A Word on DUNE Computing

Ken Herner, Fermilab

Computational HEP Traineeship Summer School

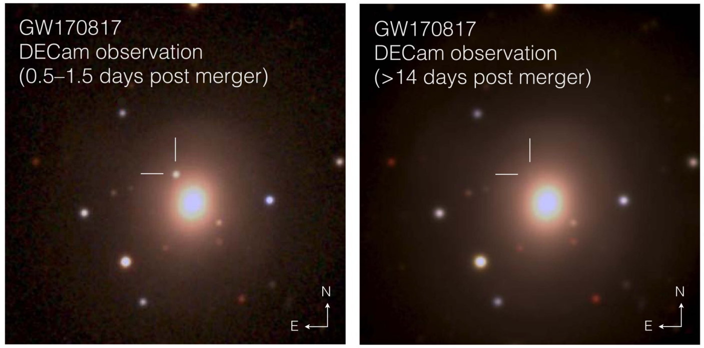
24 May 2024

Outline

- Brief Introduction to DUNE and its science goals
- Set the scale
- DUNE's uniqueness (and unique challenges)
- A Big and Unique problem: supernova burst processing

Introduction to Ken

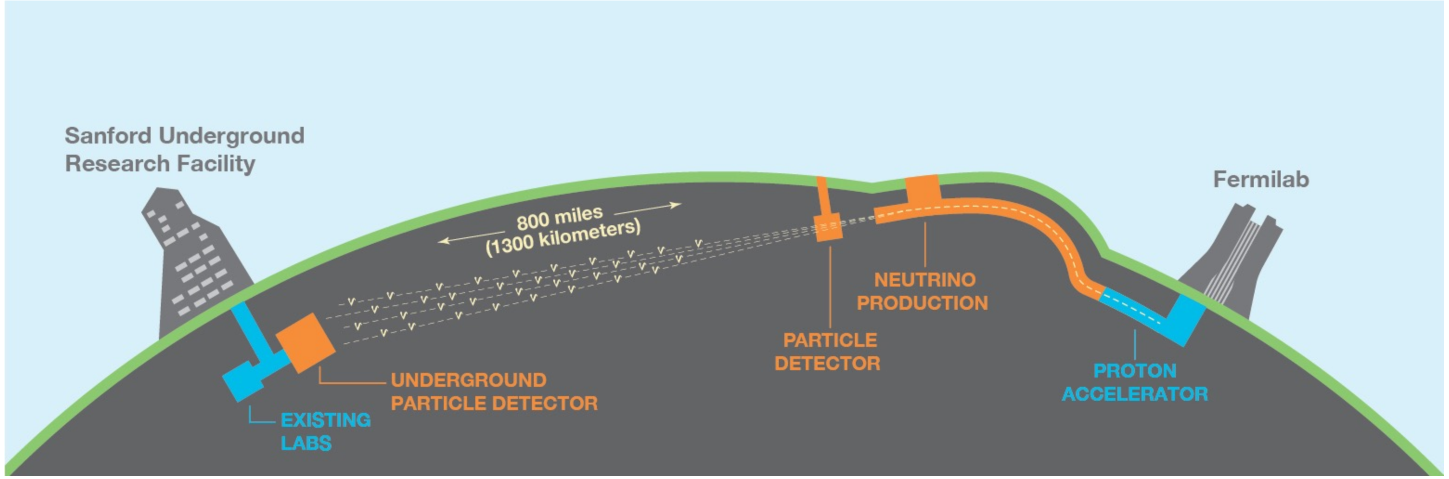
- Ph.D. on the D0 (Tevatron) experiment; most of postdoc as well (centered on Higgs boson searches)
- At Fermilab in Scientific Computing Division (now Computational Science and AI Directorate) since late 2012
  - Started with long-term preservation of D0 dataset
  - Distributed computing support for nearly all lab experiments
  - FabrIc for Frontier Experiments Project lead 2018-2021 (modular SW toolkit for non-CMS experiments)
- DUNE
  - Production Group coordinator 2018-2022: ProtoDUNE data processing, MC generation, new compute site integration, infrastructure R&D (e.g. GPUaaS); Since October 2023: Host Lab Technical Lead and DUNE-US software and computing lead
- Some other projects (not exhaustive list)
  - Various projects on Dark Energy Survey, including optical followup of GW events
    - Currently co-convener of Transient and Moving Objects Science Working Group
  - Vera Rubin Observatory
    - Work in Data management on alert production systems and campaign management



Soares-Santos et al., ApJL 848:L16 (2017)

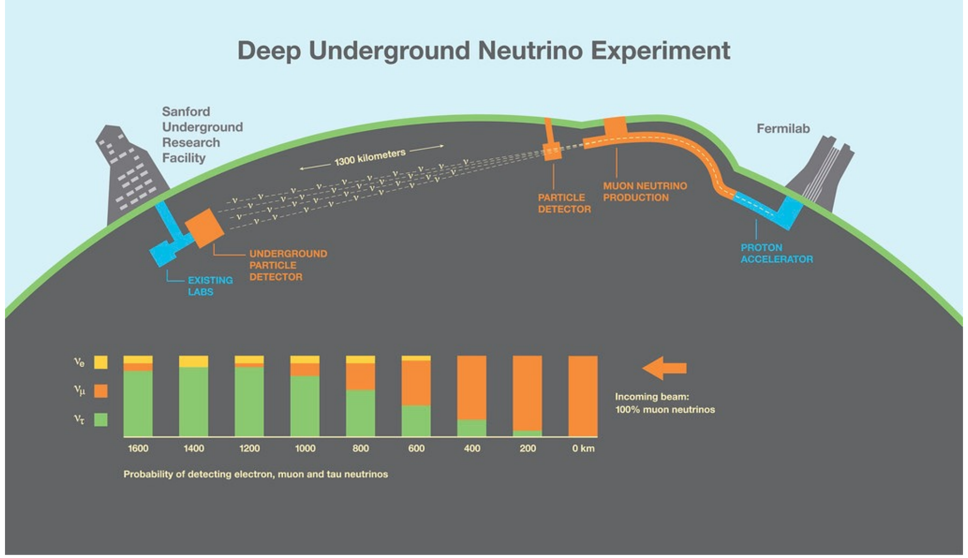
The Deep Underground Neutrino Experiment

- Future flagship experiment of Fermilab; primary focus is extending our understanding of the neutrino sector
- Consists of a Near Detector Complex (FNAL) and a Far Detector Complex (SURF in SD)



