BEAMLINE TO HPC: CODED APERTURE LAUE MICRODIFFRACTION

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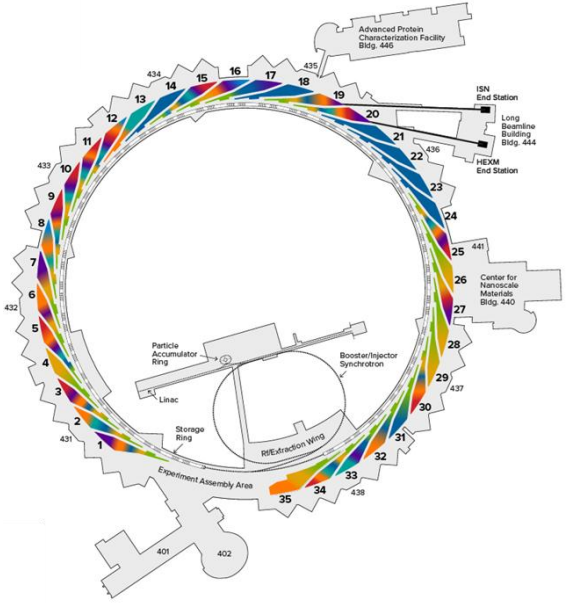
A NOTE ON THIS PRESENTATION

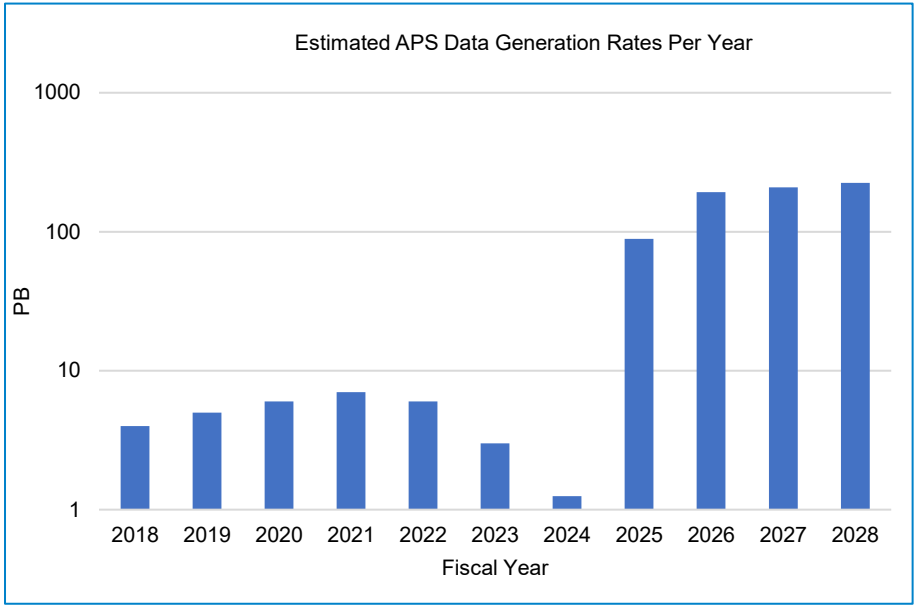
- Most work done in late 2022-2023
  - Pre-AI
- Beamline has been down since mid-2023
  - Early 2D experiments ~2 weeks ago
  - HPC-scale experiments starting in winter

ADVANCED PHOTON SOURCE

- 72 beamlines
- 5,500 users per year
- ~2000 publications per year
- 20% of AlphaFold's training data was characterized at the APS

