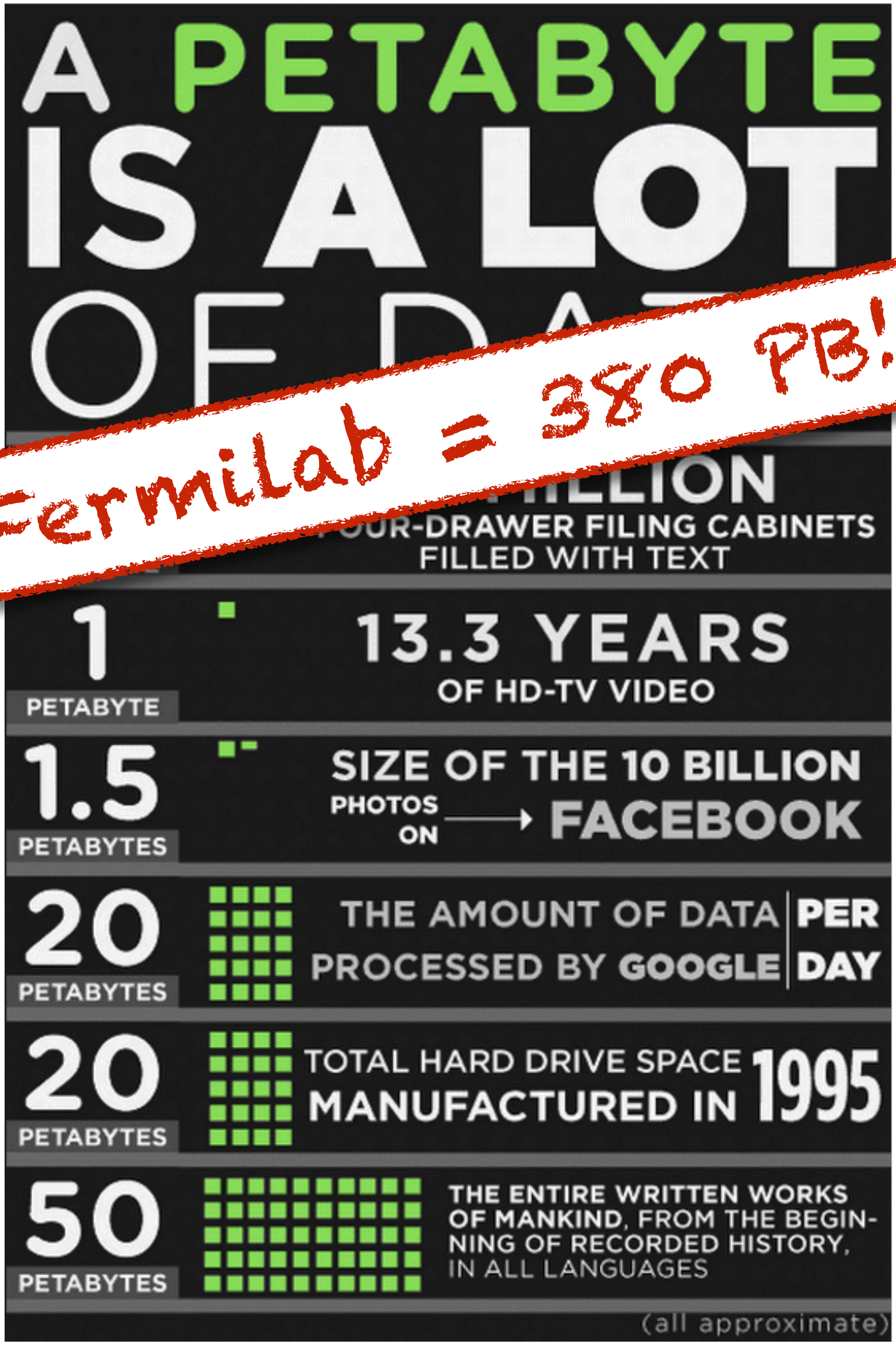
A PETABYTE IS A LOT OF DATA

1 PETABYTE	20 MILLION FOUR-DRAWER FILING CABINETS FILLED WITH TEXT
1 PETABYTE	13.3 YEARS OF HD-TV VIDEO
1.5 PETABYTES	SIZE OF THE 10 BILLION PHOTOS ON → FACEBOOK
20 PETABYTES	THE AMOUNT OF DATA PROCESSED BY GOOGLE PER DAY
20 PETABYTES	TOTAL HARD DRIVE SPACE MANUFACTURED IN 1995
50 PETABYTES	THE ENTIRE WRITTEN WORKS OF MANKIND, FROM THE BEGINNING OF RECORDED HISTORY, IN ALL LANGUAGES

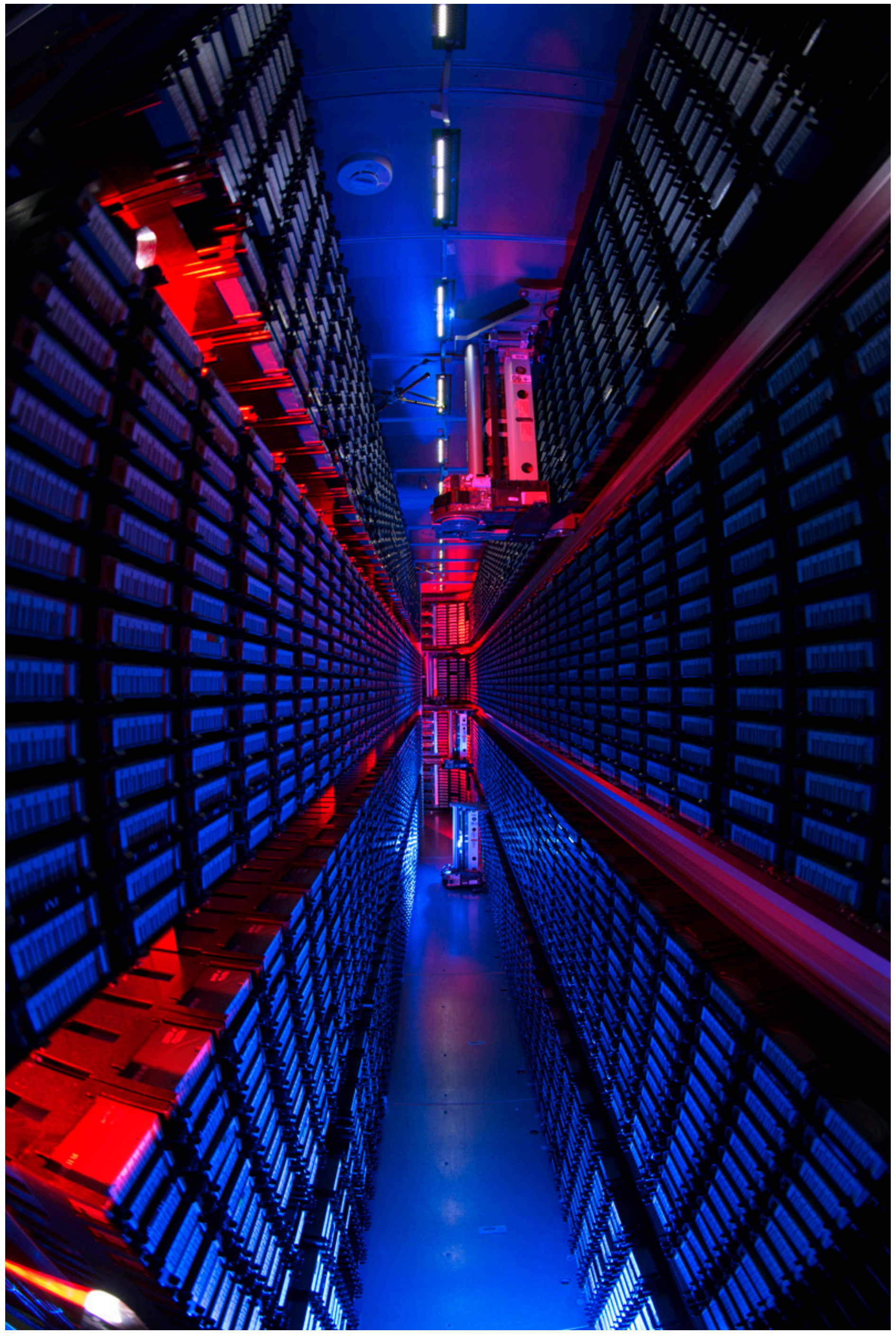
(all approximate)

Storage: understanding units

Scientific data stored at Fermilab = 380 PB!



Storage: tape



- Primary storage medium for scientific data at Fermilab: **magnetic tape**
- Still the most efficient way to store petabytes of data if:
  - Not all of it is accessed at the same time
  - Access patterns are fairly linear
  - Sufficient disk for **staging**
- Fermilab has seven **robotic tape libraries**
  - Each library can hold up to 10,000 tapes
- Current tapes hold ~12TB of data each (1km of tape!)

