CAPS: CODES APS MODEL

MODELING X-RAY DATA ACQUISITION WORKFLOWS AT THE APS

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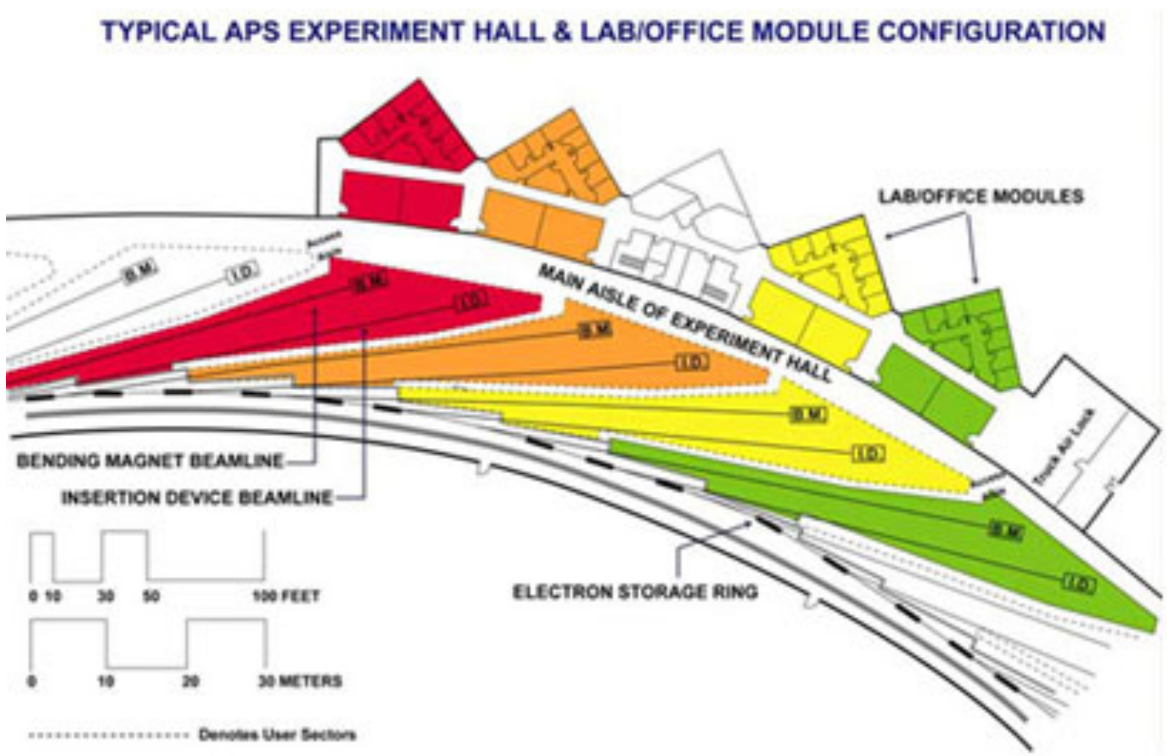
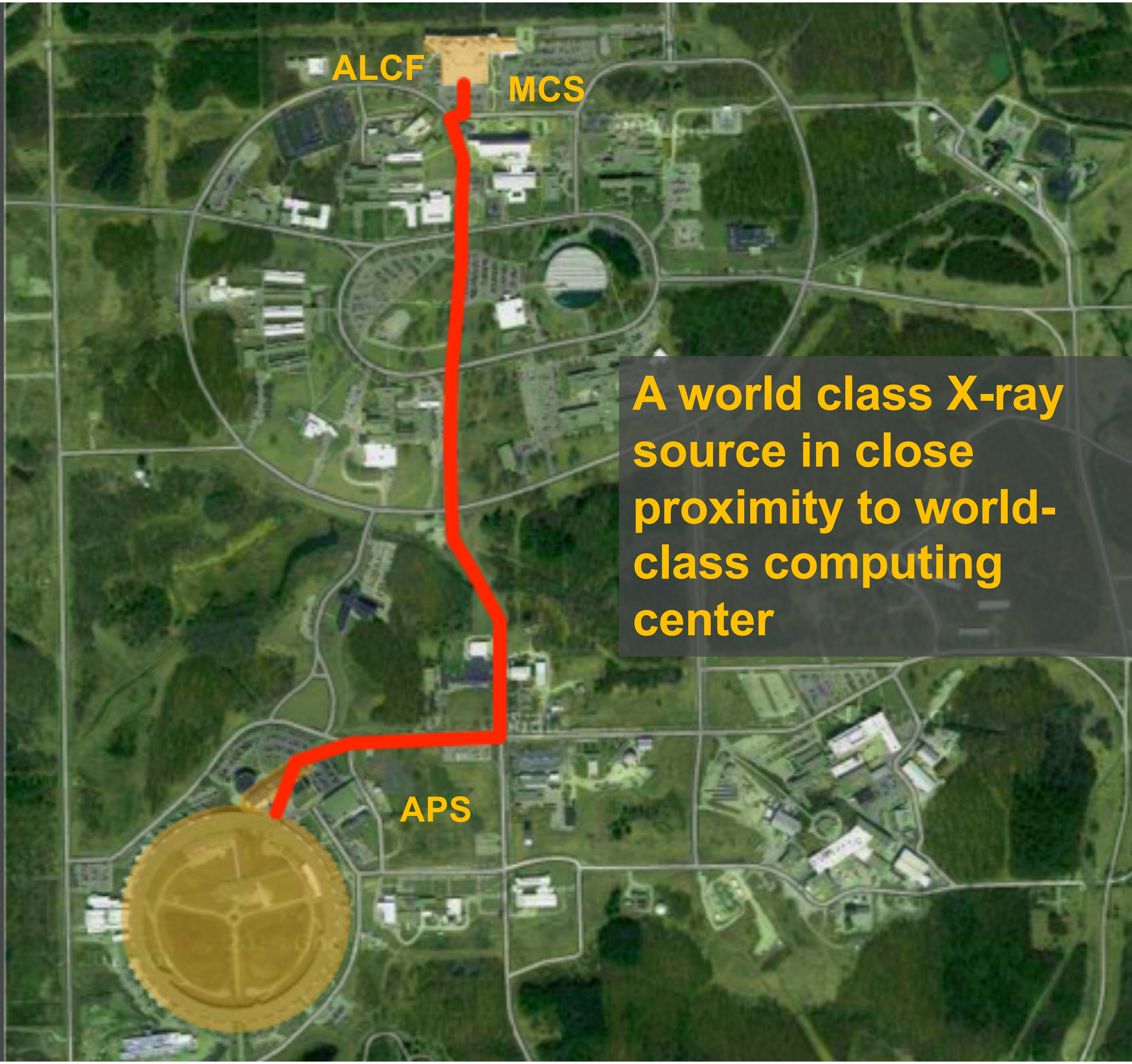
THE ADVANCED PHOTON SOURCE (APS)