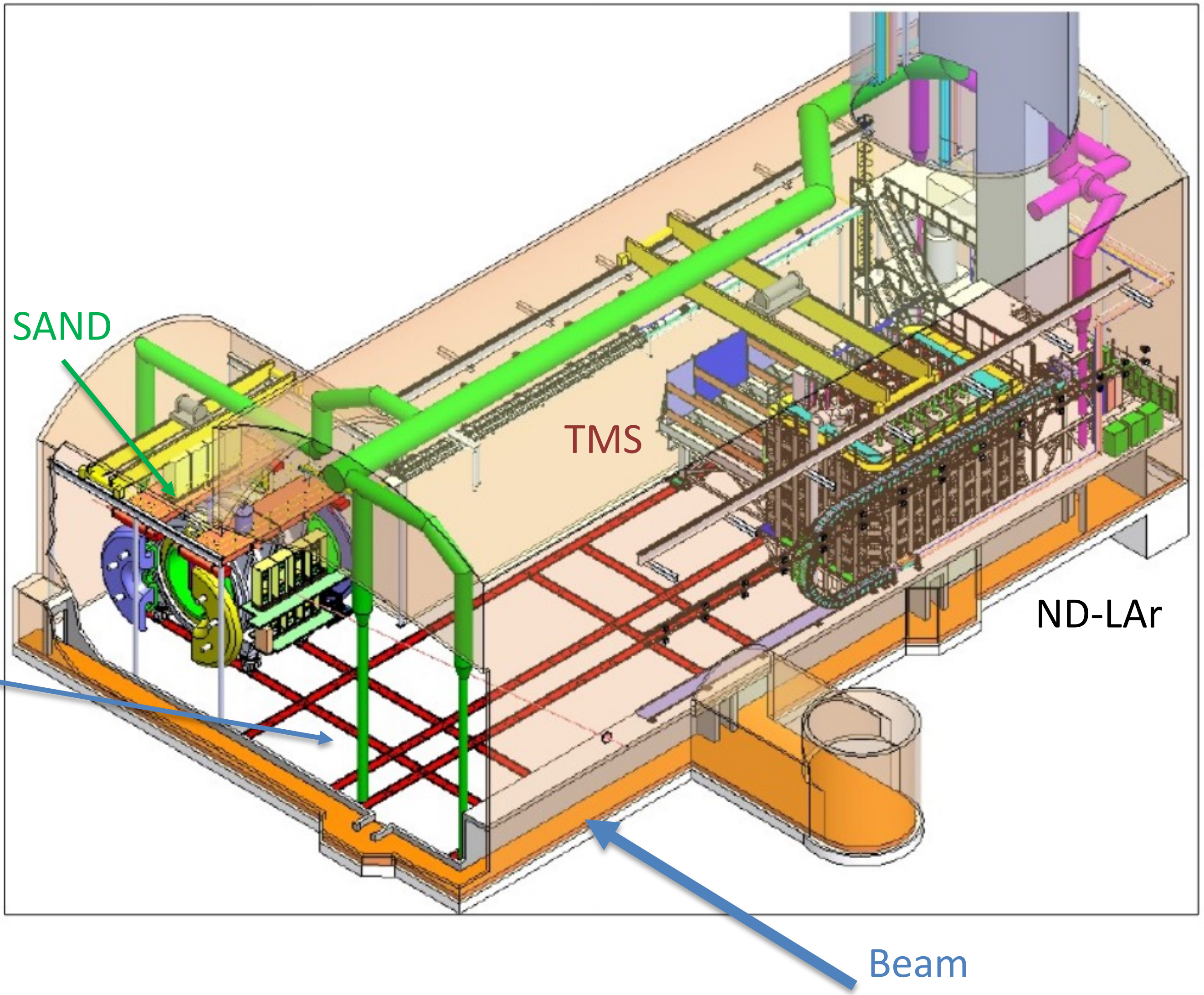
Science Goals

- Three main physics goals:
  - Origin of matter (neutrino oscillation parameters, mass ordering, ...)
  - Unification of forces (BSM physics, e.g. proton decay)
  - Black Hole Formation (neutrinos from core-collapse SN)
- Learn more at https://www.dunescience.org



Near Detector Complex

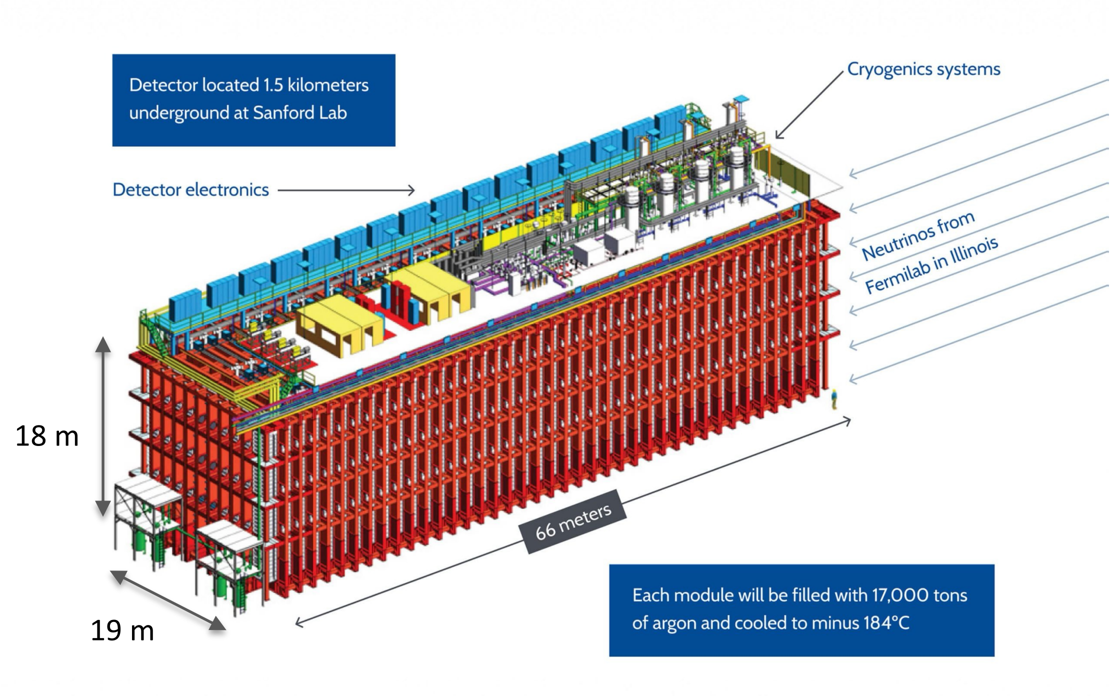
- Really, three detectors:
  - ND-LAr: Liquid argon TPC
  - TMS: Temporary Muon Spectrometer
  - SAND: System for on-Axis Neutrino Detection
- PRISM system allows ND-LAr and TMS to move off-axis to perform measurements at different angles to beam (SAND fixed).
- TMS to be replaced

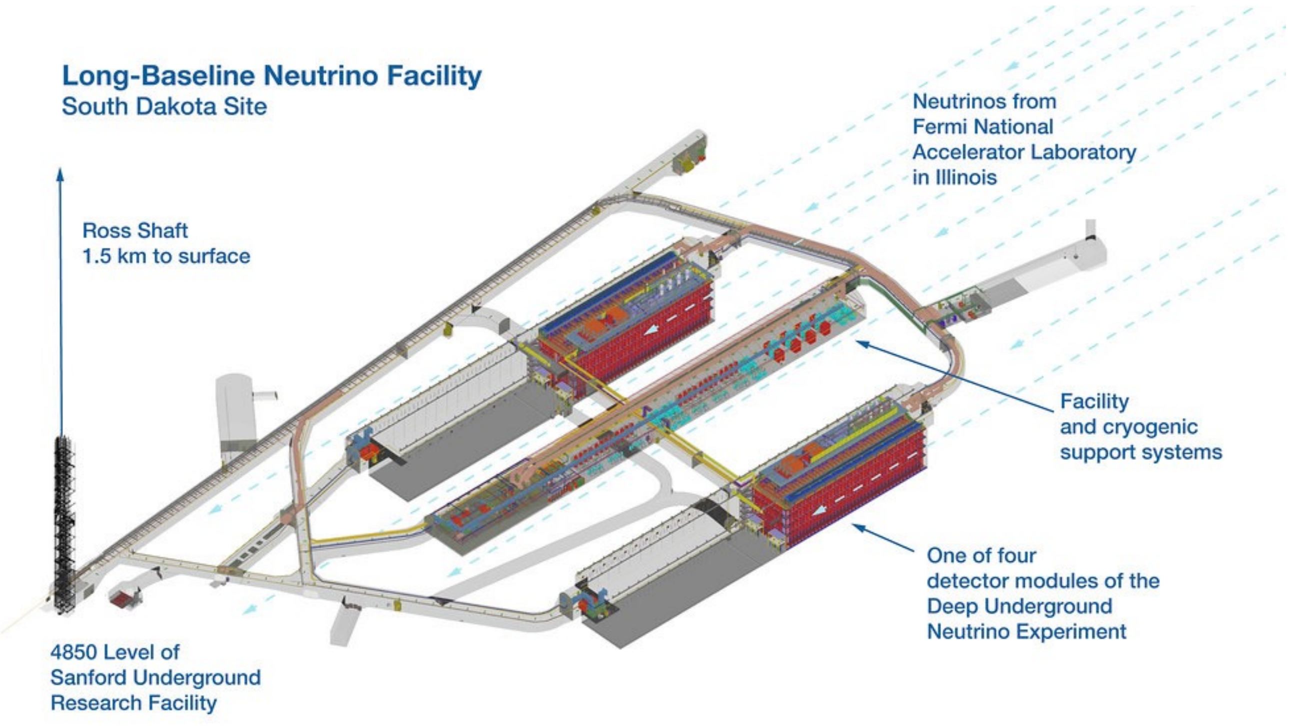


Far Detectors

- Far Detector will eventually consist of four LAr-based* TPC modules
- Installed in two stages (FD1 and FD2 for DUNE Phase 1)