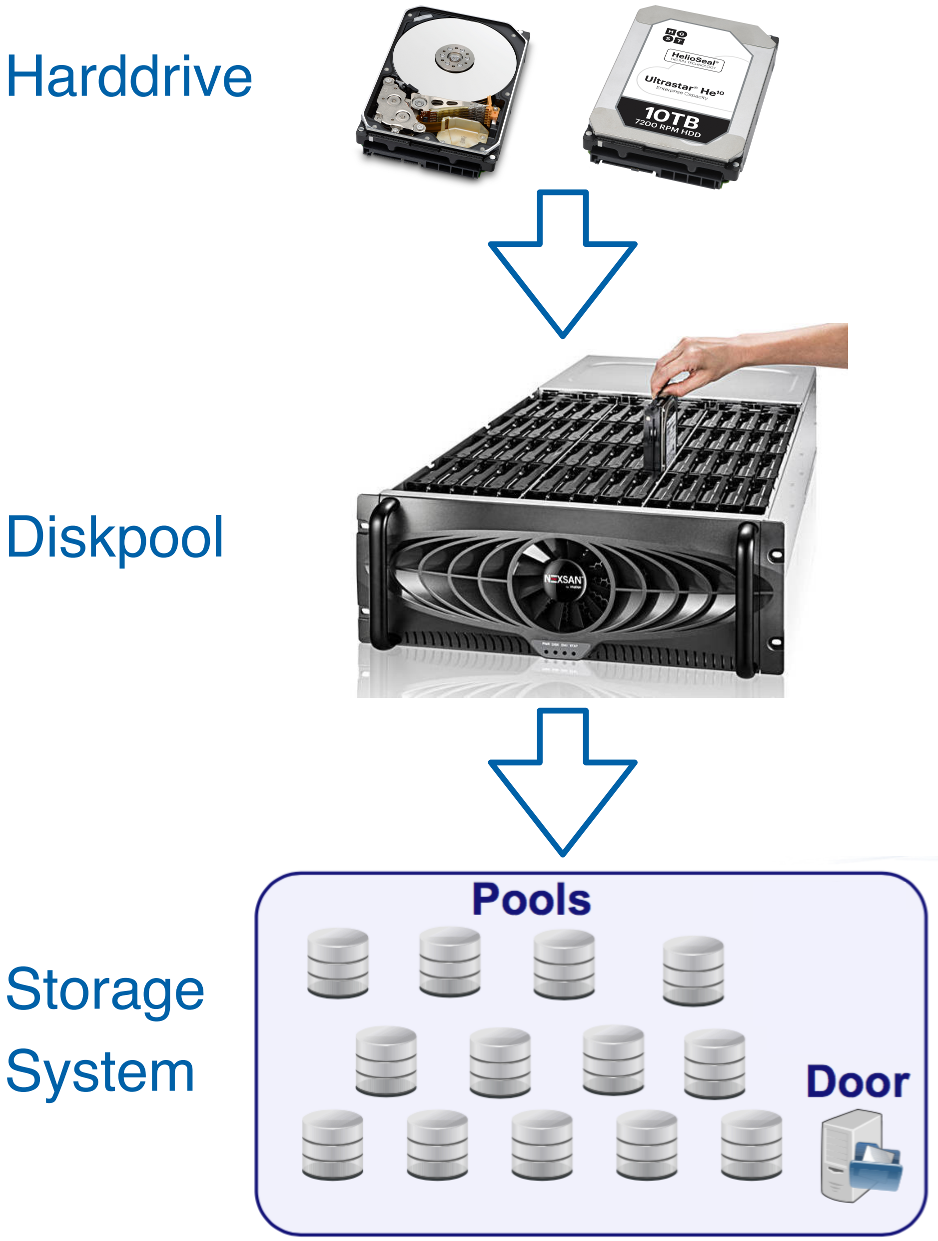
- Total active on tape: 300 PB
  - CMS, 89.69
  - NOVA, 53.65
  - uBoone, 28.48
  - gm2, 17.51
  - DUNE, 15.06