THE ADVANCED PHOTON SOURCE

X-RAY PRODUCTION

- Moves electrons at electrons at >99.999999% of the speed of light.
- Magnets bend electron trajectories, producing x-rays, highly focused onto a small area
- X-rays strike targets in 35 different laboratories – each a lead-lined, radiation-proof experiment station




ALCF
MCS
A world class X-ray source in close proximity to world-class computing center
APS

DISTANCE FROM TOP LIGHT SOURCES TO TOP SUPERCOMPUTER CENTERS

Light Source	Distance to Top10 Machine
SIRIUS, Brazil	> 5000Km, TACC, USA
BAP, China	2000Km, Tihane-2, China
MAX, Sweden	800Km, Jülich Germany
PETRA III, Germany	500Km, Jülich Germany
ESRF, France	400Km, Lugano, Switzerland
Spring 8, Japan	100Km, K-Machine, Kobe, Japan
APS, IL, USA	~1Km, ALCF & MCS*, ANL, USA

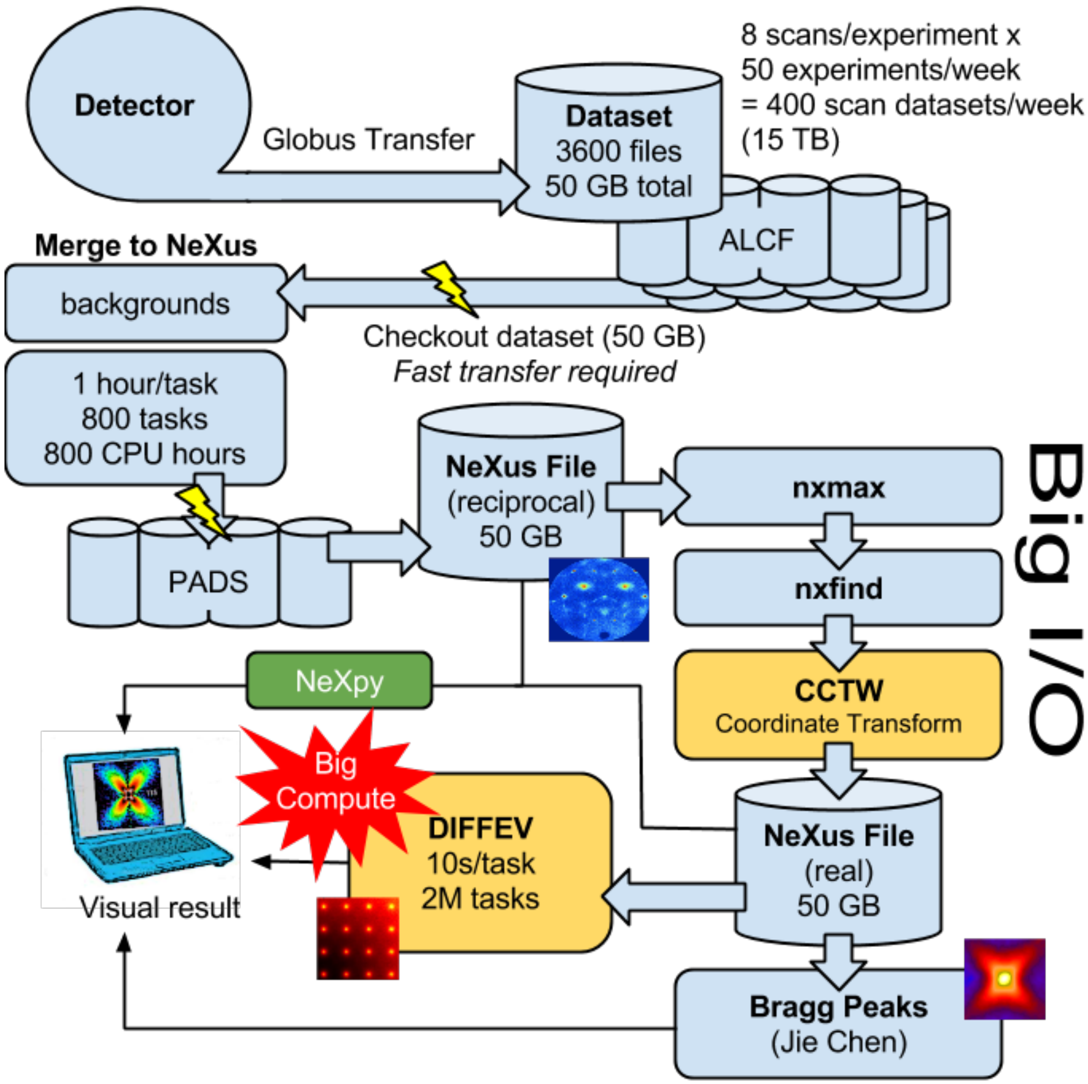
*ANL Computing Divisions
ALCF: Argonne Leadership Computing Facility
MCS: Mathematics & Computer Science