* fourth module is still officially the "module of opportunity"





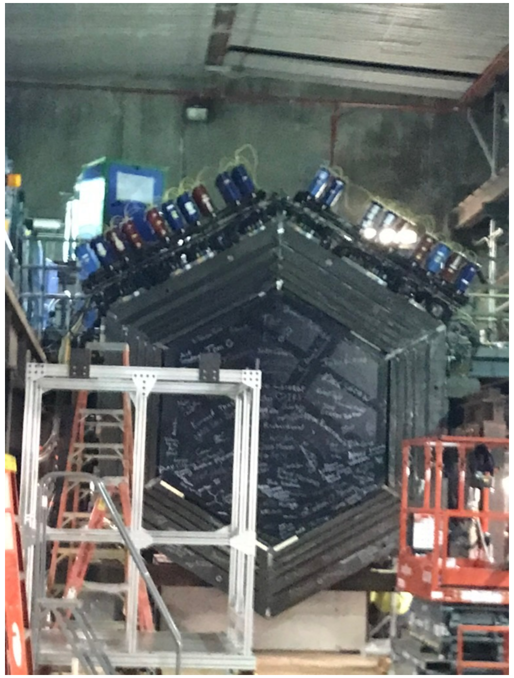
Fermilab DUNE

Prototype Detectors

- ProtoDUNE horizontal and vertical drift detectors (Far detector technology; CERN-Prevessin)

[Link to image]

- NDLAr **2x2** prototype (Near detector technology; FNAL)



Rough DUNE Timeline and Goals

- 2024
  - ProtoDUNE II beam run @ CERN; ND 2x2 prototype run @ FNAL
    - Aside: DAQ outputs HDF5 files (new to neutrino experiments)
- ca. 2025-2028
  - Phase 1 far detector installation
- ca. 2029-2031
  - ND installation, FD commissioning, first science runs with all Phase 1 detectors (ND and FD1/2)
- Late 2030s
  - Phase 2: full far detector, upgraded near detector, upgraded neutrino beam (all together: 4x Phase 1 event rate)

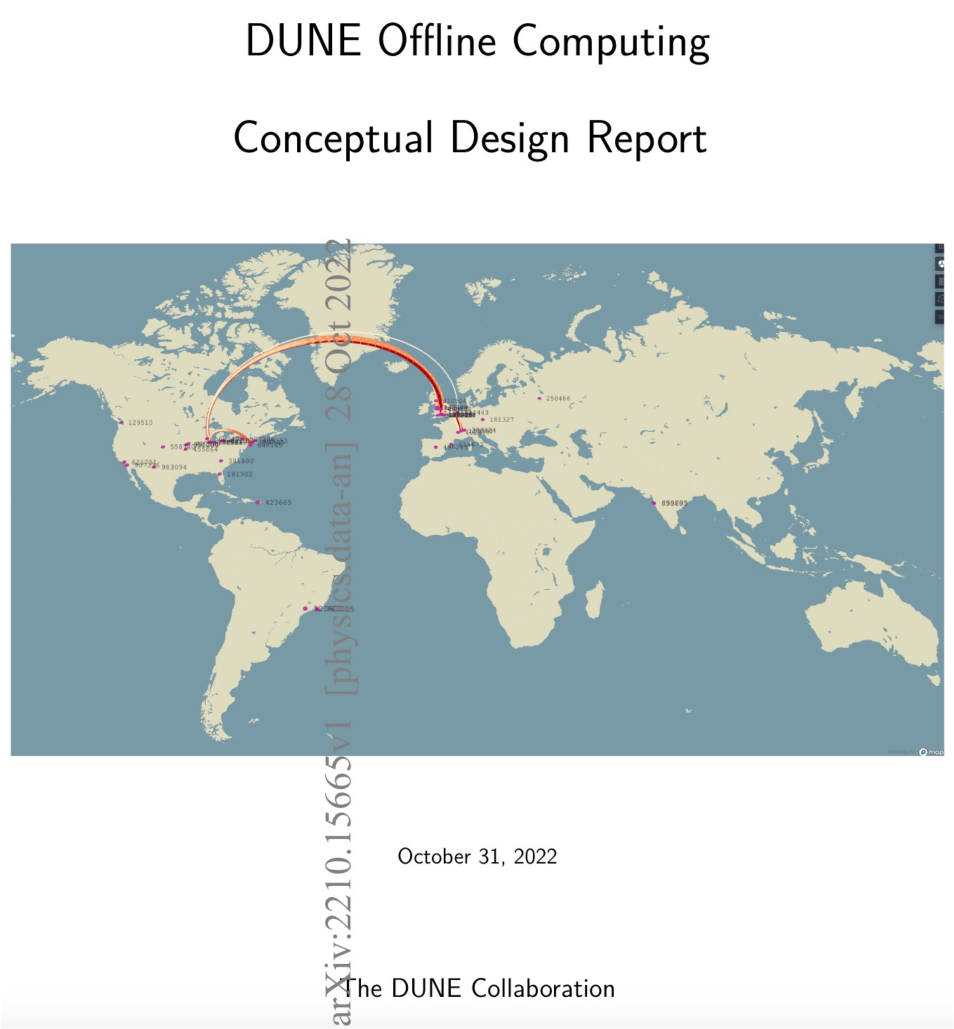
Experiment Stage	Physics Milestone	Exposure (kt-MW-years)	Years (Staged)
Phase I	5σ MO ($\delta_{\rm CP} = -\pi/2$)	16	1-2
	5σ MO (100% of $\delta_{\rm CP}$ values)	66	3-5
	3σ CPV ($\delta_{\rm CP} = -\pi/2$)	100	4-6
Phase II	5σ CPV ($\delta_{\rm CP} = -\pi/2$)	334	7-8
	$\delta_{\rm CP}$ resolution of 10 degrees ($\delta_{\rm CP} = 0$)	400	8-9
	5σ CPV (50% of $\delta_{\rm CP}$ values)	646	11
	3σ CPV (75% of $\delta_{\rm CP}$ values)	936	14
	$\sin^2 2\theta_{13}$ resolution of 0.004	1079	16

Snowmass 2021

5 sigma needs a LOT of pseudoexperiments....