Storage: tape libraries

- 9000 to 10000 tapes per library
- A few dozen drives
- Fire suppression system

https://drive.google.com/open?id=1caM9JoUONtfIgqxrcJBBN5OlmGrpnYy5

Storage: disk



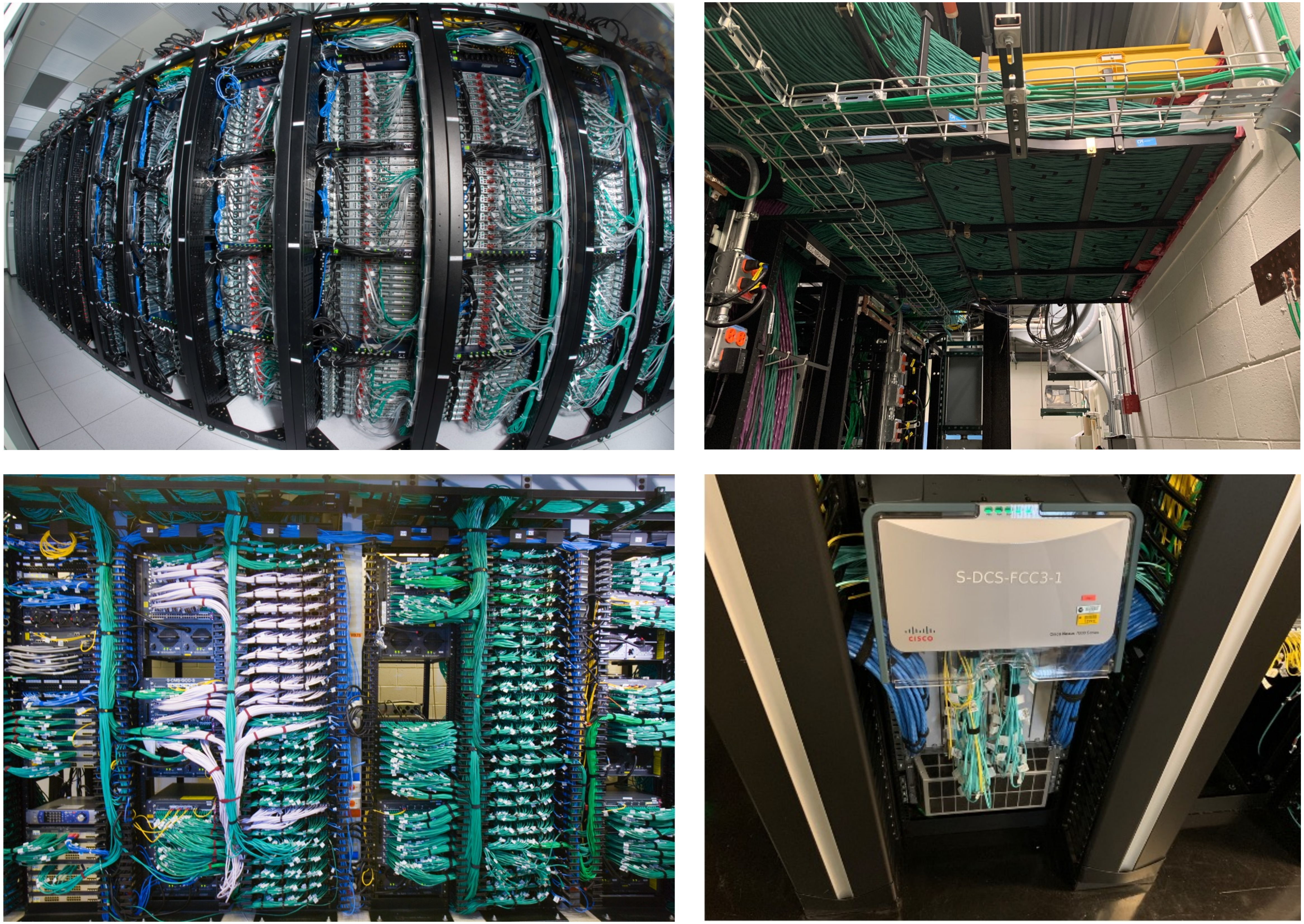
Harddrive

Diskpool

Storage System

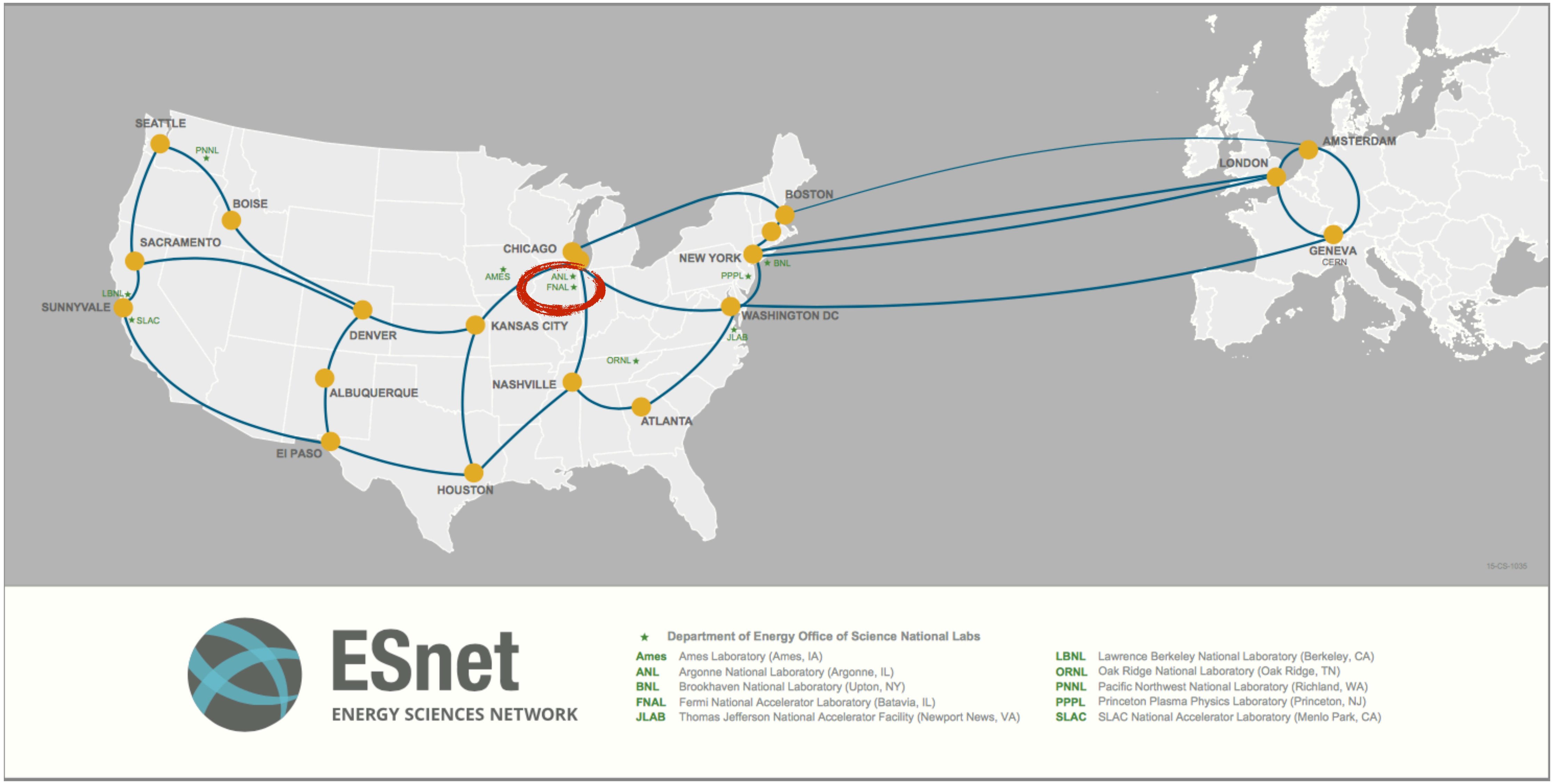
- ~80PB of disk (hard drive) storage
  - Most used as staging area from tape
- Disks are organized into **pools**
- Software allows collections of pools to appear to a user as a **single storage device**
  - Fermilab uses a system called “dCache”
  - In a typical week, data throughput in the Fermilab dCache pools average **30GB/s**

Networking: Local Networks

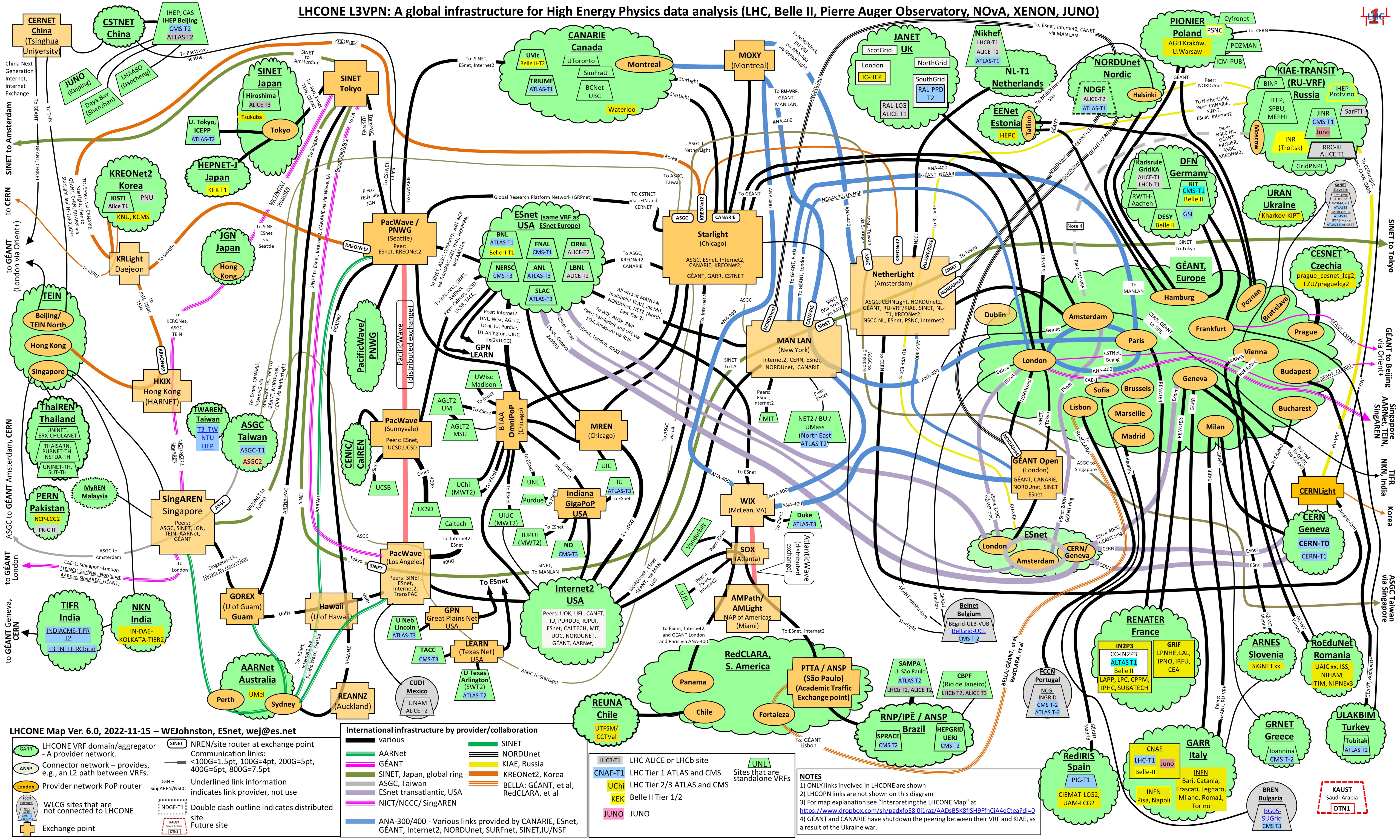


Networking: Wide Area Networks

- Distributed computing requires **fast** and **reliable networks**
- **Dedicated fiber optic links** (typically 100 Gbps) connect **experiments** and major labs
- e.g. ESNet at national labs, GÉANT in Europe
- Dedicated LHC links connect these together (LHCONE, LHCOPN)



Networking



LHCONE L3VPN: A global infrastructure for High Energy Physics data analysis (LHC, Belle II, Pierre Auger Observatory, NOvA, XENON, JUNO)

LHCONE Map Ver. 6.0, 2022-11-15 – WEJohnston, ESnet, wej@es.net

GARR	LHCONE VRF domain/aggregator - A provider network.
ANSP	Connector network – provides, e.g., an L2 path between VRFs.
London	Provider network PoP router
FCCN Portugal NCG-INGRID CMS T-2 ATLAS T-2	WLCG sites that are not connected to LHCONE
	Exchange point
SINET	NREN/site router at exchange point
	Communication links: <100G=1.5pt, 100G=4pt, 200G=5pt, 400G=6pt, 800G=7.5pt
JGN – SingAREN/NSCC	Underlined link information indicates link provider, not use
NDGF-T1	Double dash outline indicates distributed site
KAUST Saudi Arabia DTN1	Future site

International infrastructure by provider/collaboration

- various
- SINET
- AARNet
- NORDUnet
- GÉANT
- KIAE, Russia
- SINET, Japan, global ring
- KREONet2, Korea
- ASGC, Taiwan
- BELLA: GÉANT, et al, RedCLARA, et al
- ESnet transatlantic, USA
- NICT/NCCC/ SingAREN
- ANA-300/400 - Various links provided by CANARIE, ESnet, GÉANT, Internet2, NORDUnet, SURFnet, SINET,IU/NSF

LHCB-T1	LHC ALICE or LHCb site
CNAF-T1	LHC Tier 1 ATLAS and CMS
UChi	LHC Tier 2/3 ATLAS and CMS
KEK	Belle II Tier 1/2
JUNO	JUNO
UNL	Sites that are standalone VRFs

NOTES

1) ONLY links involved in LHCONE are shown
2) LHCOPN links are not shown on this diagram
3) For map explanation see "Interpreting the LHCONE Map" at https://www.dropbox.com/sh/padxfo58j0j1raz/AADsB5K8fISH9FfhCjA4eCtea?dl=0
4) GÉANT and CANARIE have shutdown the peering between their VRF and KIAE, as a result of the Ukraine war.