DATA MANAGEMENT FOR ENERGY SCIENCES

- "Despite the central role of **digital data** in Dept. of Energy (DOE) research, the methods used to manage these data and to support the information and **collaboration processes** that underpin DOE research are often **surprisingly primitive**…"
  - *DOE Workshop Report on Scientific Collaborations (2011)*
- Significant recent work has been invested in improving data analysis and management practices as the APS:
- **Automated data capture and analysis pipelines**
  Boost productivity during beamtime
- **Integration with high-performance computers**
  Integrate experiment and simulation
- **Effective use of large data sets**
  Maximize utility of high-resolution, high-frame-rate detectors and automation
- **High interactivity and programmability**
  Enable scientists to manage their own workflows

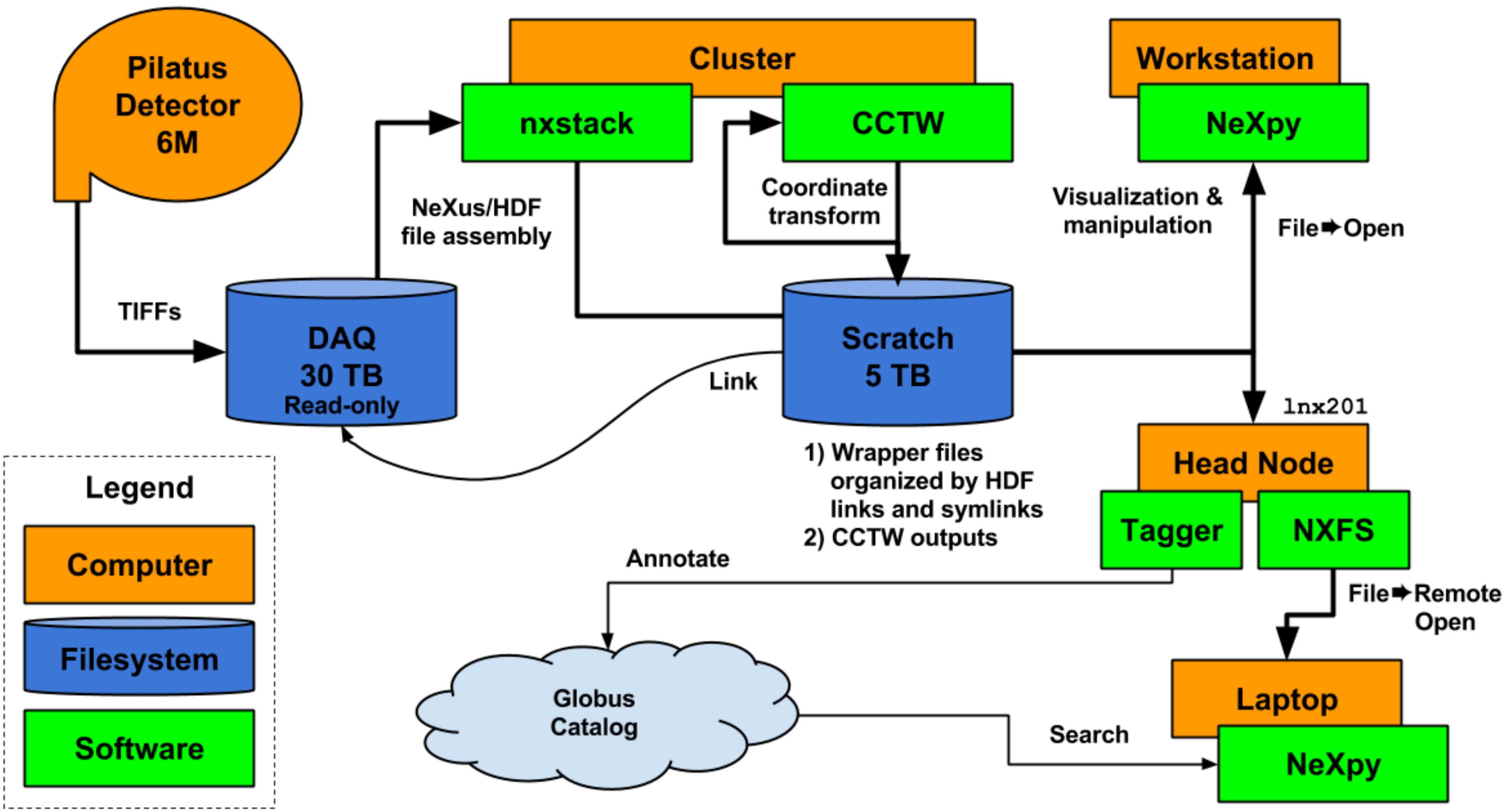
TYPICAL APS DATA ANALYSIS WORKFLOW

Diffuse Scattering Analysis and Inverse Model



X-RAY SCIENCE WORKFLOW AT CHESS

Cornell High-Energy Synchrotron Source



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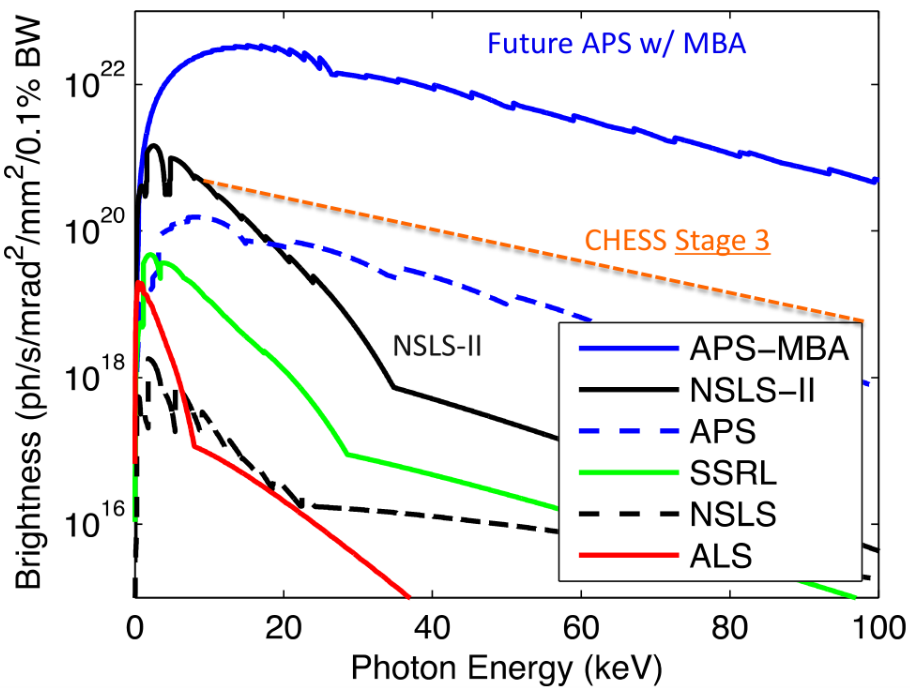
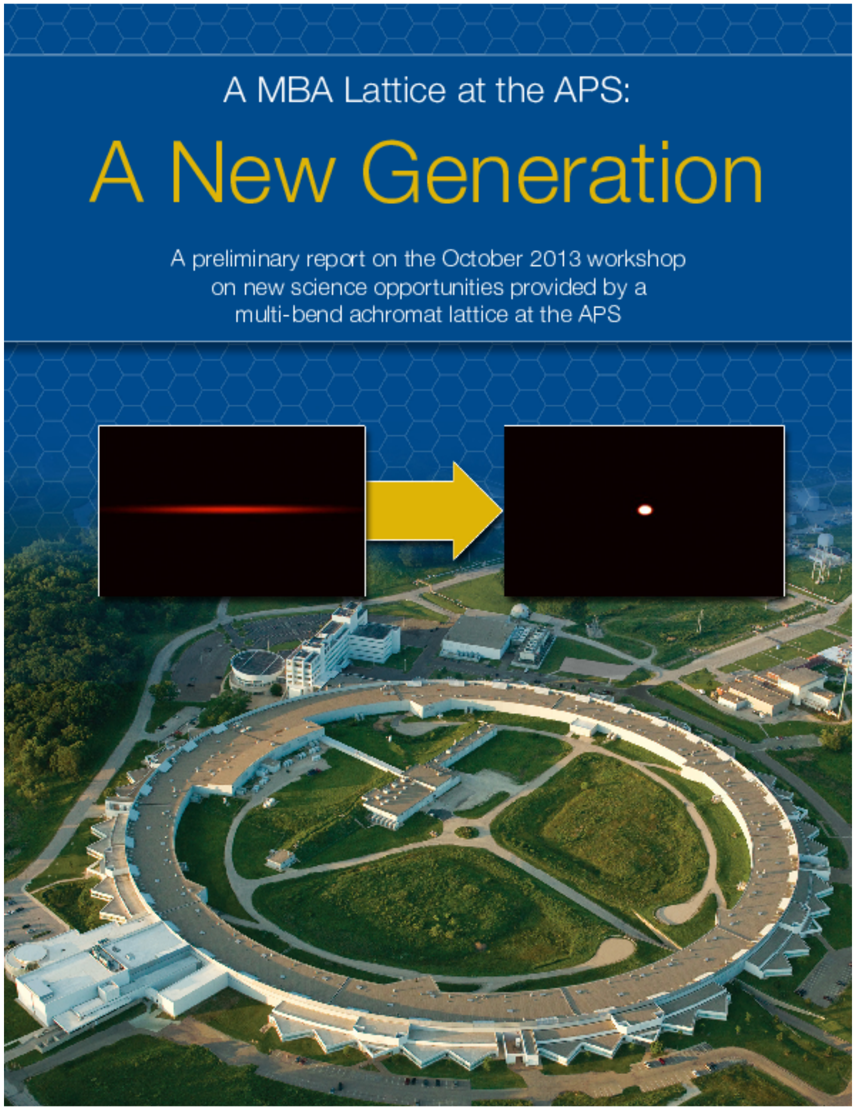
APS UPGRADE (APS-U)