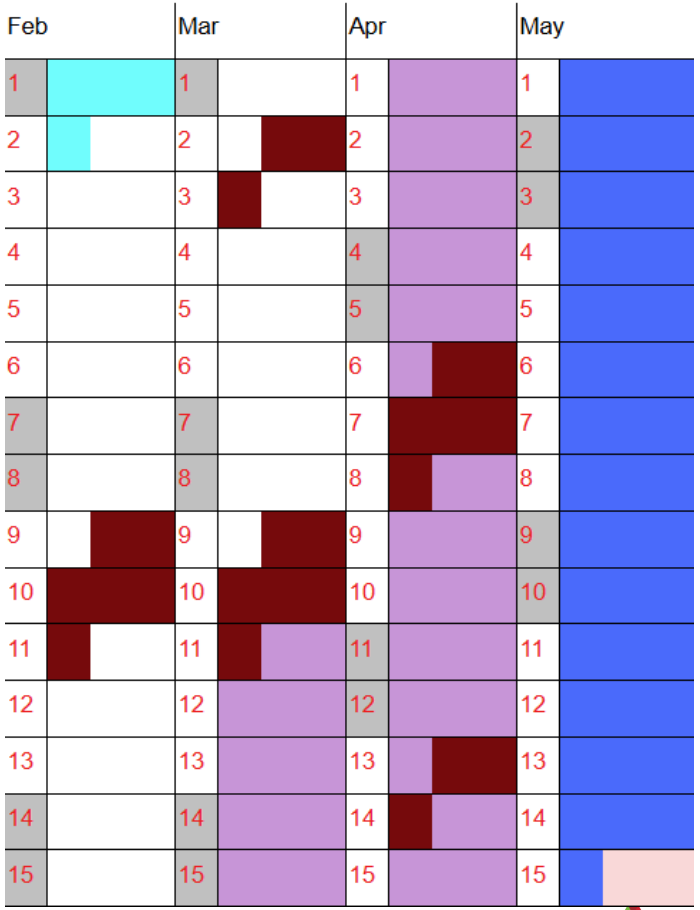


HANDLING THE APS UPGRADE

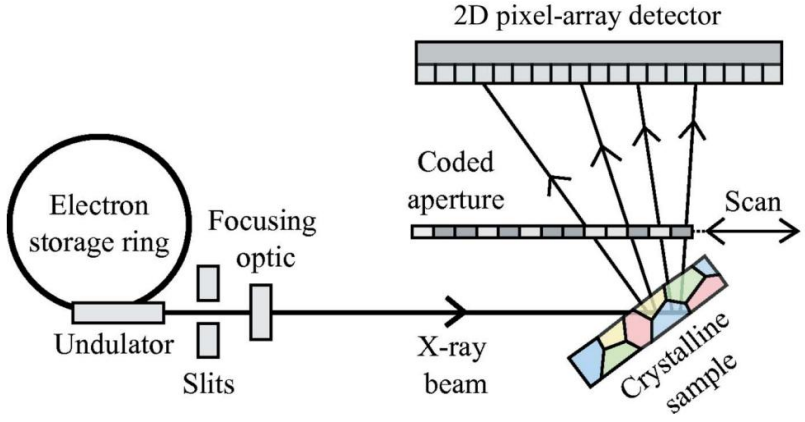


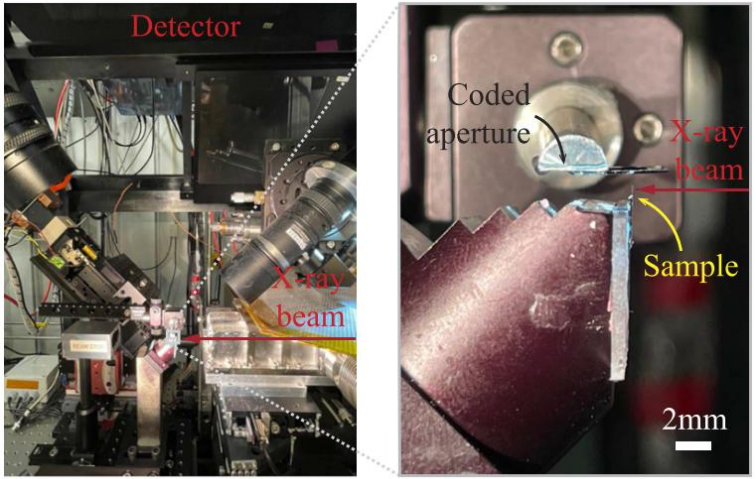
BEAMTIME IS EVERYTHING

- Users are assigned shifts to conduct experiments
- ***Any*** time not putting atoms in front of beams feels wasted
- Culture of “fire and forget”



CODED APERTURE LAUE MICRODIFFRACTION





MatSci applied to microelectronics, batteries, geology, etc

Up to a 5x reduction in beamtime vs wire scans

Gürsoy, Doğa, Dina Sheyfer, Michael Wojcik, Wenjun Liu, and Jonathan Z. Tischler. "Depth-resolved Laue microdiffraction with coded apertures." Journal of Applied Crystallography 55, no. 5 (2022).

Gürsoy, Doğa, et al. "Digital autofocusing of a coded-aperture Laue diffraction microscope." Review of Scientific Instruments 94.1 (2023): 013702.

TRADEOFF: COMPUTATIONAL COMPLEXITY

- ~450 points per scan
  - ~1.5 min per point
  - **~11 hours per scan**

- Est. Processing (CPU Implementation, Oct. 2022)
  - Single core: 15 days/point (**18.75 years/scan**)
  - 1 Polaris Node: 20 hours/point (**375 days/scan**)

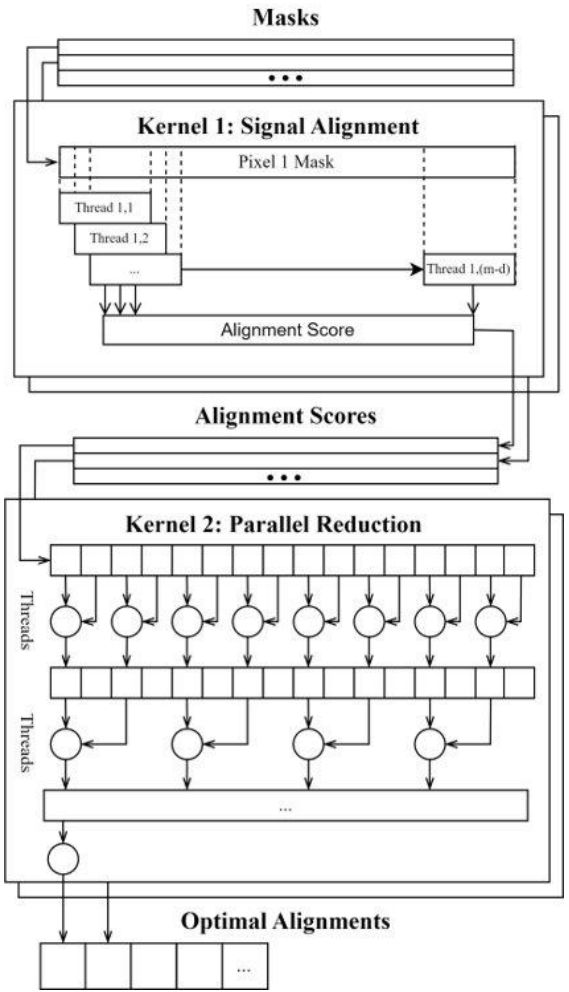
- **Unique Position**: reason to use HPC pre-APS-U
  - Allocated 55 Polaris nodes & preemptable queue
  - Experiments scheduled in 6 months
  - Can we keep up with the detector?