LHCONE - intermediate detail from William Johnston - https://www.dropbox.com/sh/padxfo58j0j1raz/AADsB5K8fISH9FfhCjA4eCtea?dl=0

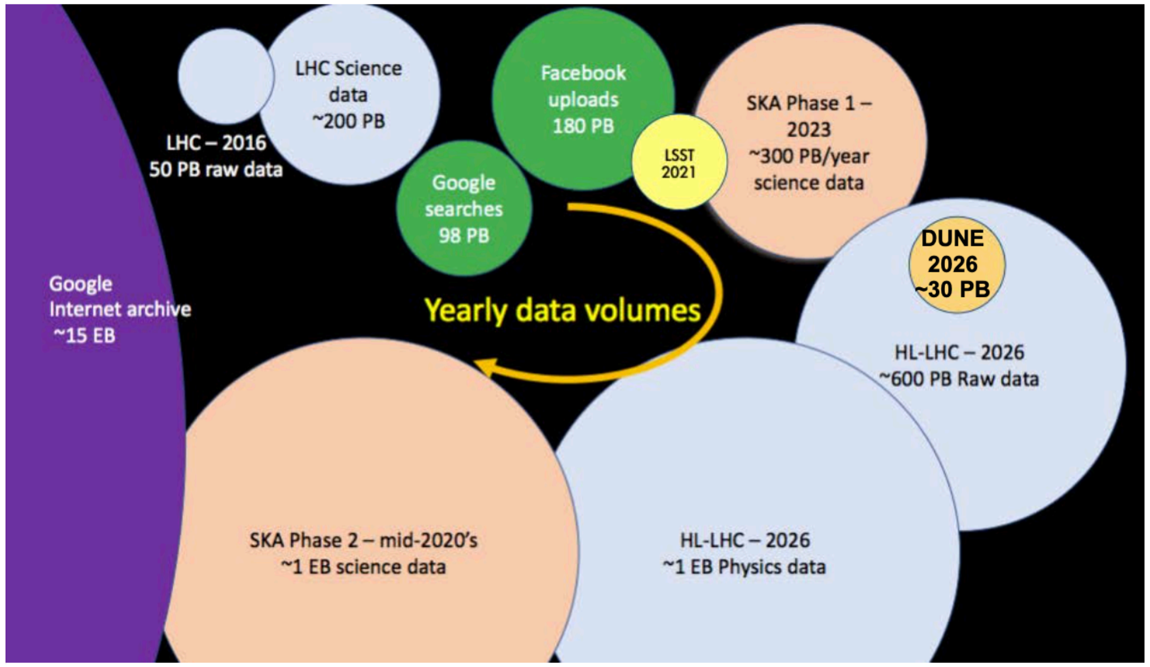
The Future

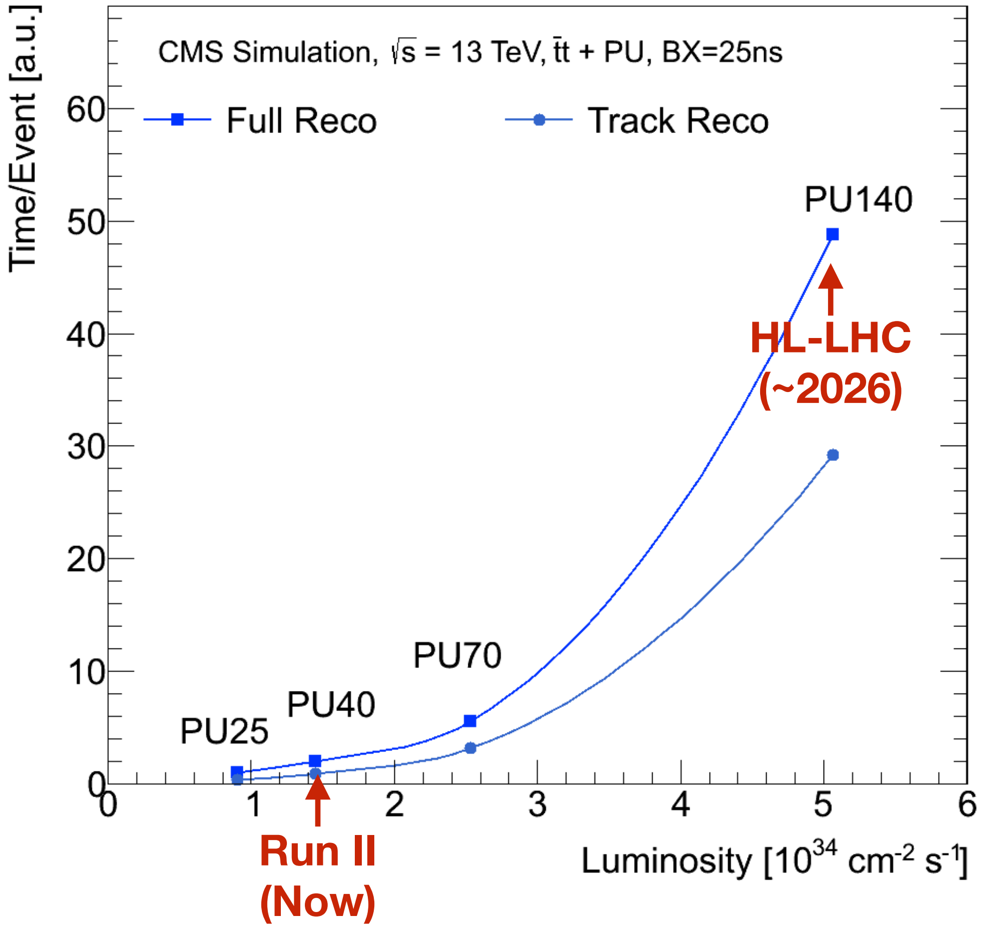
Explosion of data and ever-growing need for CPU

- HL-LHC, DUNE, LSST, SKA will produce up to **exabytes of data** per year
- More than one order of magnitude above current dataset sizes

- And more **complex** data to allow **precision measurements**

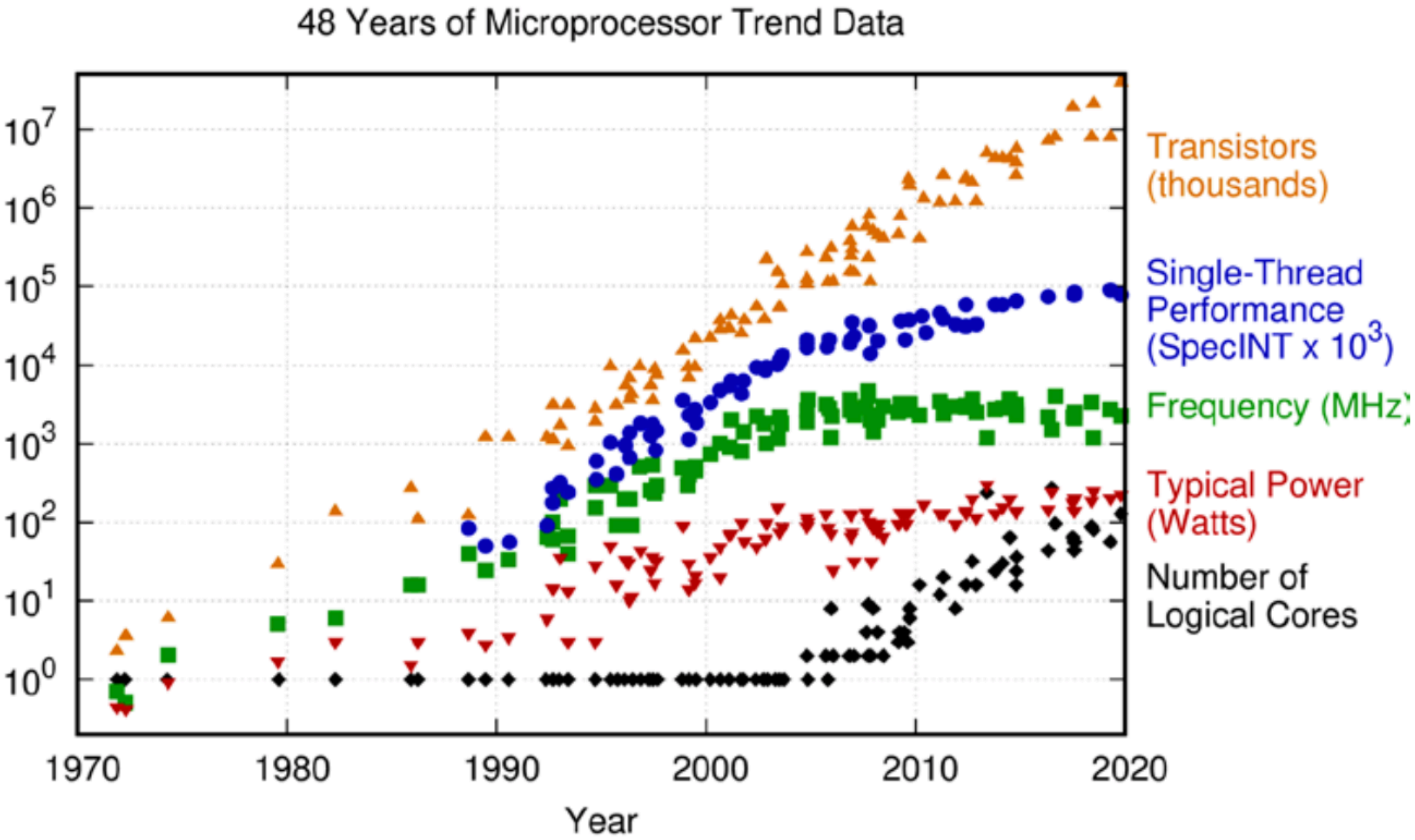
- Growing **dataset size** and **event complexity** = **more computing!**
  - If we scale **current algorithms**, the CPU needs of LHC experiments will grow by a factor of **30** in a decade
  - Similar issues faced by newer, bigger LAr experiments such as DUNE