- Will increase beam brightness by 100-1000x, primarily by making the beam cross-section smaller



- (Plot from Stuart Henderson)



A CODES-BASED MODEL (CAPS)

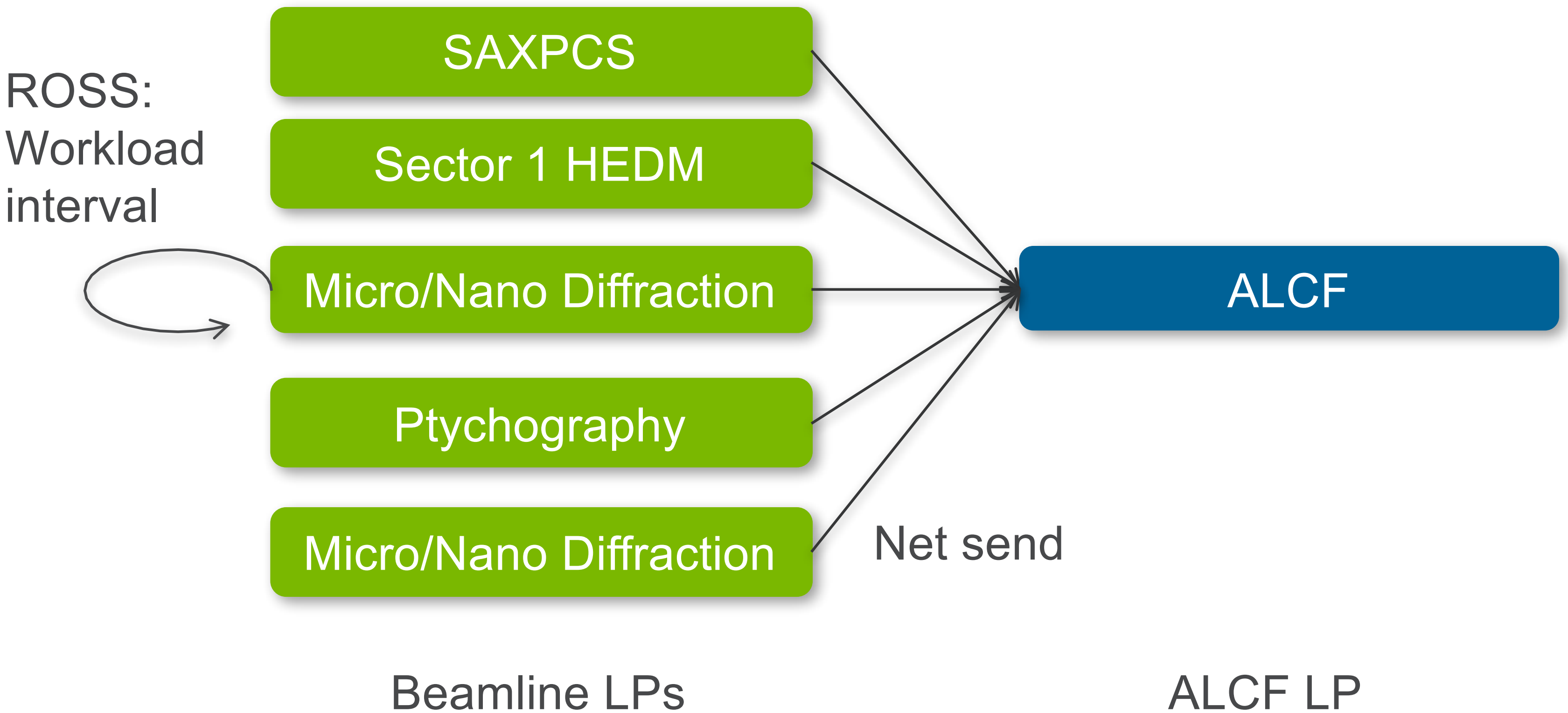
CAPS: THE CODES APS MODEL

Goals & objectives

- **Model existing APS data analysis workflows**
  - Primarily capture data movement over the network
  - Capture data sizes, acquisition rates, and workload patterns
- **Model projected APS workflows over the next 10 years**
  - Based on beamline scientists' projections
  - Data rate increases by factor of **10,000**
- **Automatic data buffers**
  - Data rates expected to be unpredictable, bursty
  - Highly volatile acquisition rates due to user-in-the-loop workflows, ad hoc experiment setup procedures, beam or detector downtime, etc.
- **Interaction with other users and systems**
  - On the network
  - At endpoints like the ALCF

MODEL CAPS1: BASIC DATA TRANSFER

- Simply models multiple beamlines over a shared network to the ALCF
- Based on data acquisition rates for 2016, 2021, and 2026