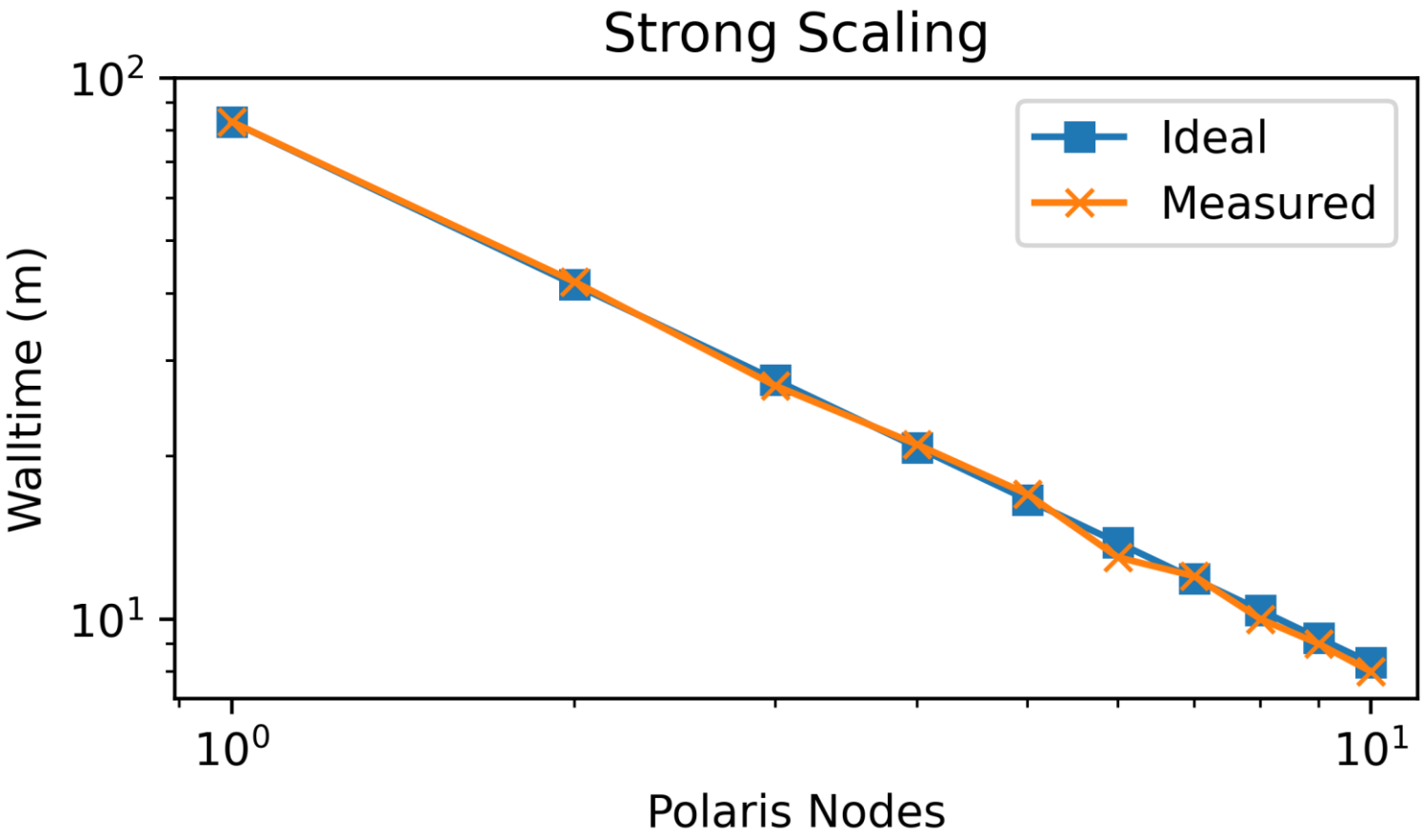
OPTIMIZATION

- GPU: Custom CUDA kernels
  - Heavy memory optimization
  - 800x segment speedup
  - (When GPT-o1 came out, this is the first thing I tested on it)

- CPU: Jax JIT compilation
  - Cache & memory optimizations
  - 4x segment speedup

– **14-15x speedup in practice**
  – ~~20 hours/point* (375 days/scan)~~
  – **1.4 hours/point (26 days/scan)**




Strong Scaling
10^2
10^1
Walltime (m)
10^0
10^1
Polaris Nodes
Ideal
Measured

POINT-LEVEL PARALLELISM

- Increases throughput
  - ~~26 days/scan~~
  - **12 hours/scan @ 55 nodes**

- Mostly there for optimization.