Solving the Computing Problem

- Computing CDR written in 2022
- https://arxiv.org/abs/2210.15665
- Covers offline model, use cases, resource estimates
- Must eventually integrate information from seven distinct detectors
- Of course, things evolve even on the timescale of two years
- **Every single item you've discussed this week is relevant to DUNE in some way, shape, or form (many are absolutely critical to its success)**


DUNE Offline Computing

Conceptual Design Report

October 31, 2022

The DUNE Collaboration

arXiv:2210.15665v1 [physics.data-an] 28 Oct 2022

Storage Status and Requirements

- Combination of disk cache and tape for archiving
- Roughly 10% of LHC experiments in 2030s (also true of CPU needs)
- 2 geographically separate copies of raw detector data

[rucio] Replicas per site

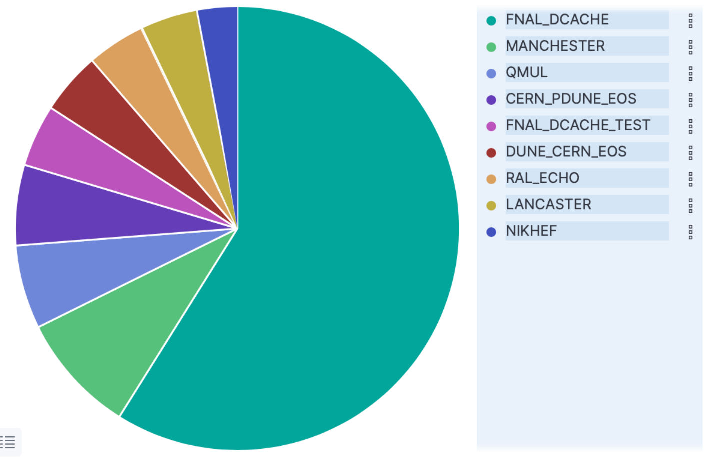
Export

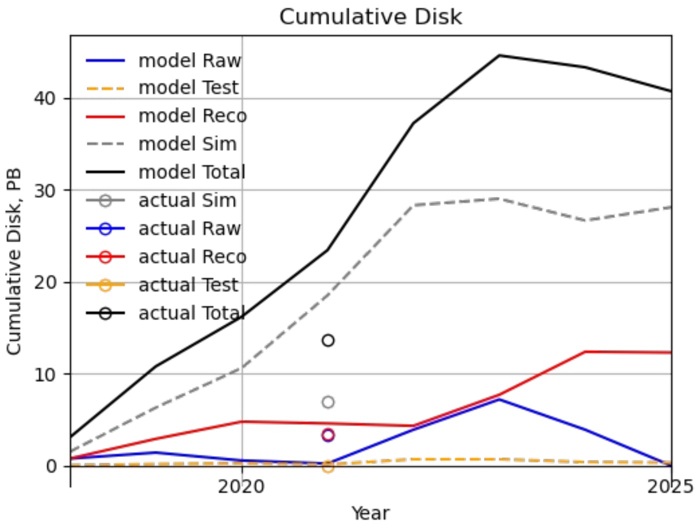
RSE	Replicas	Total bytes
FNAL_DCACHE	2,848,795	9.83PB
MANCHESTER	423,817	996.55TB
QMUL	294,794	624.06TB
CERN_PDUNE_EOS	282,793	975.33TB
FNAL_DCACHE_TEST	218,228	626.21TB
DUNE_CERN_EOS	217,975	626.0TB
RAL_ECHO	204,115	884.85TB
LANCASTER	200,066	471.49TB

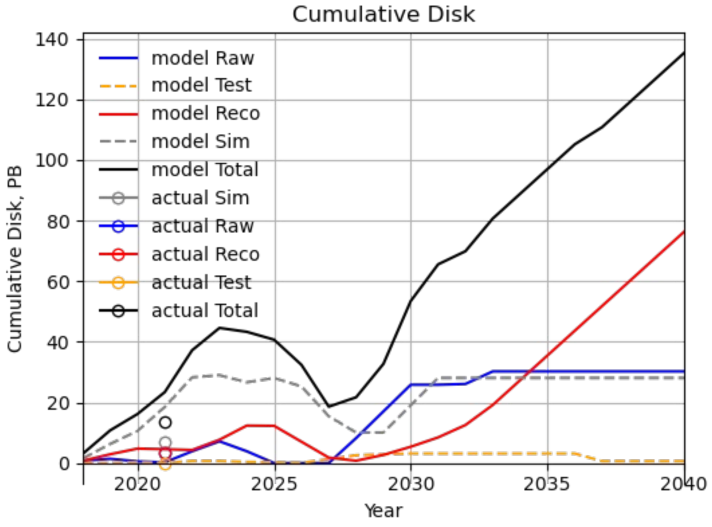
1 2

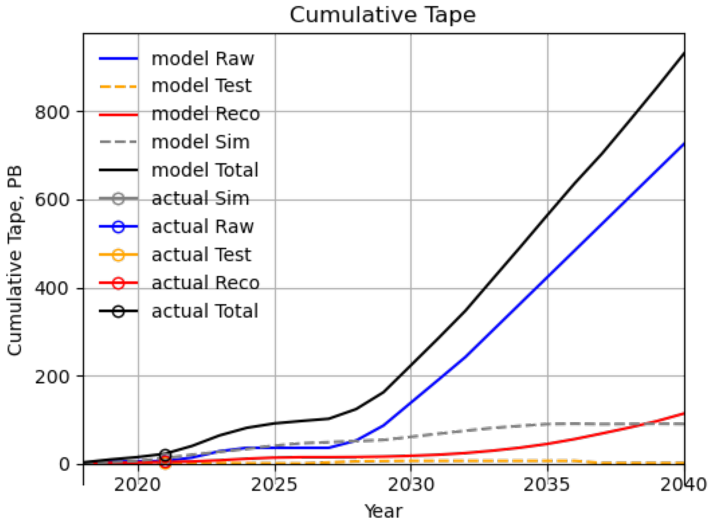
July 2022

[rucio] Replicas pie



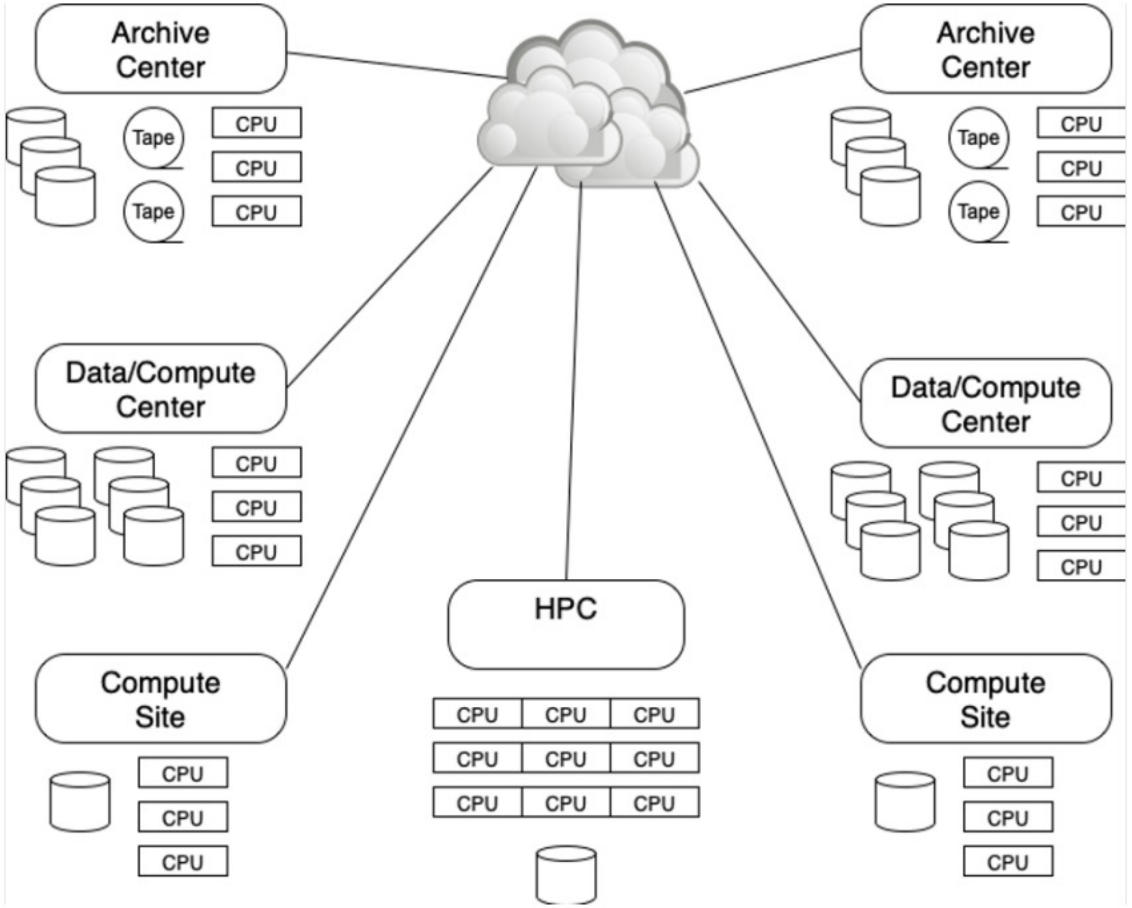






Distributed Computing Tools in DUNE

- Mostly High Throughput Computing-style (many single-core) jobs so far, similar to Large Hadron Collider experiments
  - However, more of a service-based model than a tiered model. Sites provide one of more services (standard compute, High Performance Computing, storage/compute, archiving, user analysis, etc.)
- Use variety of sites; mix of dedicated/pledged resources and opportunistic access through OSG
- Mostly stream input data over network with XRootD
- Rucio for dataset transfer and replication
- CVMFS for core software distribution; jobs run in containers (image also distributed via CVMFS)
- New software developed for bookkeeping and workflow management, known as justIN
- Good network design and performance are critical to success, especially in a "flatter" architecture