Moore’s Law probably won’t help

- Moore’s Law: **Number of transistors** on a chip doubles every 2 years
- That’s still true, but **single-thread performance** has stopped increasing
- Instead, **number of cores** is now dramatically increasing



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2019 by K. Rupp

To take advantage of these:

Intel Many Integrate Core (MIC) CPU

NVIDIA GPU

We need to rewrite a lot of software!

What about supercomputers?

ASCR* Computing Upgrades At a Glance

System attributes	NERSC Now	OLCF Now	ALCF Now	NERSC Upgrade	ALCF Upgrade	OLCF Upgrade	ALCF Upgrade
Name	**Cori**	**Summit**	**Theta**	**Perlmutter**	**Polaris**	**Frontier**	**Aurora**
Installation (planned or actual)	2016	2018	2017	2021	2021	2021-2	2022-3
System peak (PF)	30	200	12	>120	35-45	1500	> 1000
Peak Power (MW)	3.7	10	<2.1	6	<2	29	60

This is the hard part - getting the computing power without melting the building.

PF = petaflops, floating point operations per second

1,000 PF = 1 exaflops

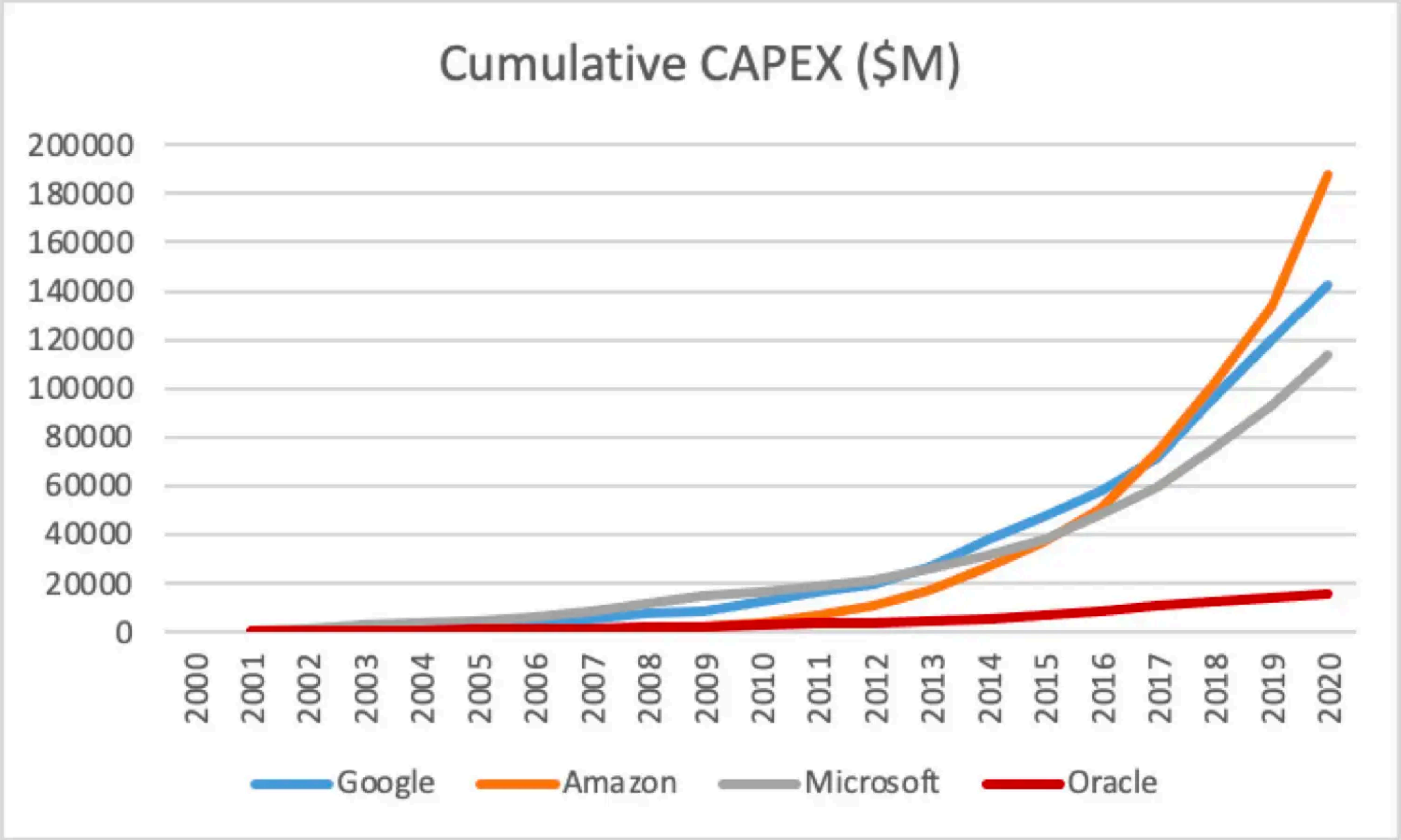
“Excascale”

*Advanced Scientific Computing Research (Dept. of Energy)

http://exascaleproject.org/

Commercial cloud computing (>> HEP computing)

- Total spending on cloud computing is now > $200 billion per year
- Many huge companies (Netflix, for example) don’t buy their own clusters but rely entirely on cloud computing
- HEP experiments are using these resources as well



https://www.infoworld.com/article/3639017/cloud-costs-a-lot-of-money.html

Analysis techniques: tools from industry

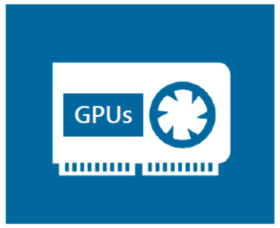
- HEP experiments were some of **the first** cases where people had to deal with analyzing really big datasets
  - Had to develop our own tools to get the science done (ROOT, for example)
- Not true anymore. Basically every big company you can think of has huge amounts of data at their fingertips
  - Many tools of been developed outside labs and universities to help store, process, and analyze all this data

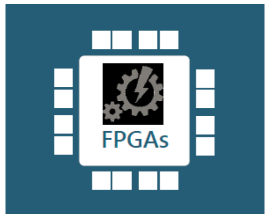
- Fermilab's approach for CMS analysis is COFFEA (the COmpact Framework for Elaborate Algorithms)
  - Instead of a **for loop** over events, use **array programming** expressions to process many events simultaneously
  - Uses Apache Spark and tools from the scientific python "ecosystem" based on numpy