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440154.polaris-p* laue_aps_realti* mprince           25:30:56 R demand
440155.polaris-p* laue_aps_realti* mprince           19:05:28 R demand
440156.polaris-p* laue_aps_realti* mprince           11:18:02 R demand
440157.polaris-p* laue_aps_realti* mprince           08:57:42 R demand
440158.polaris-p* laue_aps_realti* mprince           02:00:51 R demand
440159.polaris-p* laue_aps_realti* mprince                  0 Q demand
440160.polaris-p* laue_aps_realti* mprince                  0 Q demand
440161.polaris-p* laue_aps_realti* mprince                  0 Q demand
440162.polaris-p* laue_aps_realti* mprince                  0 Q demand
440163.polaris-p* laue_aps_realti* mprince                  0 Q demand
440164.polaris-p* laue_aps_realti* mprince                  0 Q demand
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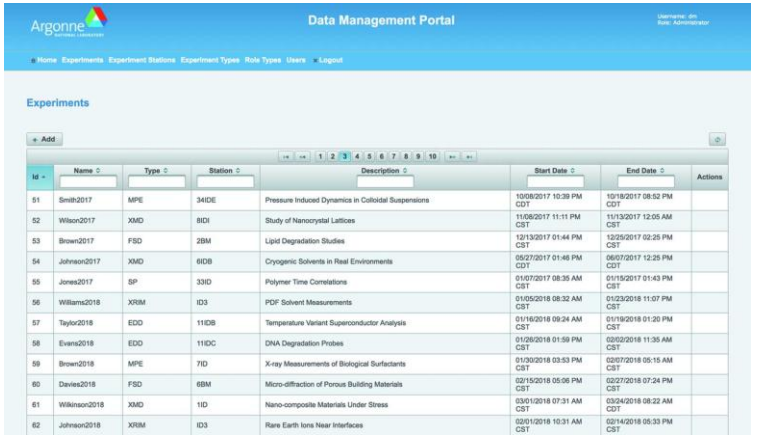
DATA TRANSFER SYSTEM REQUIREMENTS

- Autonomously detect and process new data from the APS
- Transfer data to and from the facilities
- Create and monitor jobs on Polaris