BEAMLINE WORKLOAD CONFIGURATION

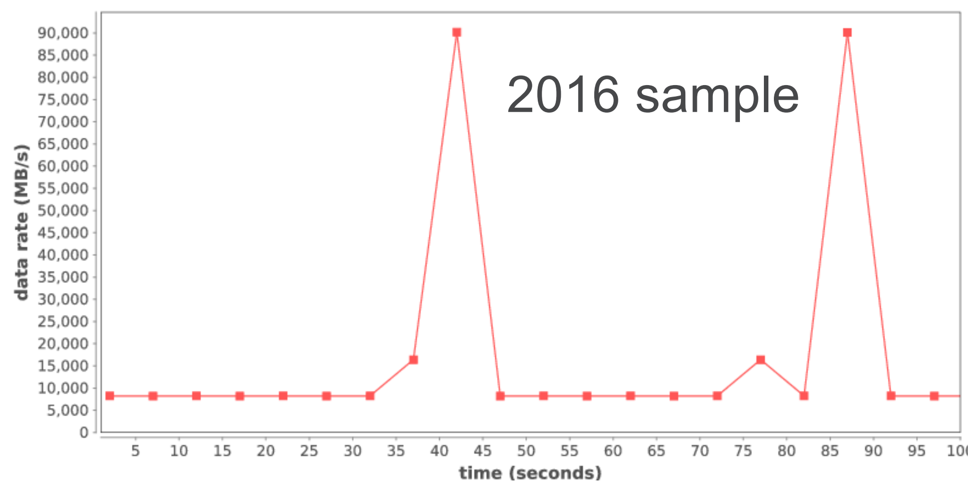
Reuse of CODES conf file processing

- Creates section for CAPS workloads alongside CODES network configuration
- Current parameters include acquisition rate and data chunk size
- Future workload models will incorporate more complex acquisition rate models, including sample changes, downtime, etc.

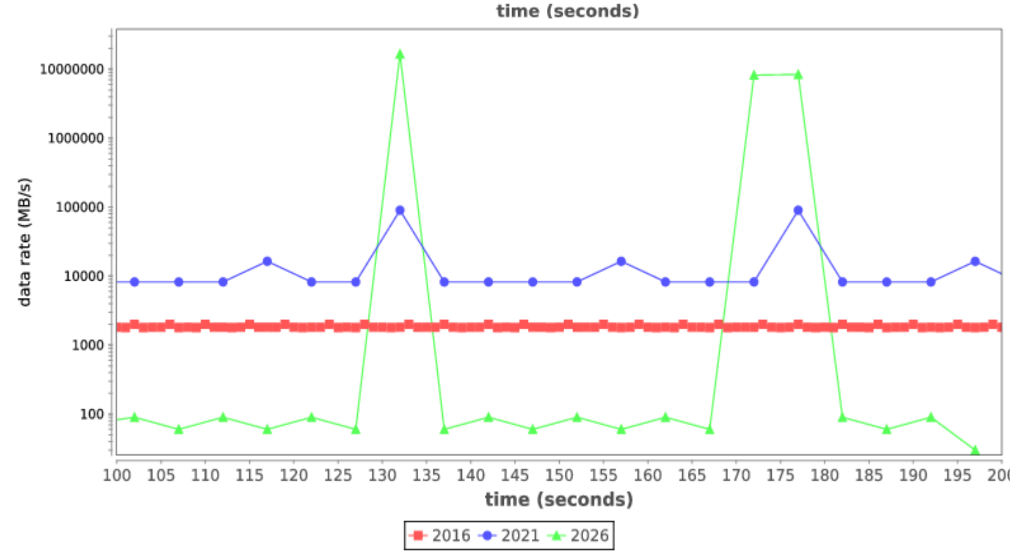
```
LPGROUPS
{
   MODELNET_GRP
   { ... }
}
PARAMS
{ ... }
APS
{
   # beamline names should be unique
   DynamicsAndStructure_SWD
   {
        delay="0.1";   # delay between transmissions (s)
        mbytes="200";  # gbytes/transmission
   }
   Sector1_HEDM
   {
        delay="1.5";   # delay between transmissions (s)
        mbytes="8";    # mbytes/transmission
   }
   MicroNanoDiffraction
   {
        delay="1";     # delay between transmissions (s)
        kbytes="840";  # kbytes/transmission
   }
   Ptychography
   {
        delay="1";     # delay between transmissions (s)
        kbytes="1680"; # kbytes/transmission
   }
   Sector8_SAXPCS
   {
        delay="0.1";    # delay between transmissions (s)
        mbytes="200";   # mbytes/transmission
   }
}
```

DATA TRANSFER TIMELINE PLOTS

- Goal: Provide visual feedback about network usage over time
- Log data arrival events, post-process to construct timeline



- Overlay of projections for 5 beamlines in years 2016, 2021, and 2026
- Assumes faster network in the future
- Initial observation: network usage burstier in future than now