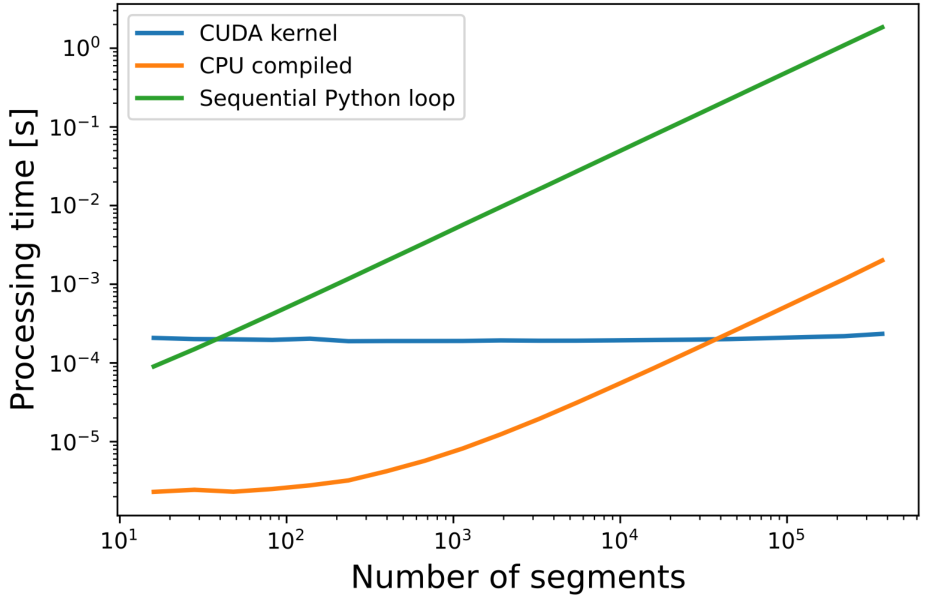
Fermilab DUNE

Some DUNE-ique items

- There are some differences wrt LHC experiments
  - "Events" don't really mean the same thing ("Trigger records")
  - Trigger records are *much* bigger than LHC events: O(100 MB) vs. O(1 MB)
  - Current and future DAQs creating HDF5 files (before, essentially root files).
- Earlier: "Mostly High Throughput Computing-style (many single-core) jobs so far..."
- HPC becoming increasingly important, especially with GPU availability
  - Also critical for performing final oscillation parameter fits and systematic variations (mentioned a bit earlier); phase space is large and requires MPI processing; exception to above rule of thumb (but a vital one!)
- Speaking of GPUs...

GPU needs example: ND-LAr

- ND needs to be able to make measurements close to the neutrino production point and contain a large fraction of the (hadronic side) of the
- events to fulfill basic requirements like constraining the flux*cross
- section model in a way that can be transferred to the FD.
- Design (~5x5mm pixels, segmentation) driven by energy resolution requirements (see ND conceptual design report) and need to disentangle the ~50 events per beam spill.
  - Leads to roughly 12 million channels.
- Large number of independent channels lends itself very well to parallelization, which is why GPUs were adopted pretty early on (see larnd-sim paper; shown on this slide)
- **Also significant use of ML in reconstruction**

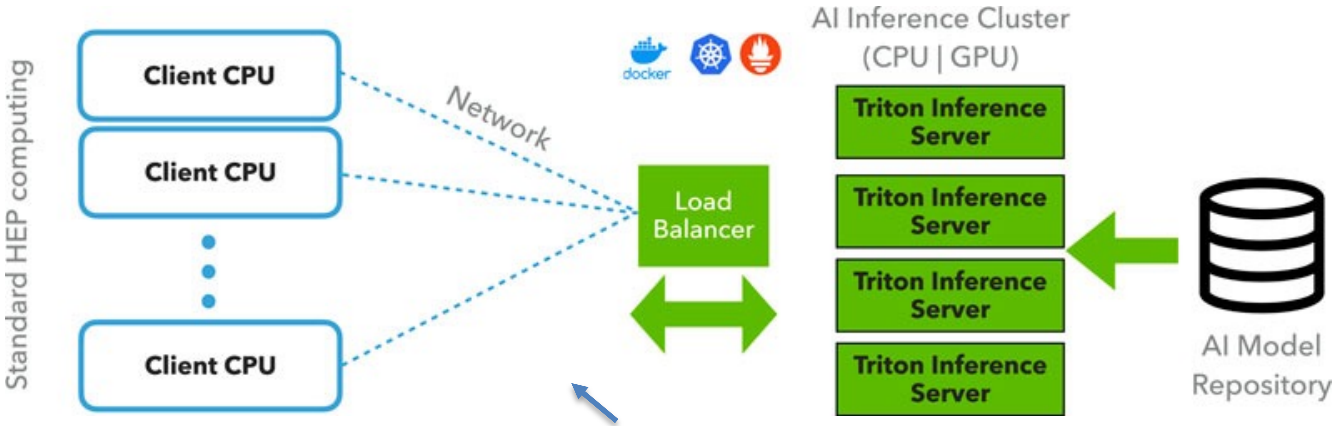


Calculation	Loop over	Quantity	GPU speed-up factor
Recombination factor	Segments	10^5	shown in plot ×3
Induced current	Pixels	10^3	most expensive task ×7314
Charge electronics response	Pixels	10^3	×985
Light time profile	Time ticks	10^5	×228
Scintillation profile	Time ticks	10^3	×568
Light electronics response	Time ticks	10^3	×1883

DUNE Collaboration, JINST 18 P04034 (2023)