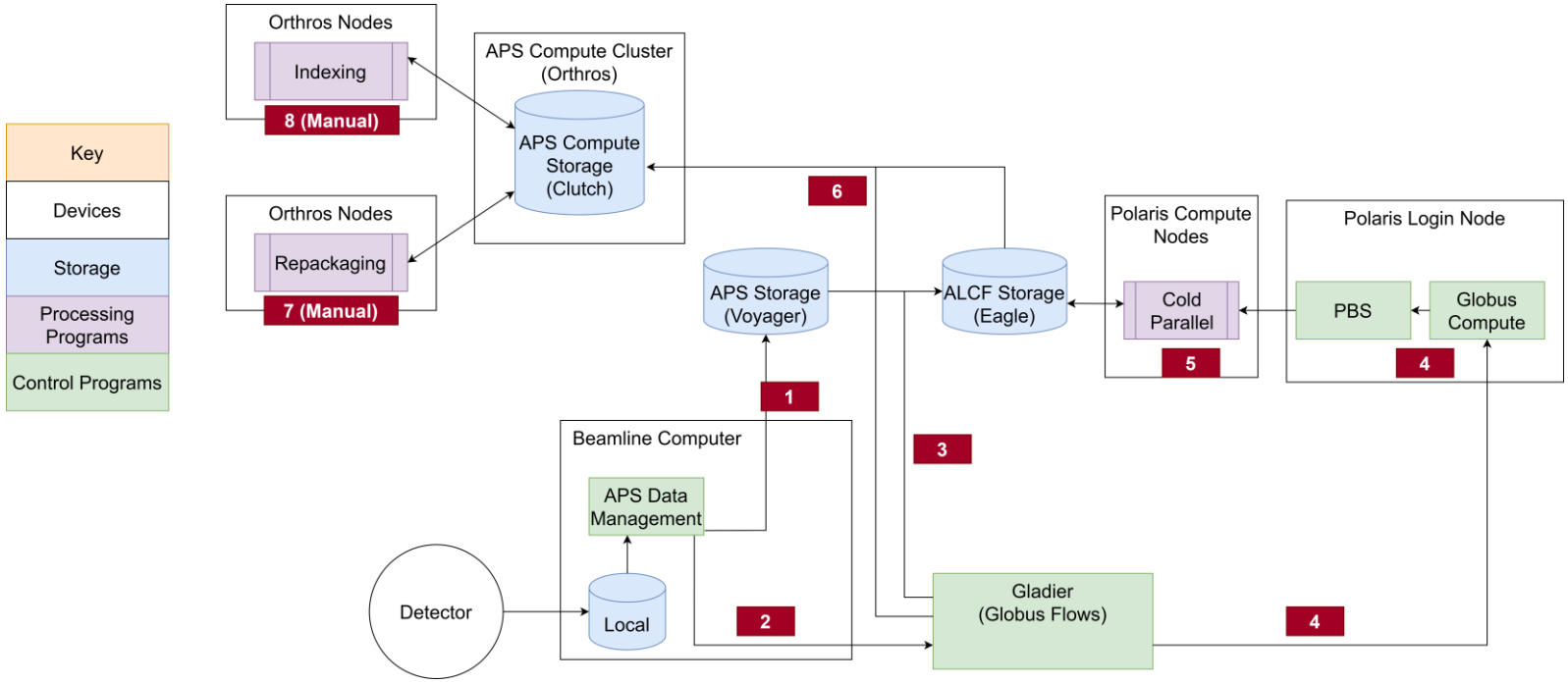
DATA TRANSFER SYSTEM TOOLS

- Data Management System
  - User Isolation
  - Internal Data Processing

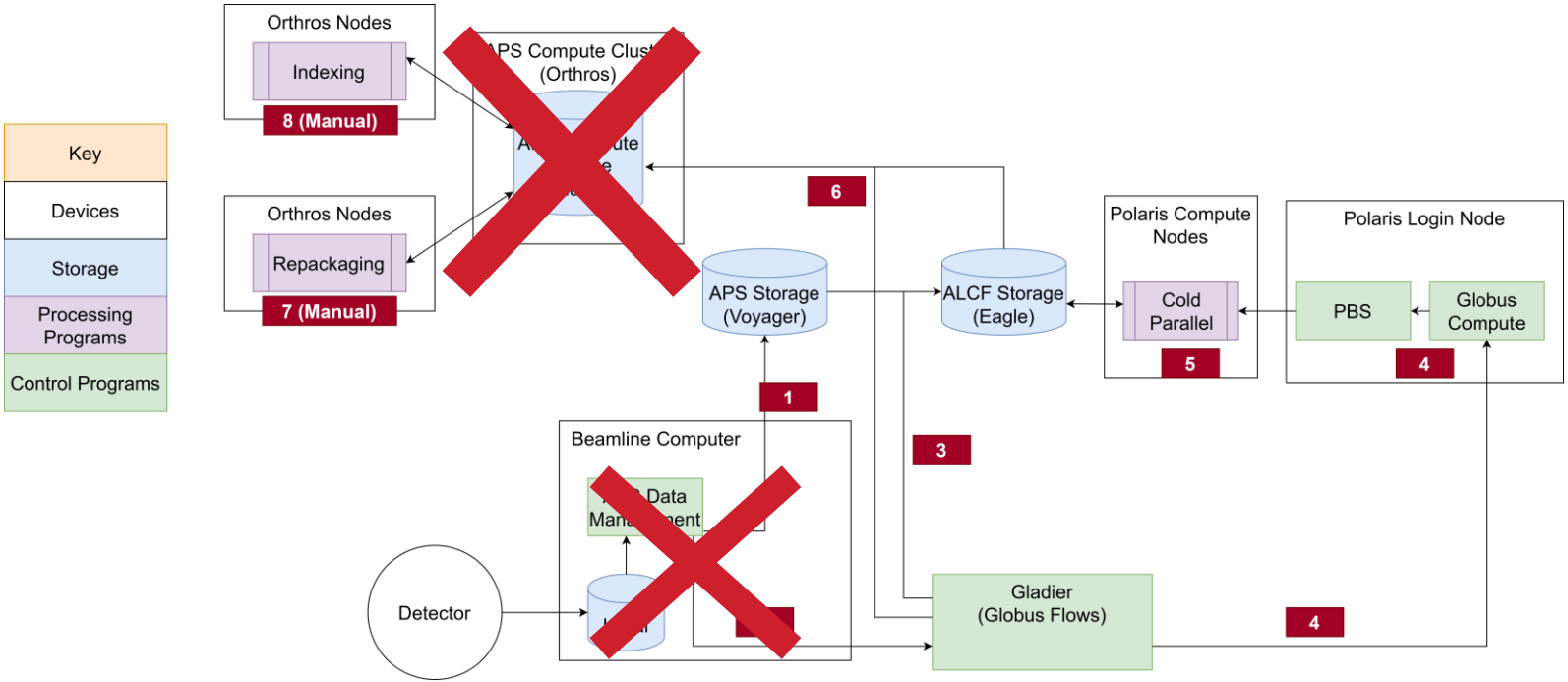


- Globus
  - Grid FTP
  - Remote SSO
  - Remote Queue Access

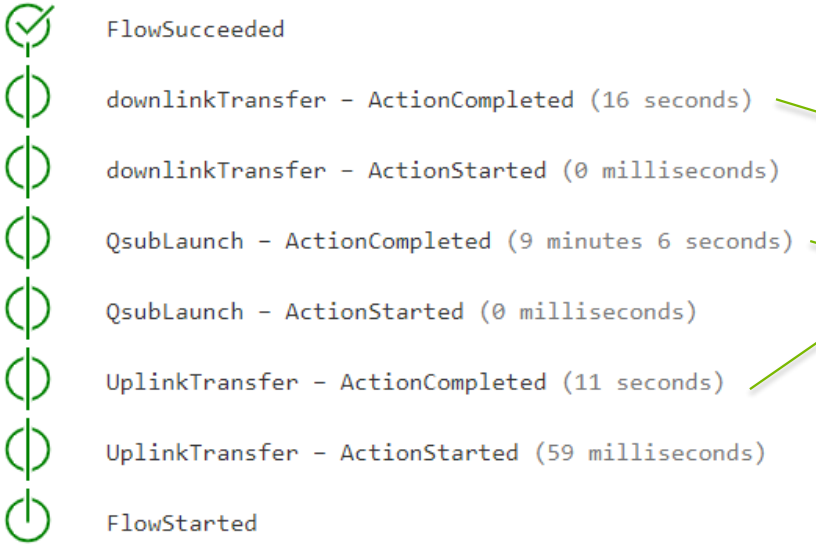
DATA TRANSFER SYSTEM



DATA TRANSFER SYSTEM 2026



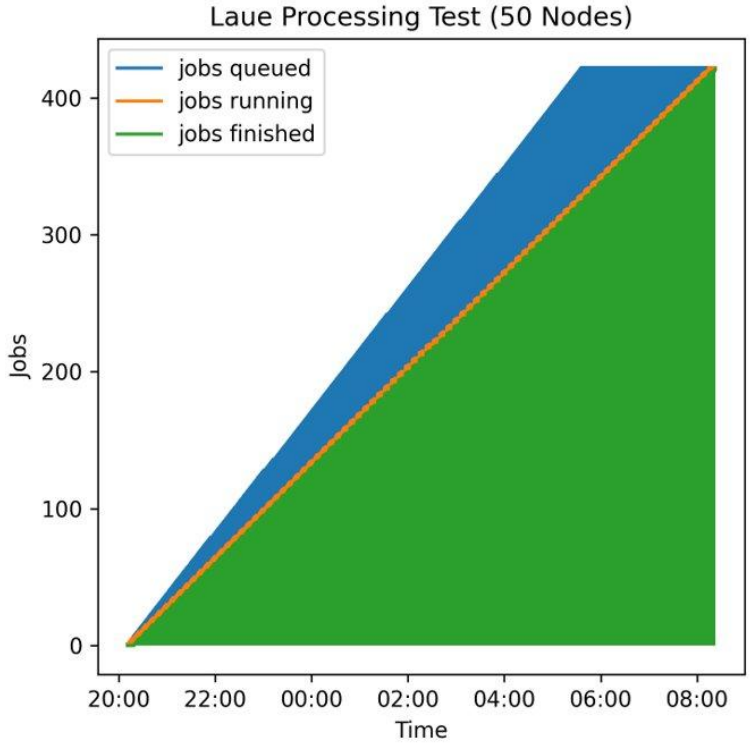
DATA TRANSFER SYSTEM OVERHEAD