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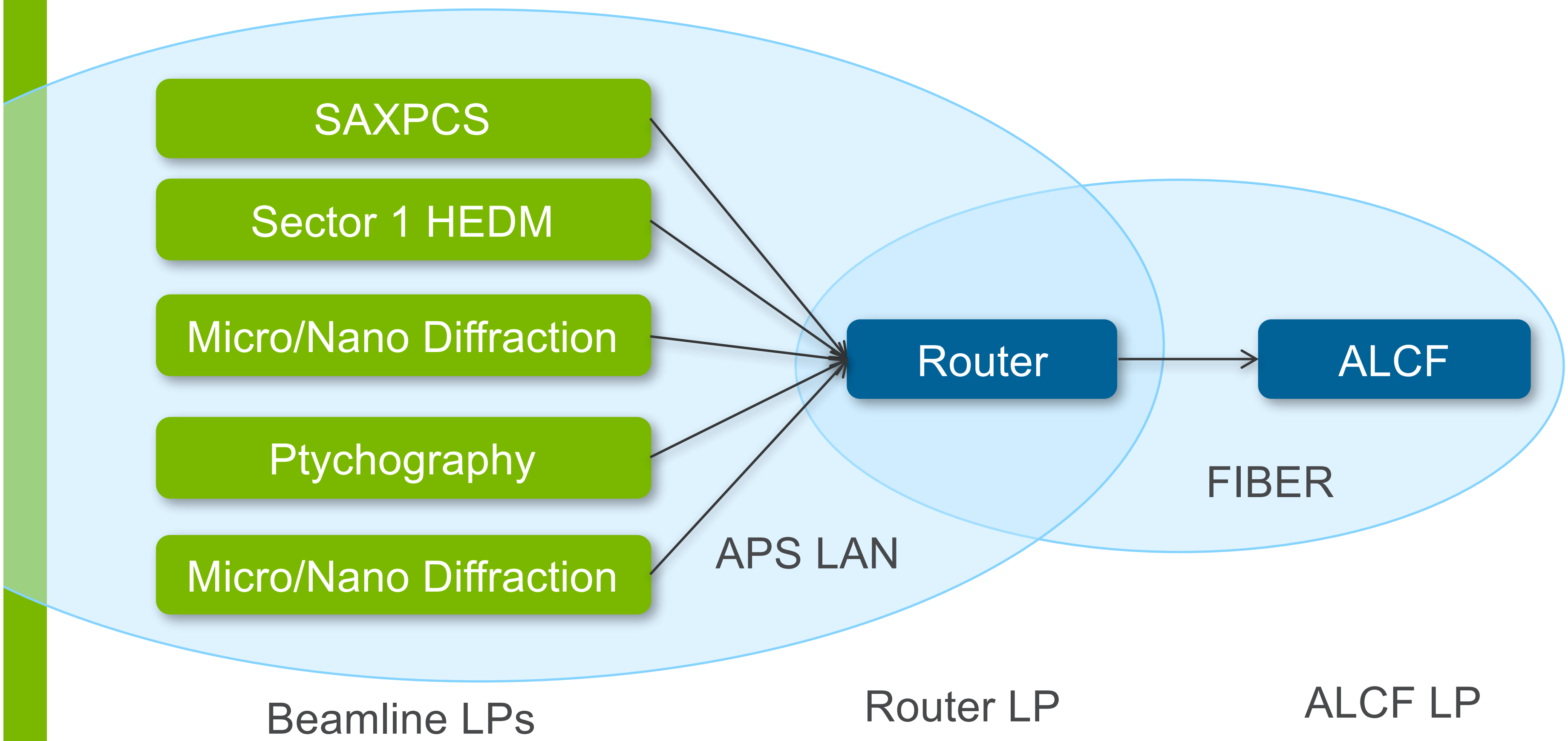
MODEL CAPS2: FUNNELED DATA TRANSFER

- Simply models multiple beamlines with a shared router to the ALCF
- Based on data acquisition rates for 2016, 2021, and 2026



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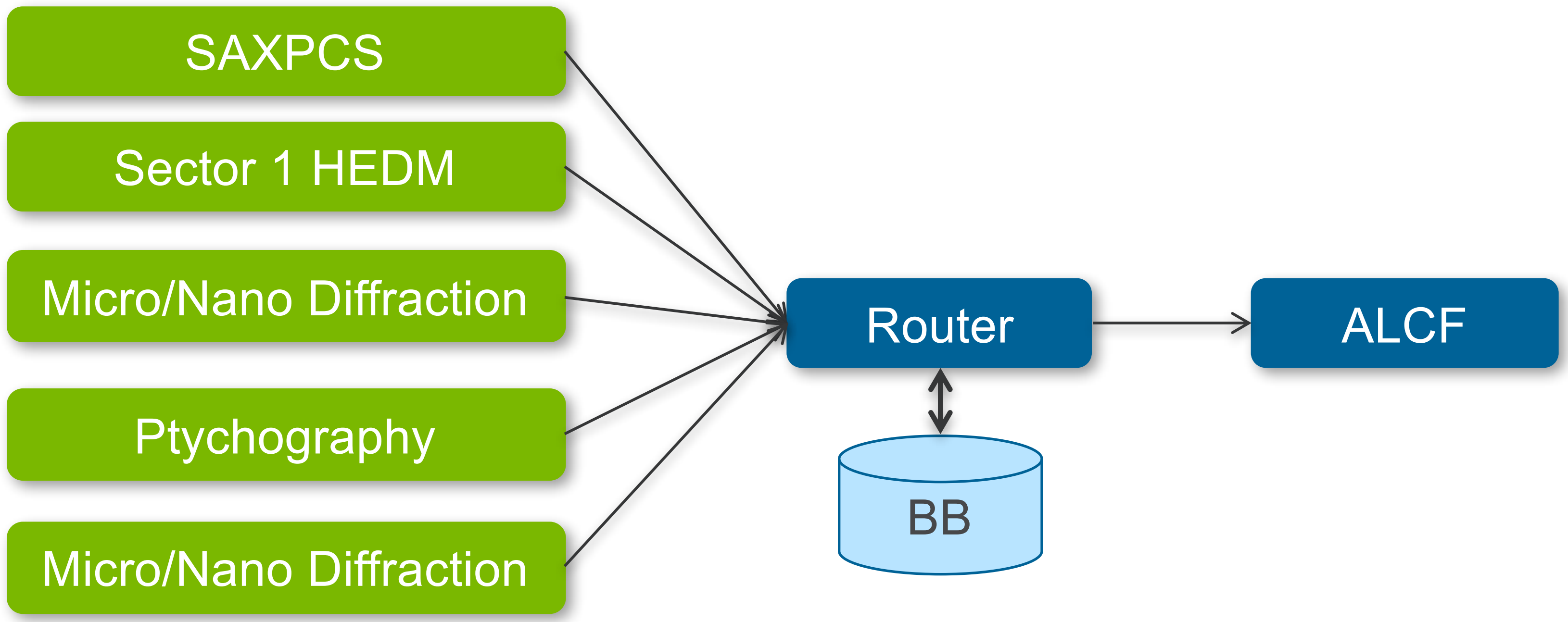
MODEL CAPS3: FUNNELED DATA BUFFER