APACHE Spark™

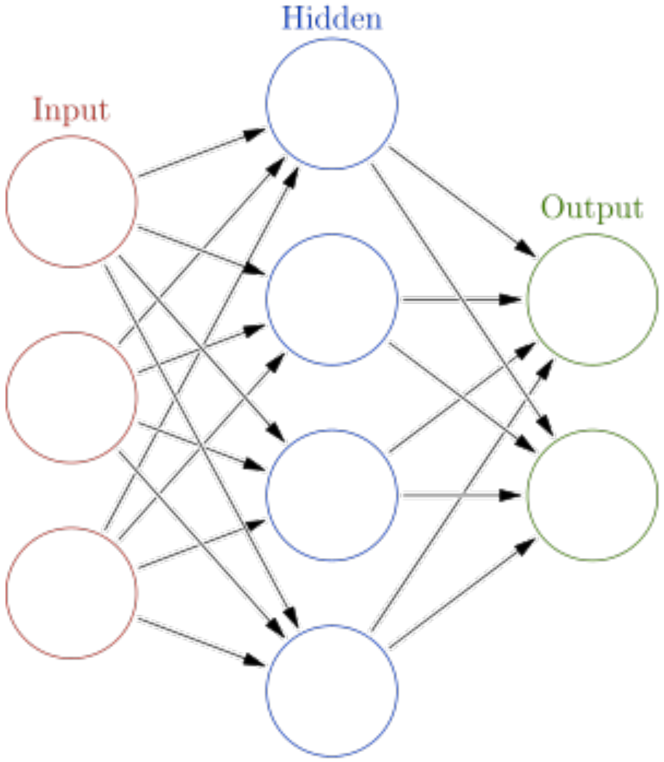
NumPy

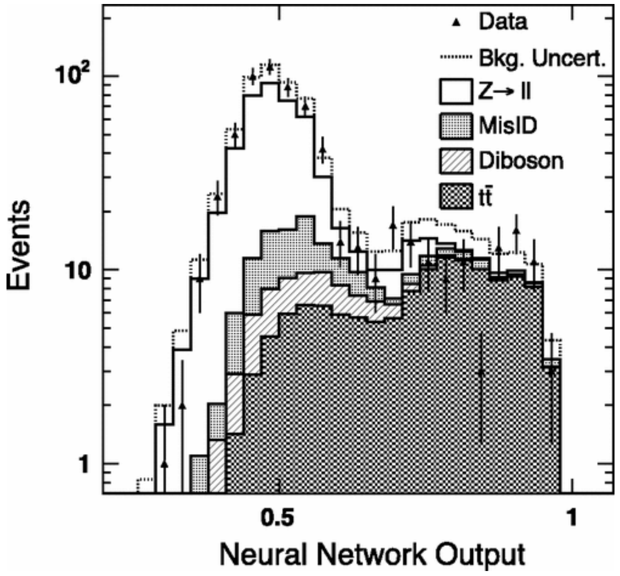
Analysis techniques: Machine Learning



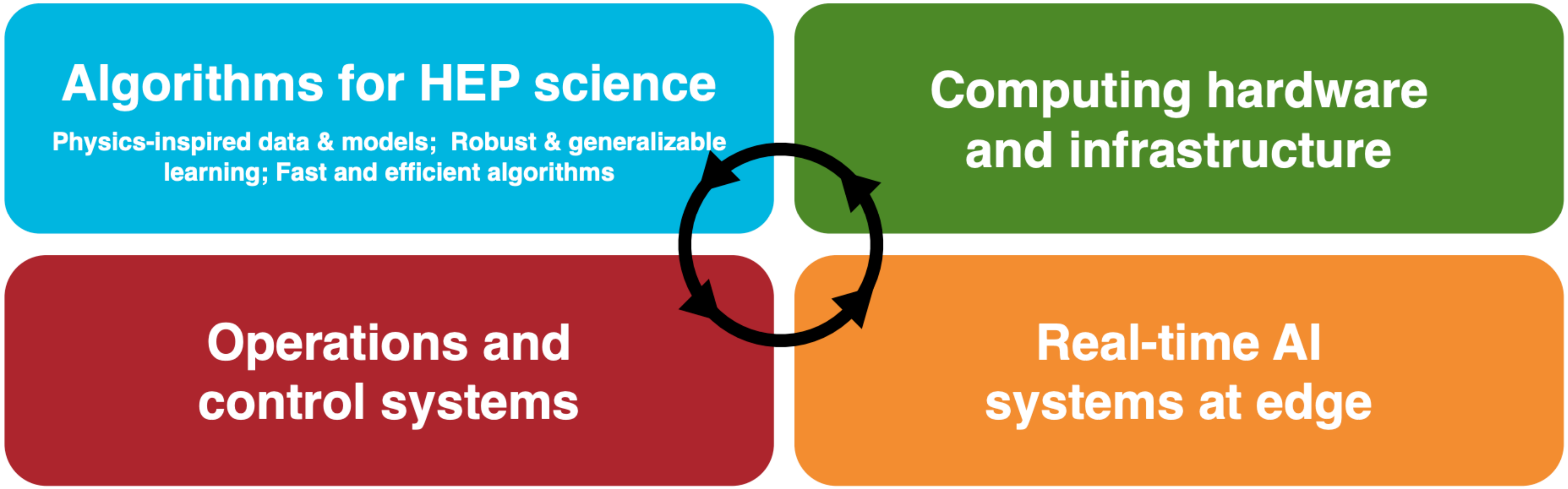


- Machine Learning is a very good fit for heterogeneous computing
- ML is function approximation $\vec{x} \mapsto \vec{y}$
  - Maps inputs to outputs by optimizing weights $\vec{y} \approx F'(\vec{x}; \vec{w})$
- Deep Learning uses Neural Networks with many hidden layers to derive features from inputs (the Neural Networks Zoo)
- More neurons --> more multiplications, weights
  - Training: optimizing weights to improve function approximation
  - Inference: applying optimized function to new data to make predictions
- Used in HEP and Astrophysics since the turn of the century
- Fermilab Artificial Intelligence Project





AI at Fermilab



Algorithms for HEP science

Physics-inspired data & models; Robust & generalizable learning; Fast and efficient algorithms