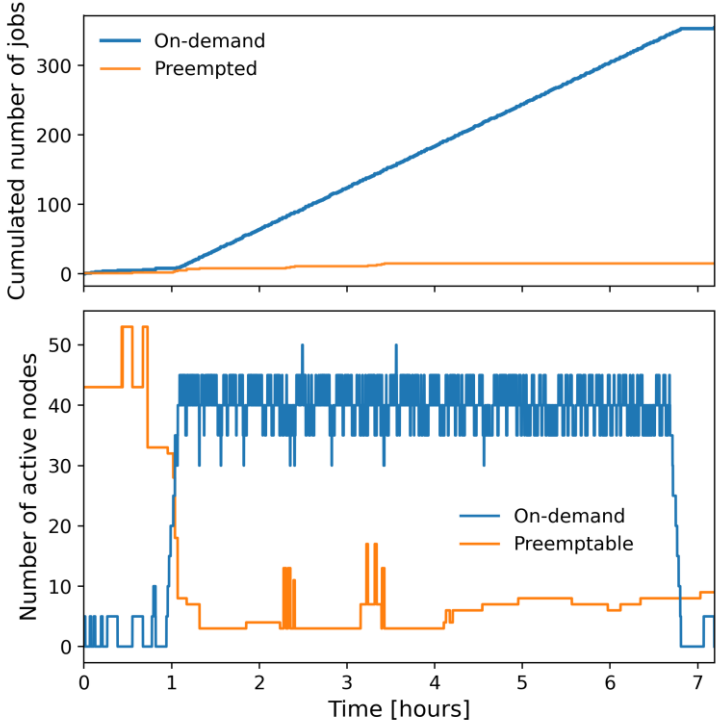
- 20-30s from Globus data transfer
- ~~30-60s from DM~~ (2026)
- 30-60s from queue (on first 5 jobs)

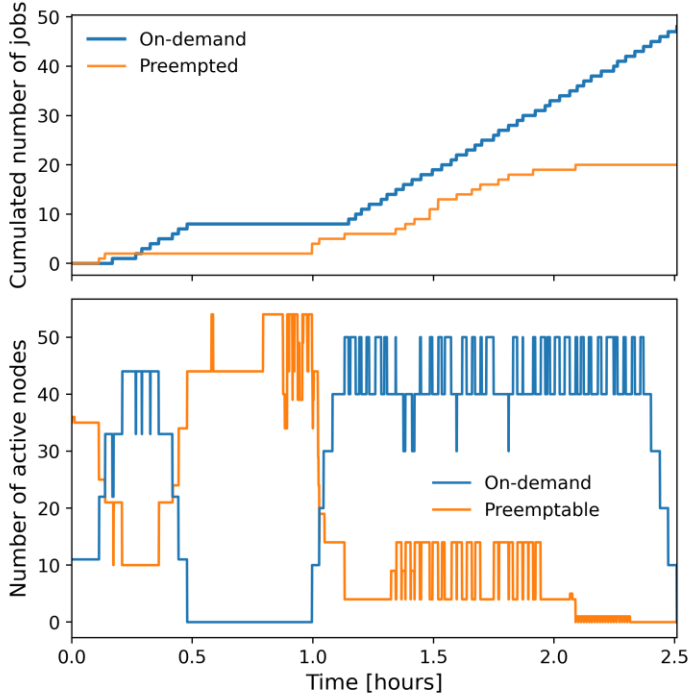
FEB 23, 2023 FIRST FULL-SCALE RUN

- Data Rate
  - 1 point every 72 s
  - 428 points (9 hrs)
- Data Volume:
  - Input: 673 GB
  - Output:
    - Test 1: 2.6 TB
    - Test 2: 9.4 TB
- Success Rate:
  - 844/856 (98.5%)
  - (Failed file copies on eagle)