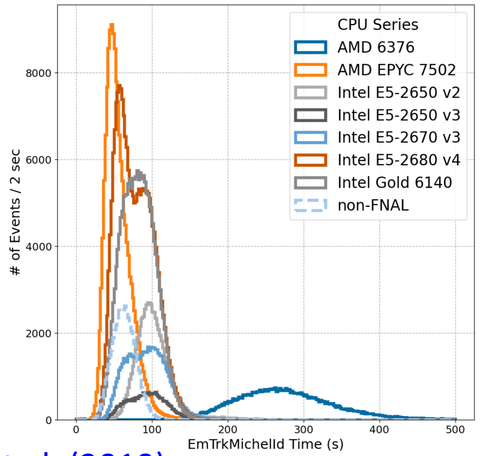
GPUaaS Studies

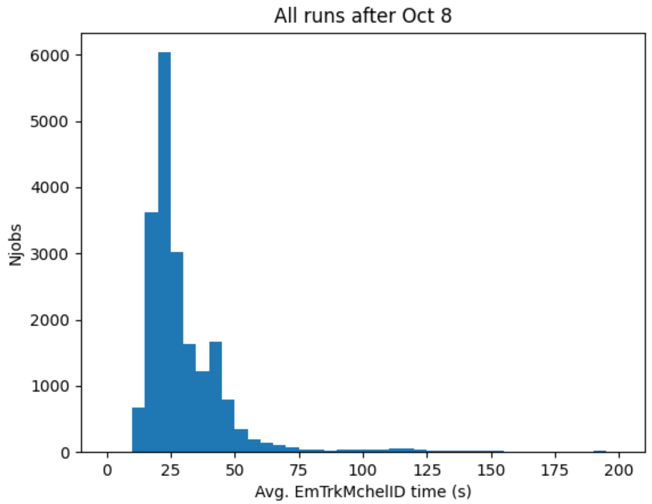
- Tests with MC show large decrease in processing time for part of track reconstruction if run on a GPU
  - Use Triton inference server and gRPC in job for communication, allows many-to-1 model of CPU jobs to single GPU (the SONIC Model)
  - Rest of stack uses standard CPU, can thus run on any site with ext. network without needing local GPU
- ProtoDUNE beam data reprocessing campaign in 2021 utilized approach at scale (few thousand concurrent jobs), used cloud-based GPU server. See Cai et al. 2023 for details
  - Clear overall speed increase wrt CPU-only version, but overall amount of data movement per job increased *significantly* (10x) wrt CPU-only versions
  - Must take care not to saturate network capacity or time gains will be lost
  - Have also run with local servers on NERSC Perlmutter nodes



M. Wang *et al.*, Front. Big Data 3, 604083 (2021)

	ML module	non-ML modules	Total
	Wall time (s)		
CPU only	220	110	330
CPU + GPUaaS	13	110	123





Further reading on SONIC model:
Duarte et al. (2019), Krupa et al. (2021), Pedro et al. (2019)

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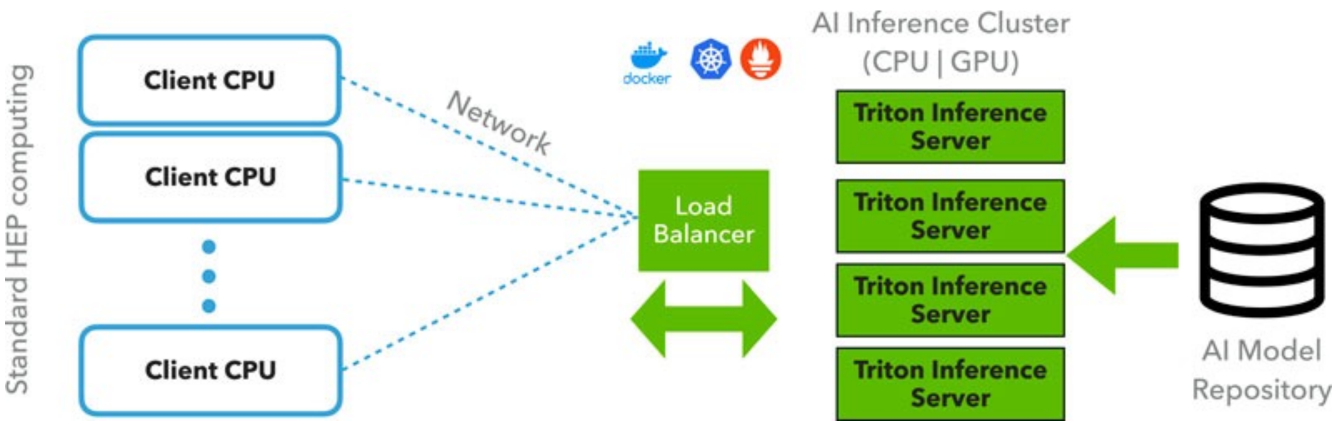

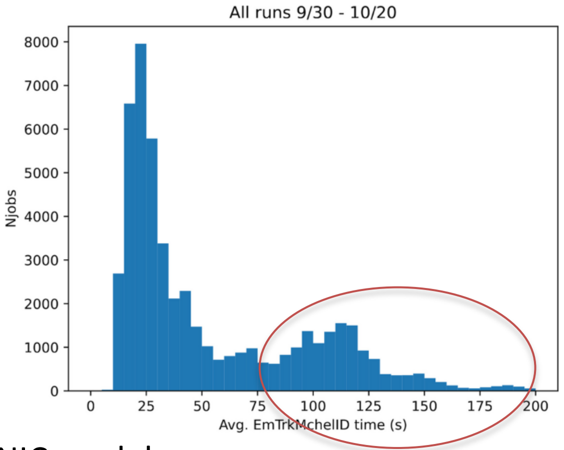

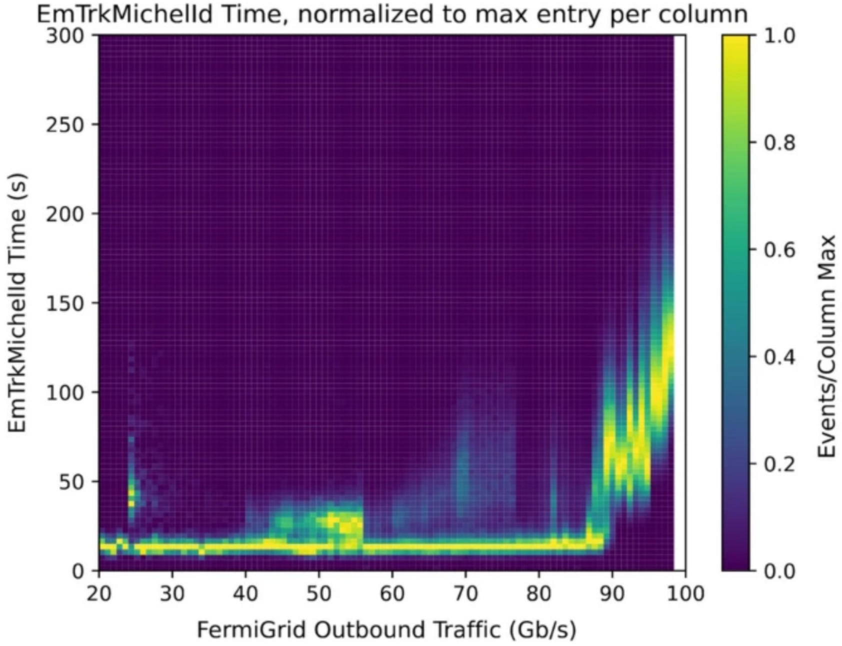

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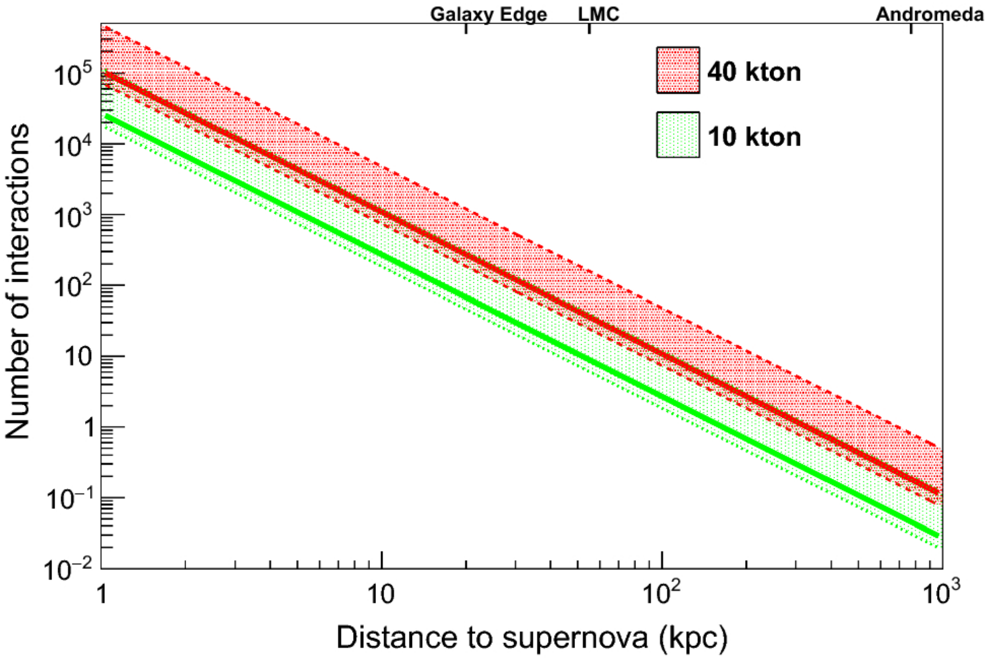
Fermilab DUNE