Computing hardware and infrastructure

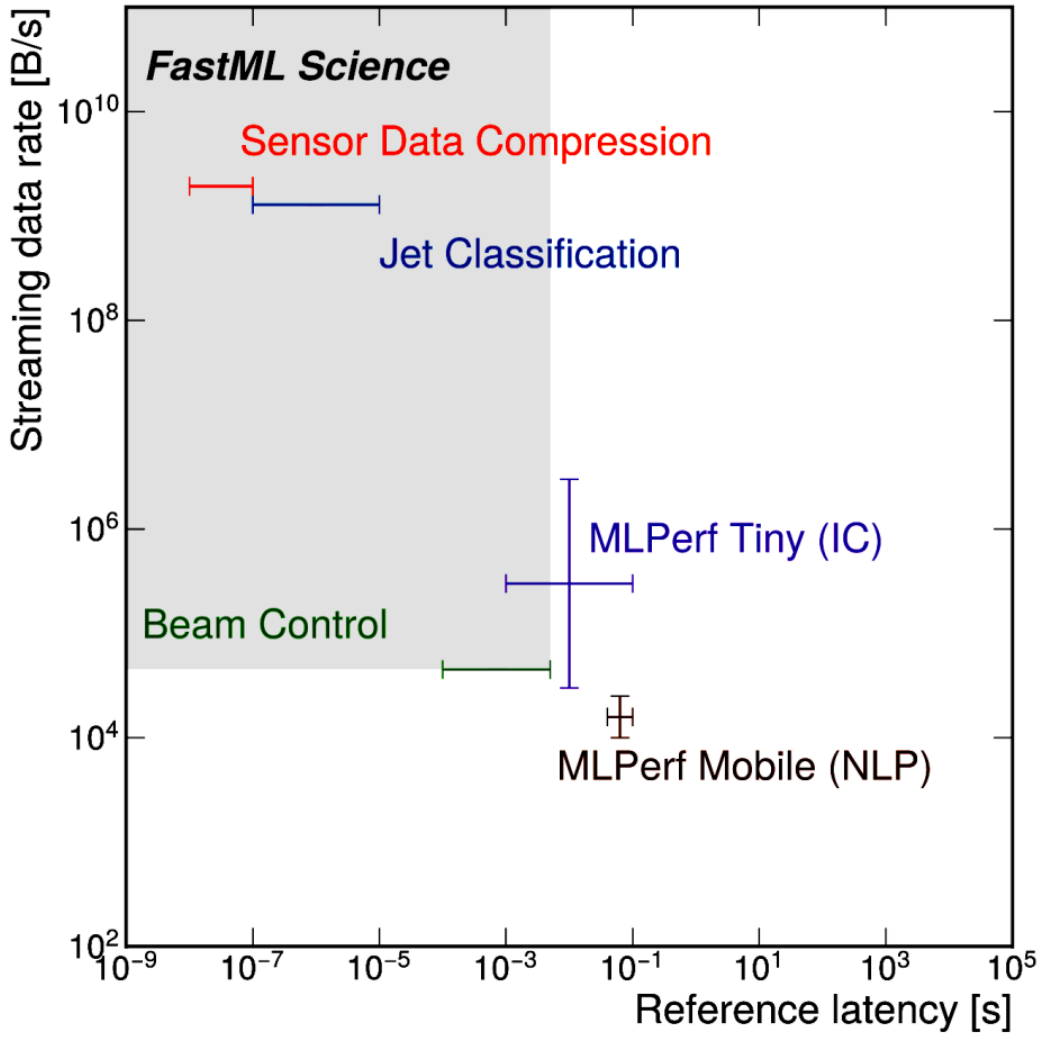
Operations and control systems

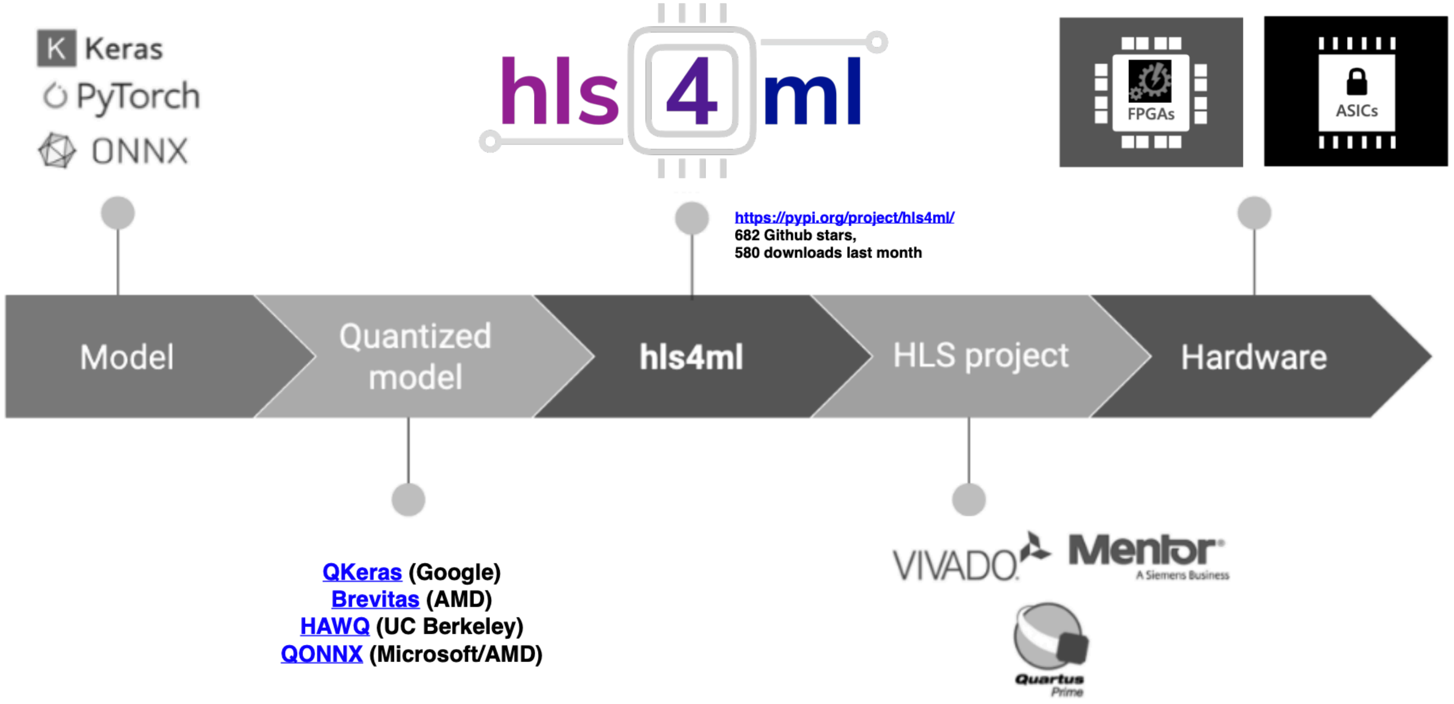
Real-time AI systems at edge

Tia Miceli - AI at Fermilab - https://indico.fnal.gov/event/59656/contributions/269042/attachments/168498/225755/20230629_AI_at_Fermilab_TiaMiceli.pdf

Real Time AI

- Fast ML at the extreme edge
- Efficient ML hardware-software codesign





Model → Quantized model → hls4ml → HLS project → Hardware

https://pypi.org/project/hls4ml/
682 Github stars,
580 downloads last month

QKeras (Google)
Brevitas (AMD)
HAWQ (UC Berkeley)
QONNX (Microsoft/AMD)

Tia Miceli - AI at Fermilab - https://indico.fnal.gov/event/59656/contributions/269042/attachments/168498/225755/20230629_AI_at_Fermilab_TiaMiceli.pdf

Algorithms for HEP science

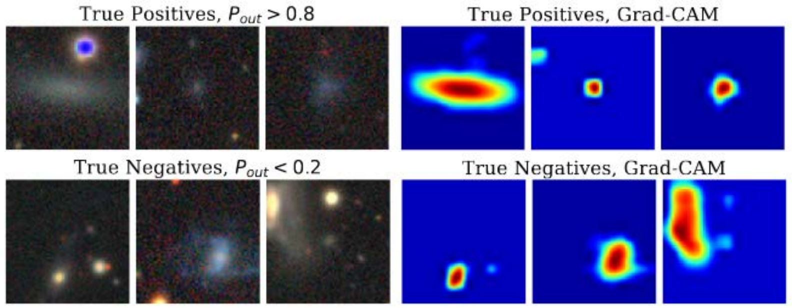
AI Techniques	HEP Projects	Impact
CNN	LArTPC Reconstruction	Uboldi et al, Nucl. Instrum. Meth. A 1028 (2022) 166371 ArgoNeuT JINST 17 (2022) P01018 DUNE Eur.Phys.J.C 82 (2022) 10, 903
GNN	CMS Reconstruction: HGCal, ECal, +	2x signal H->bb γγ improve 7%
SBI flexible likelihoods	Cosmic analyses	10^5 x faster
Generative models	Particle sim through matter	20-50x faster than GEANT4
Neural networks & importance sampling	Many-body schrodinger equation	Rocco et al., arXiv: 2206.10021 Issacson et al., arXIv:2212.06172
Deep Universal Domain Adaptation	Cosmic analyses, LHC Stealth SUSY background estimation	Mitigate bias, reduce hyper parameter tuning
Auto Encoders for anomaly detection	LHC QCD showers, Accelerator controls @ Linac (L-CAPE)	Pedro et al., JHEP 02 (2022) 074 Ngadiuba et al., arXiv: 2107.02157 Ngadiuba et al., Nature Machine Intelligence 4, 154 (2022) Ngadiuba et al., arXiv: 2110.08508
GNN	CMS pileup mitigation	Improve algo > 20%

⋮ ⋮ ⋮

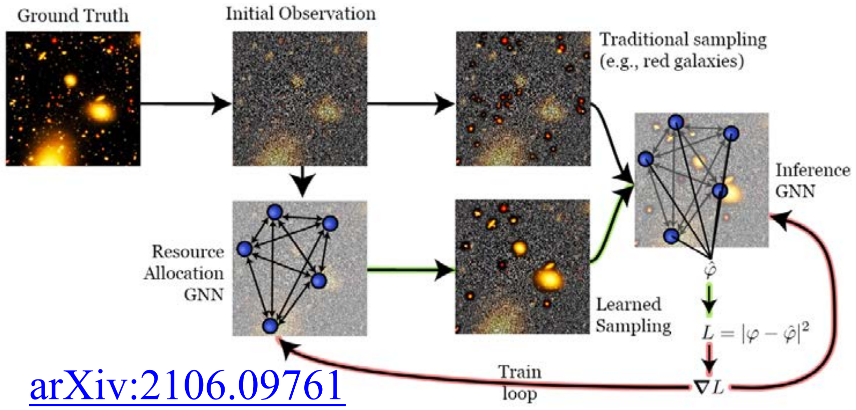
Tia Miceli - AI at Fermilab - https://indico.fnal.gov/event/59656/contributions/269042/attachments/168498/225755/20230629_AI_at_Fermilab_TiaMiceli.pdf

Algorithms for HEP science (cont)

- DeepShadows: (arXiv:2011.12437)
  - Convolutional NN to distinguish Low Surface Brightness Galaxies from artifacts in DES data
  - 92% accuracy, vs. ~80% accuracy for simpler ML methods

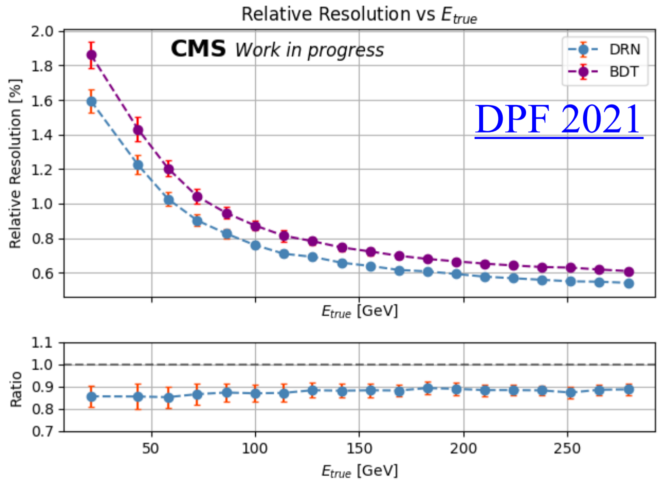


- Graph NN for unsupervised optimization of telescope time: pick best galaxies to observe
  - Outperforms conventional strategies



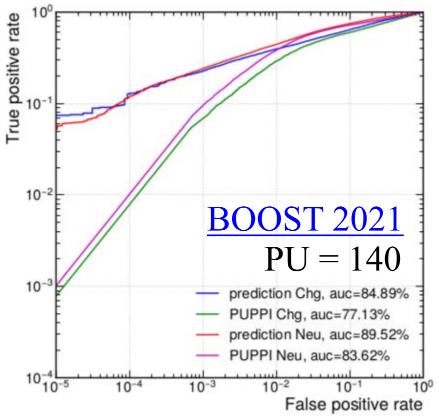
arXiv:2106.09761

- Dynamic Reduction Network (arXiv:2003.08013)
  - Learn best graph of inputs & use it for regression
  - Improve electron resolution by 10% (vs. state of the art)
  - Work in progress: apply to missing energy