PREEMPTION CHARACTERISTICS



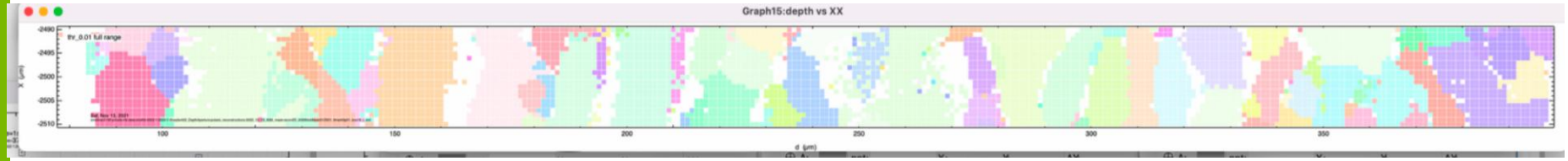


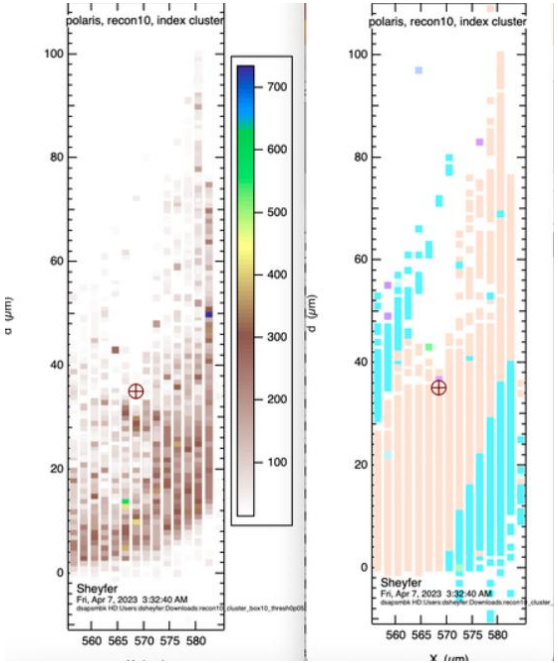
ALL TEST RUNS

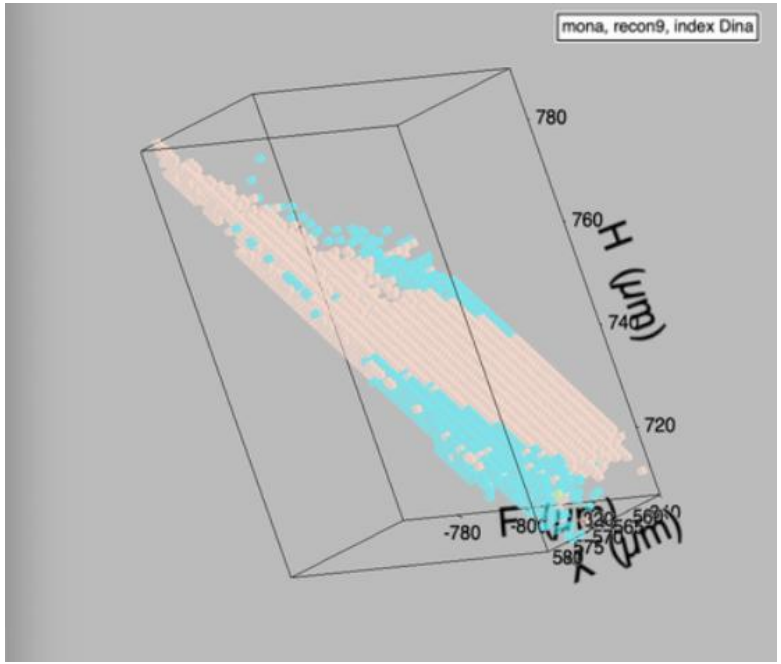
Dataset	Points	Nodes	Node H.	NH/Job (SD)
AL (2/9)	40	11	54.11	1.71 (0.22)
AL (2/10)	40	10	60.80	1.52 (0.01)
Ni2(1) (2/25)	422	10	598.68	1.42 (0.01)
Ni2(1) (2/28)	422	10	600.79	1.42 (0.72)
Ni2(2)* (4/1)	345	5	228.52	0.66 (0.04)