Core Software Framework

- ProtoDUNE and FD software based on the Art framework (descendant of CMSSW). Remember, however, that
  - DUNE and collider detector events differ in size and structure; readout not always synced to a beam timing
  - DUNE needs easy access to heterogenous computing resources
  - Some external tools and packages lend themselves more easily to Python than C++
- Therefore, DUNE has commissioned the design of a new core software framework to support both ND and FD workflows. Key features include:
  - Support for algorithms/modules in multiple languages (C++ and Python for sure)
  - Flexible, user-defined, data groupings (must sync up different detector data in differing ways)
  - More "eager writing" (don't wait until the end to write entire event to disk)
  - Configurable, composable, framework-agnostic algorithms will “plug in” to the core framework which will schedule data/workflow/hardware access (e.g. GPU) and handle data provenance tracking and other metadata, and data persistency and I/O.
- Planning to deliver during FY27 (FY starts October 1, 2026)

The Big Challenge: a supernova

- Sensitive to neutrinos from a (relatively) nearby supernova
- Would read detector out in a continuous mode for ~ 100s
- Expect approximately 400 TB (uncompressed) for four-module readout; **still 184 TB at current compression levels**
- Prelim studies of event reconstruction could lead to a source location accurate to < 5 degrees– **important for follow-up by other instruments (optical/near IR telescopes, etc.)**
  - **But time is everything in this game. 4+ hours to transfer data on a dedicated 100 Gb network, plus processing time…**
- Expect one SN trigger per month (mostly false alarms)



DUNE Collaboration, EPJC **81**, 423 (2021)

Supernova: SINGLE CHANNEL READOUT FOUR MODULE READOUT TRIGGER RATE	300 MB 460 TB 1 per month	Uncompressed 100 s Uncompressed 100 s (assumption)

Processing supernova data

- Limited space and infrastructure (i.e. cooling) at the far site means bulk processing on a local farm is impractical to impossible
- Don’t have to transfer full dataset before processing starts
  - Workflow mgmt systems must deal with dynamic datasets and shifting resource availability
- 10,000 – 40,000 present-day CPUs needed for reconstruction (30k likely) to finish within a few hours of event (goal: preliminary direction before event rises in optical bands)
  - HPC centers can probably fit the bill, but data transfer in and out is the major problem to solve
  - **Must consider redundancy as well**
- Must be able to handle large input stream as well as output at a similar rate
  - Run standard data reco or make a slimmed-down, faster version? Speed vs. accuracy tradeoff?
- Implications for additional network paths? What are those requirements? Costs?

Fermilab DUNE

Summary

- DUNE will significantly advance our understanding of one of the least understood elementary particle types
- Potential for significant paradigm-shifting discoveries (e.g. proton decay)
- A supernova in our galaxy will lead to a wealth of information, but processing detector data in a timely fashion will be one of DUNE's biggest challenges
- DUNE will not succeed without efficient, robust computing! Affects all aspects of the experiment
- General strategy: use common tools wherever possible, share information with other experiments, but don't be afraid to break new ground where needed.
- Plenty of room to get involved and work on interesting projects!

Thank You!

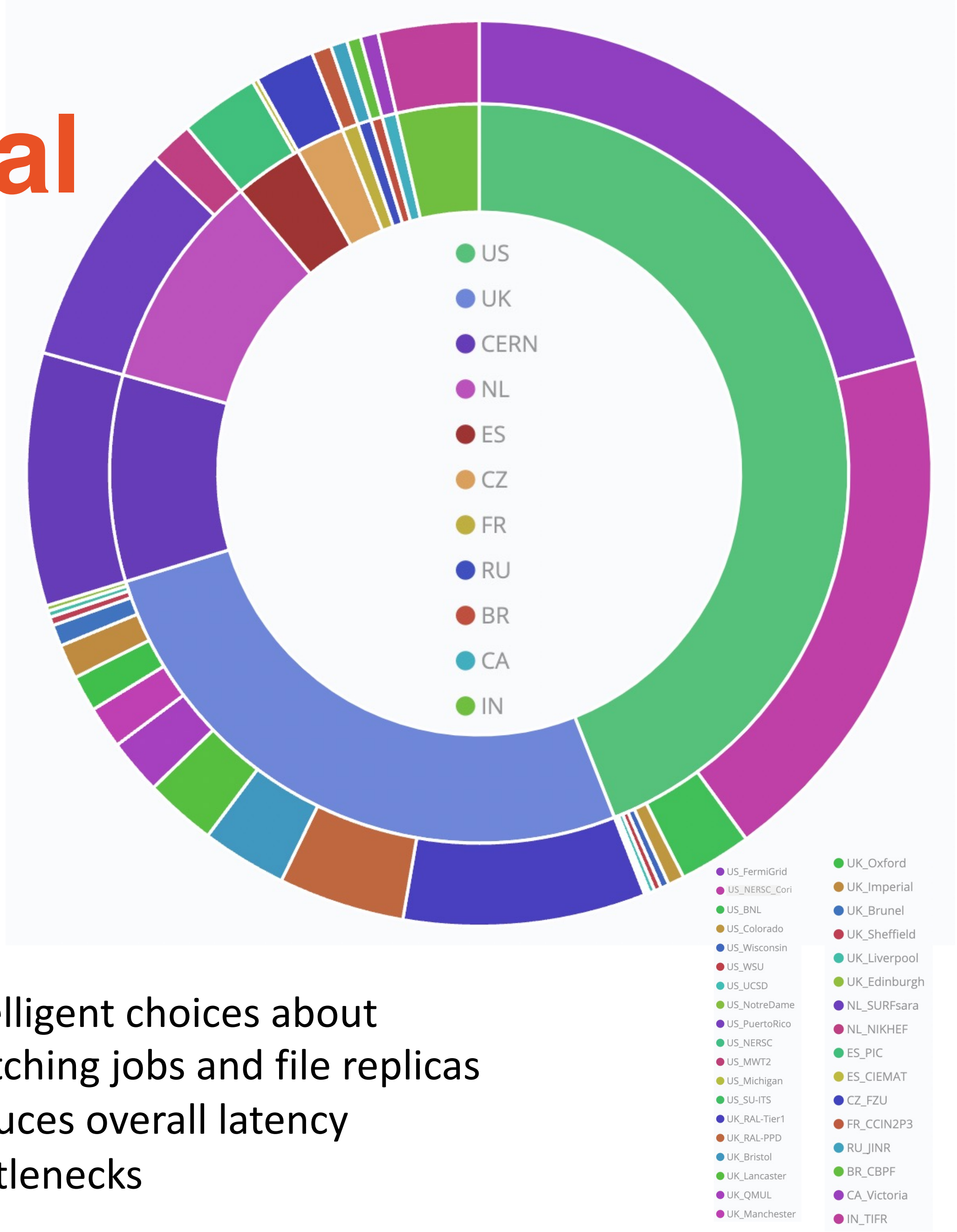
Backup

Some further reading

- dunescience.org
- https://arxiv.org/abs/2210.15665
- ML reconstruction for LAr TPCs
- DUNE Physics Snowmass Whitepaper
- ProtoDUNE performance paper (Figure 47 is a good example of how to distinguish between the different types of events)

DUNE Computing is global

- Significant efforts to add international presence began in 2018
- Compute sites in 12 countries + CERN on four continents
- Record time for adding DUNE support to a grid site (start to successful batch jobs) is **2h**.
- For October 2021-October 2022, > 50% of production wall hours outside USA; < 25% at Fermilab
- Numerous sites have also pledged storage support (19 PB in 2022)