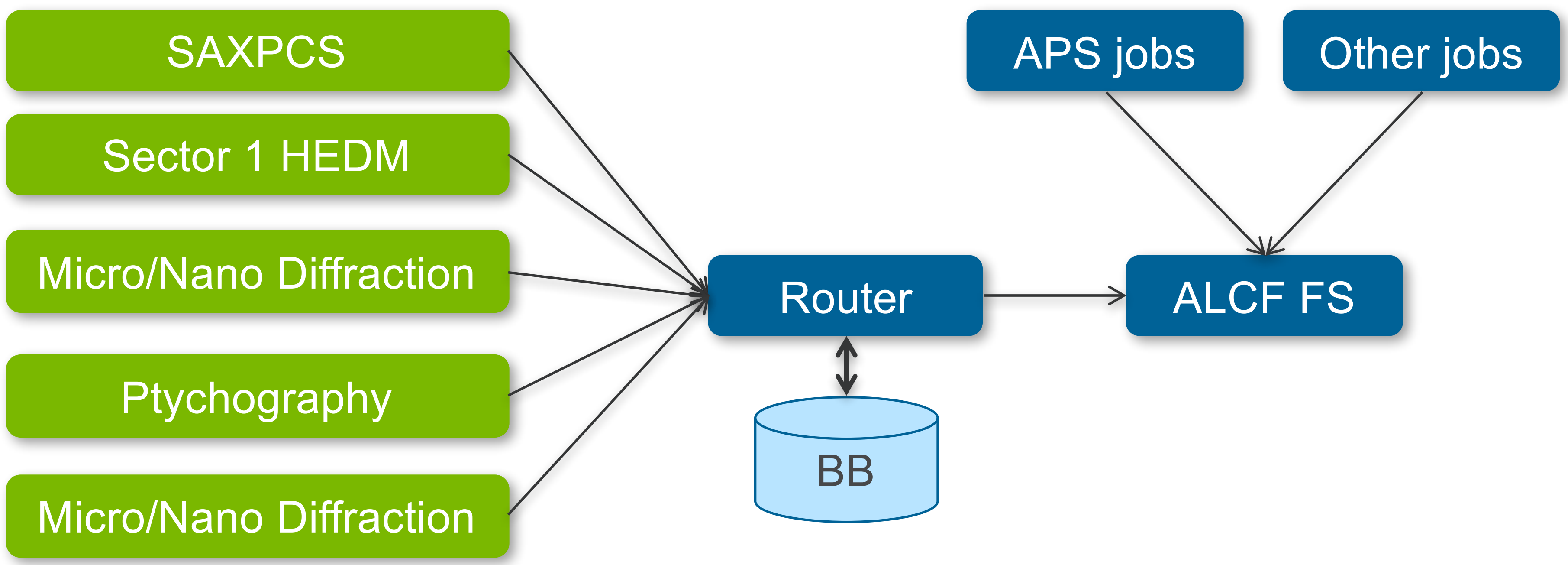
- Simply models multiple beamlines with a burst buffer to the ALCF
- Based on data acquisition rates for 2016, 2021, and 2026



- Burst buffer accommodates irregular beamline workloads

MODEL CAPS4: ENDPOINT CONTENTION

- Models multiple beamlines with contention at the ALCF
- Based on data acquisition rates for 2016, 2021, and 2026



- APS jobs triggered by data arrival
- Other jobs triggered by model workload, or absence of APS jobs

SUMMARY

- Enabling bottleneck analysis and scenario evaluation for future APS workloads

- Status:
  - Basic APS-like framework in place for APS data acquisition with real-world APS data rates and projections
  - Moving toward more complex, useful models

- Future work:
  - More CODES/ROSS usage:
    - Multiple networks
    - Rough storage model
    - Simple ALCF jobs model
  - More complex APS usage model (daily/weekly cycles)
  - Refine quality to produce actionable, co-design investigations

THANKS TO

- Many APS collaborators
- Nicholas Schwarz for the projections

QUESTIONS?