*Processing conducted on a later software version

EARLY SCIENTIFIC RESULTS





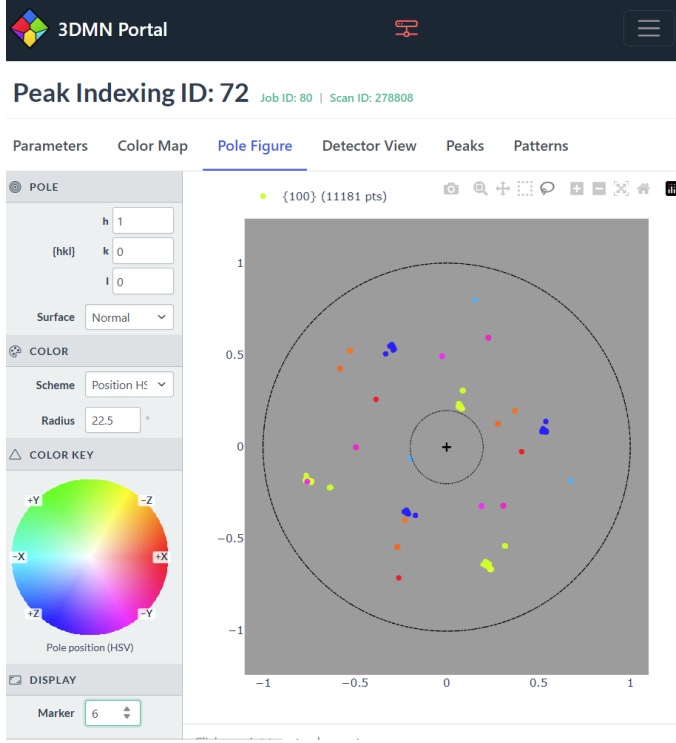


LOOKING FORWARD

- Web Portals & Viz

- LLM Agents
  - User Support
  - Automated Experimentation

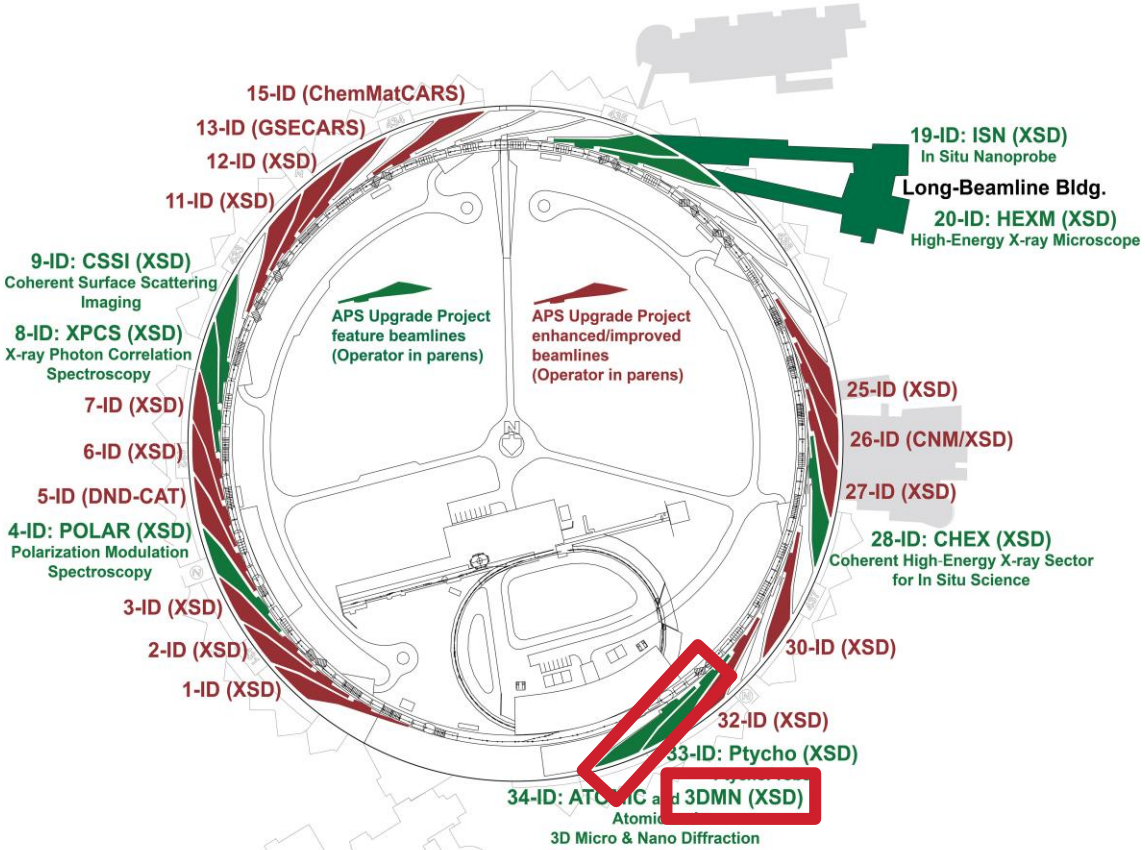
- 34-ID-E is planning to get a new detector:
  - 10x collection speed
  - 10x more processing
  - Excellent target for autoresearch/LLMs



ZOOMING OUT

- 3DMN Uses a lot more software:
  - **Coded Aperture <- Today's presentation**
  - CA Calibration
  - Wire Reconstructions (HPC possible with Eiger)
  - Indexing
  - Laue Matching (Streaming/instant views for 2D only)
  - Assorted Analysis and Viz

ZOOMING OUT… AGAIN



CONCLUSION & TAKEAWAYS

- Multifaceted, full stack problem: UI/UX -> data management + transfer -> HPC -> GPU kernels.
- More beamlines are likely to follow, and we need to learn to work in parallel
- As detector technology improves, this problem compounds

ACKNOWLEDGEMENT

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QUESTIONS?