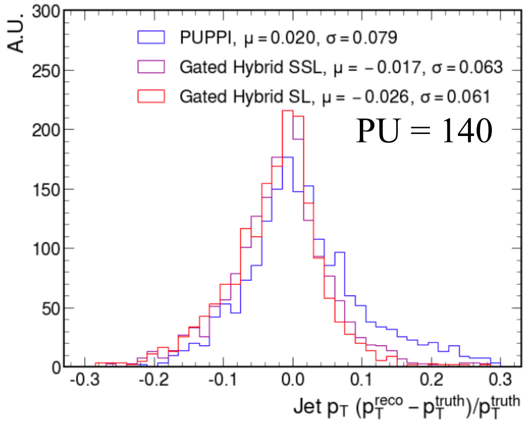


DPF 2021

- Semi-supervised Graph NN to reject pileup: trained on charged particles → can use data!
  - Significantly improves on classical algorithm
- See K.Pedro, AI at Fermilab, for more



BOOST 2021
PU = 140



Operation System Controls

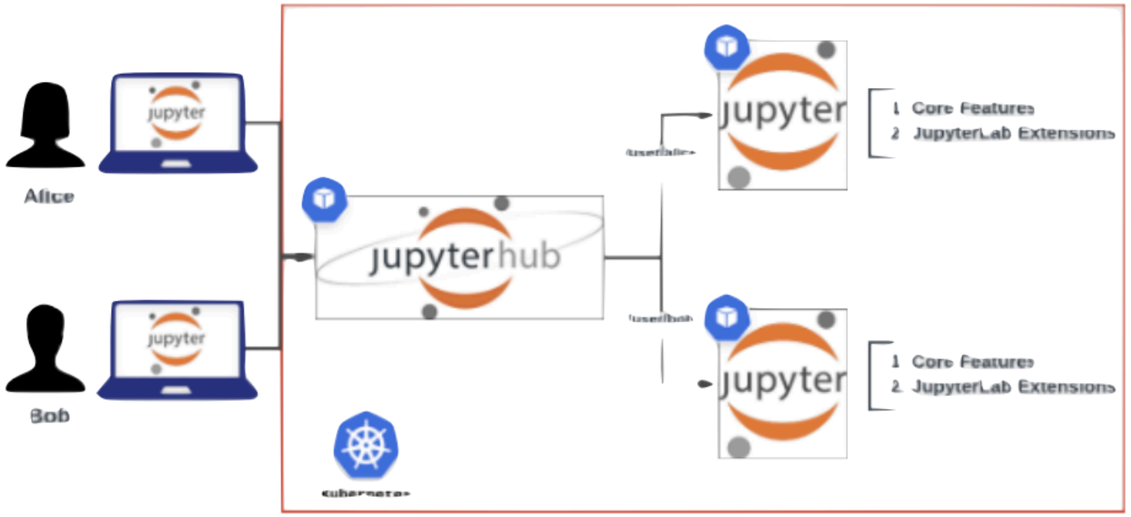
Cosmology	Quantum	Accelerator Controls
- Experiment automation for self driving telescopes (GNN & RL) - instrument design (replace expensive optics simulations with SBI and decision trees)	- AI/ML for controlling & optimizing quantum computers with micro electronics and edge AI - Theoretical & experimental work on quantum detectors	- Linac RF optimization (prevent the need for constant tuning to reduce beam losses at injection to Booster) - Booster GMPS (reinforcement learning agent on FPGA to supplement traditional PID loop) - Real-time Edge AI Distributed Systems (READS) • Disentangle Main Injector and Recycler Ring beam losses with a U-Net • Increase muon resonant extraction spill uniformity for Mu2e with reinforcement learning

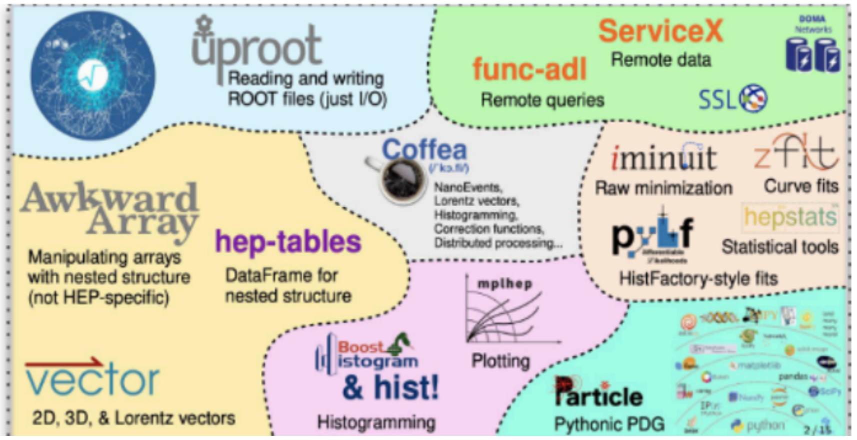
Tia Miceli - AI at Fermilab - https://indico.fnal.gov/event/59656/contributions/269042/attachments/168498/225755/20230629_AI_at_Fermilab_TiaMiceli.pdf

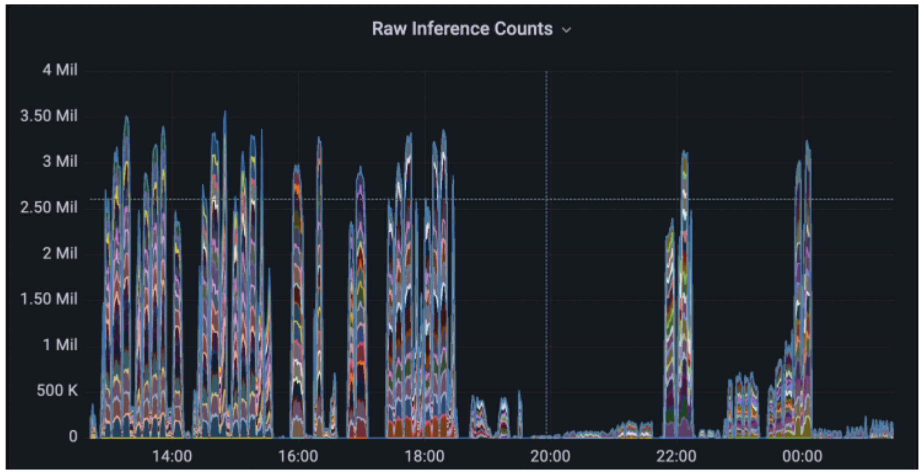
Computing hardware infrastructure

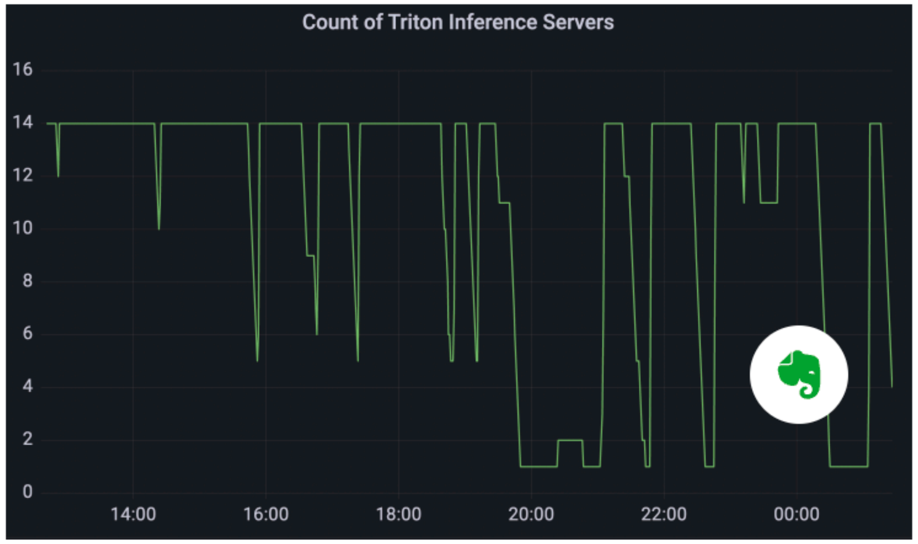
- **Elastic Analysis Facility** @ Fermilab provides **resources** and **data-science standard industry tools** for AI training and inference
- Additional GPU resources available on CMS LPC, Wilson Cluster
- Capable of **bursting** to O(100k) batch computing CPU cores

Flechas et al., arXiv:2203.10161
Benjamin et al., arXiv:2203.08010









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Conclusions

- The complexity of HEP experiments doesn't stop with the detectors
- Scientific computing permeates every aspect of how we do physics at Fermilab

- There are challenges ahead
  - Many that **you** could help solve!

- **Thanks to all those who helped with content**
  - Especially: Bo Jayatilaka, Allison Hall, Kevin Pedro, Lorena Lobato, Dmitry Litvintsev, Sophie Berkman, Oliver Gutsche, Ken Herner, Burt Holzman, Michael Kirby, Anne Schukraft, Erica Snider, Alexander Radovic, Stuart Fuess

Questions?

http://computing.fnal.gov