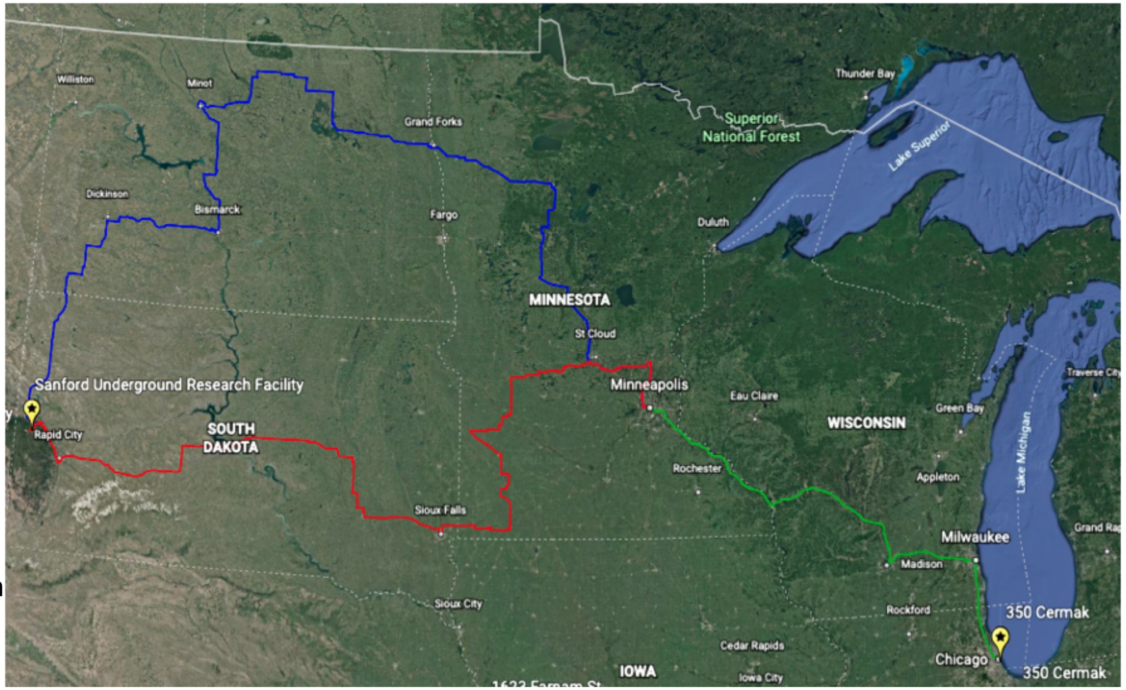
Intelligent choices about matching jobs and file replicas reduces overall latency bottlenecks

Fermilab DUNE

Networking Setup and Timeline

- Planning 100 Gb/s primary link between SURF and FNAL
  - Enables 1 wk DAQ backlog to clear in 1 day in case of connection outage. DAQ has 99% uptime
  - Primary path currently 10 Gb
  - Secondary path now 1 Gb; will go to 100 Gb when commissioning starts
  - Tertiary path capable of meeting DAQ requirements during normal physics operations
- Networking between compute sites varies; leveraging existing setups at LHC compute sites where possible (e.g. LHCONE), other large-scale infrastructure (e.g. ESnet, GÉANT, NRENs, etc.)
  - Expect larger sites w/storage to have 40+ Gb/s ext. connectivity; medium sites 20+ Gb/s
- Monitoring tools include perfSONAR

Primary Path Secondary Path



Not shown:
10 Gb Tertiary path through Denver and KC

DUNE FD WAN Bandwidth Timeline Projections:

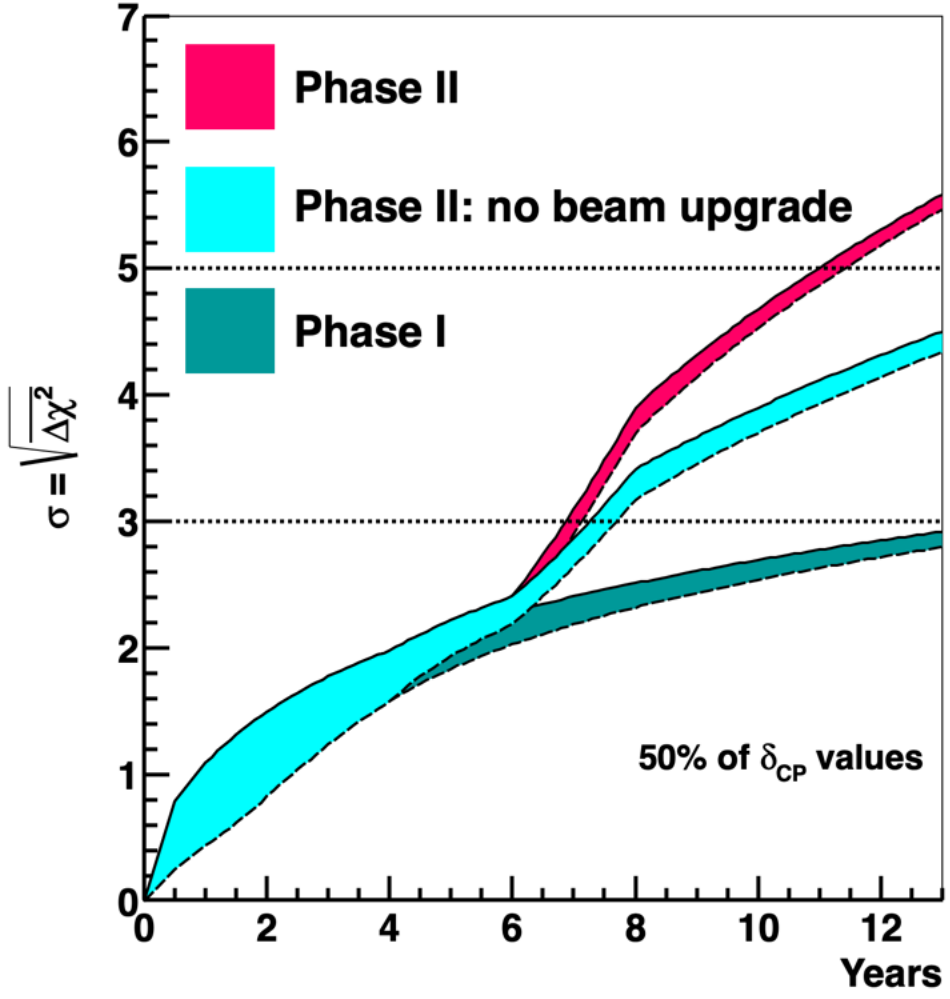
Date	*Stage of the experiment*	*Primary Path*	*Secondary Path*	*Tertiary Path*
Now	Cavern excavation	10GE	< 1GE via SURF	none
2025	Detector construction	10GE	< 1GE via SURF	none
2027	Computing/DAQ deployment	100GE	10GE	< 1GE via SURF
2028	Cryo deployment completed	100GE	100Gb/s	10GE
2029	Start of science	100GE	100Gb/s	10GE

REED: South Dakota Higher Education Network

- (pink) vLAN service provided by REED/GPN (shared)
- (green) Dedicated circuit Ross Dry Bldg. to Chicago
- (yellow) Dedicated circuit Yates Complex to Denver

Physics sensitivities

- Sensitivity to CP violation for 50% of deltacp values, as a function of time in calendar years. The width of the bands shows the impact of potential beam power ramp up; the solid upper curve is the sensitivity if data collection begins with 1.2 MW beam power and the lower dashed curve shows a conservative beam ramp scenario where the full power is achieved after 4 years. The green band shows the Phase I sensitivity and the red band showss the Phase II sensitivity.The cyan band shows the Phase II sensitivity if the beam upgrade does not occur.
- From DUNE Snowmass physics whitepaper



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