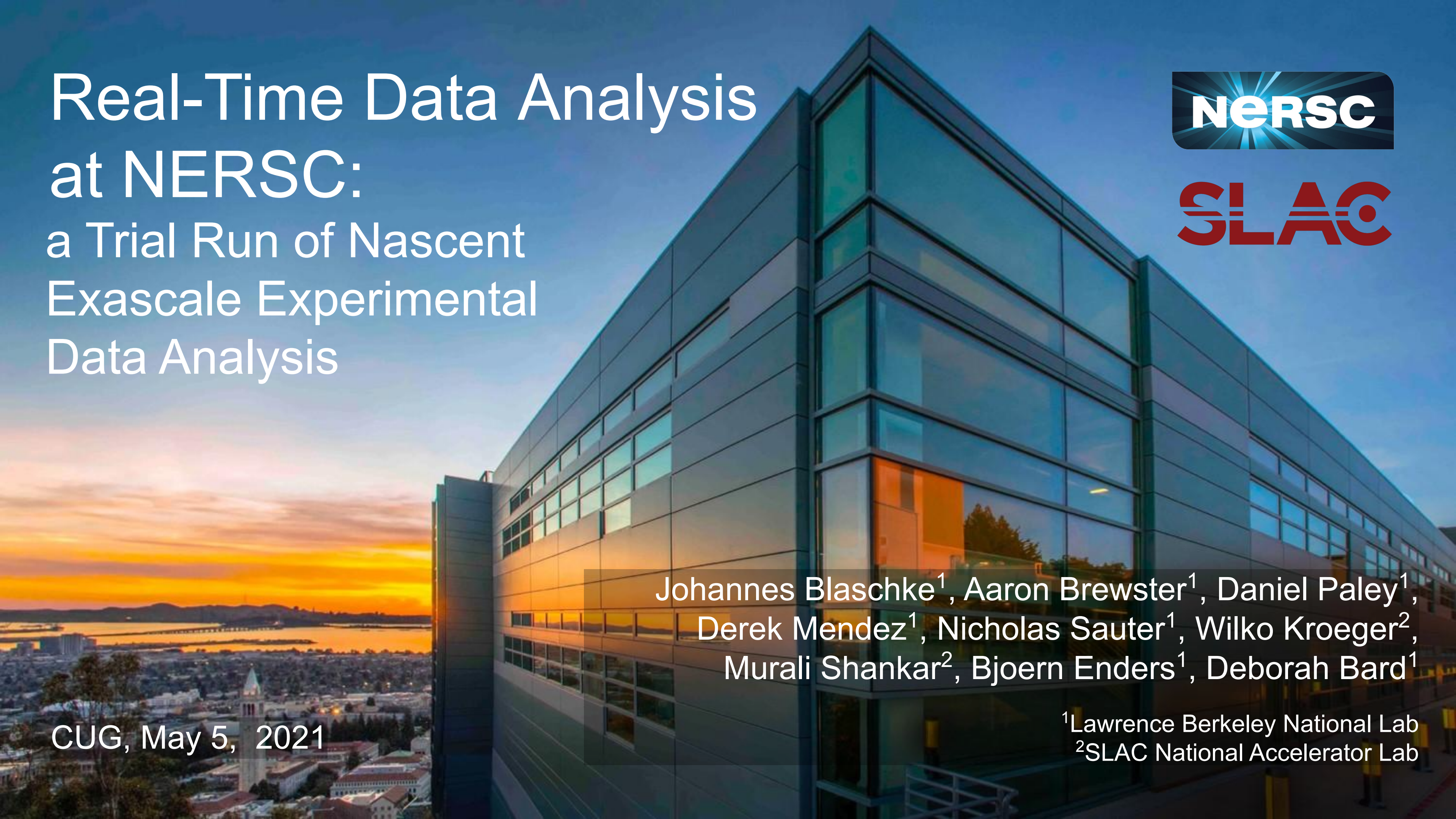


Real-Time Data Analysis at NERSC:

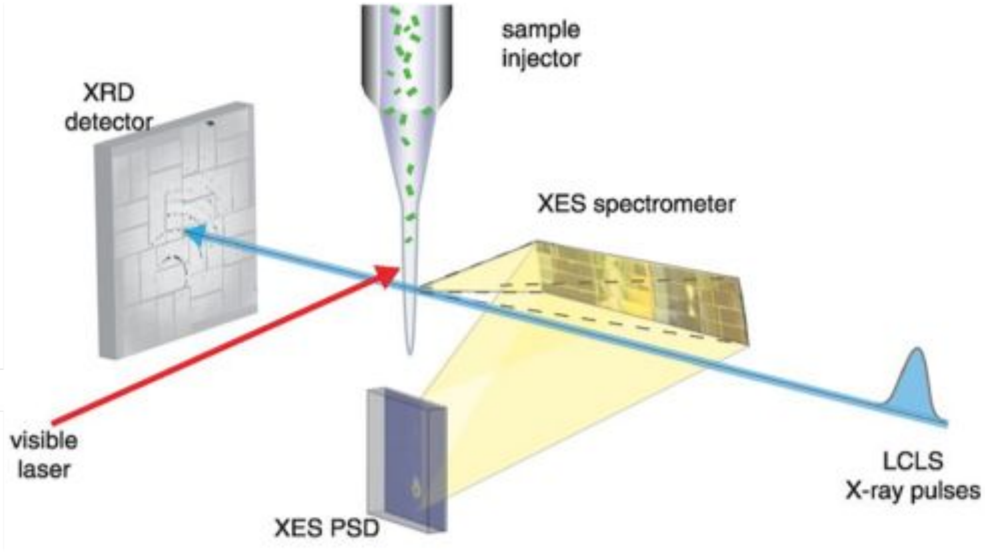
a Trial Run of Nascent Exascale Experimental Data Analysis

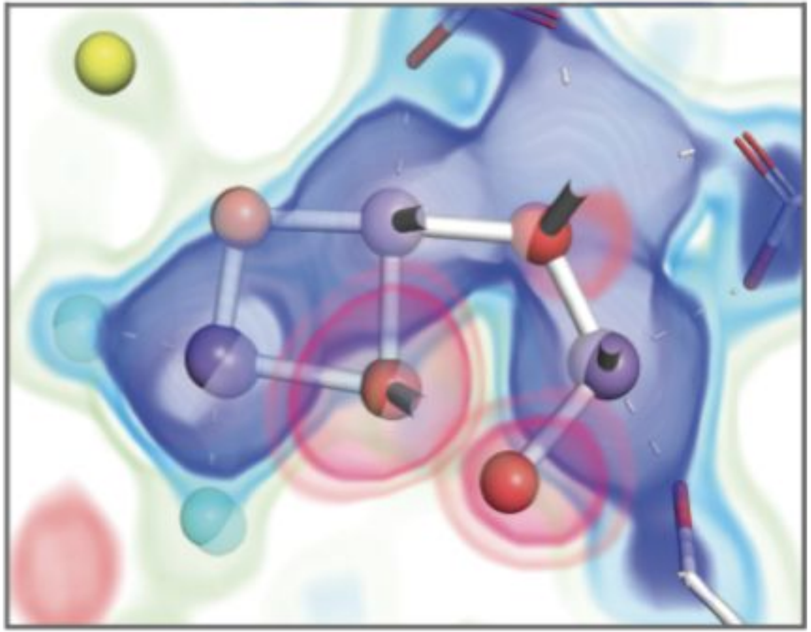
Johannes Blaschke[1], Aaron Brewster[1], Daniel Paley[1],
Derek Mendez[1], Nicholas Sauter[1], Wilko Kroeger[2],
Murali Shankar[2], Bjoern Enders[1], Deborah Bard[1]

[1]Lawrence Berkeley National Lab
[2]SLAC National Accelerator Lab

CUG, May 5, 2021

Serial Crystallography





PSII 2Fo-Fc and Fo-Fc at 2.07 Å, S3 state

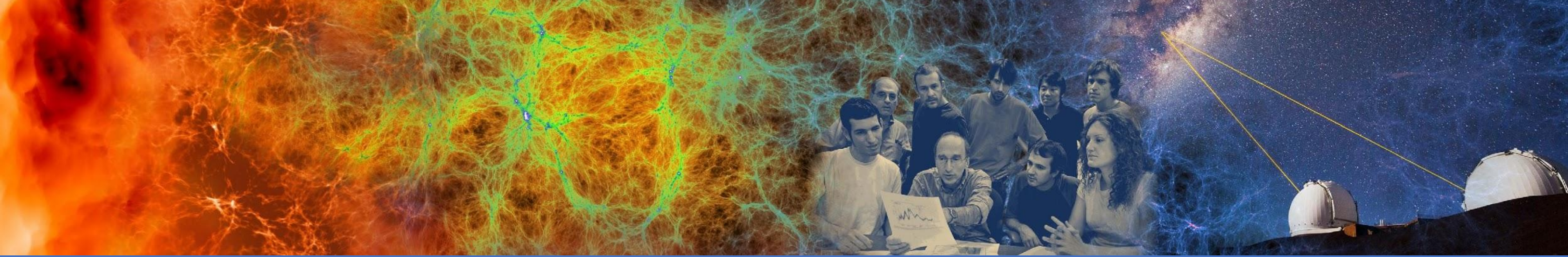
Kern et al., 2018 Nature 563:421

When should I move onto the Next Sample?

- Beamtime is scarce!

- Critical live feedback:
  - Does the beam hit the sample?
  - Do we see crystals?
  - Does the data make sense?
  - What is the quality of the data?

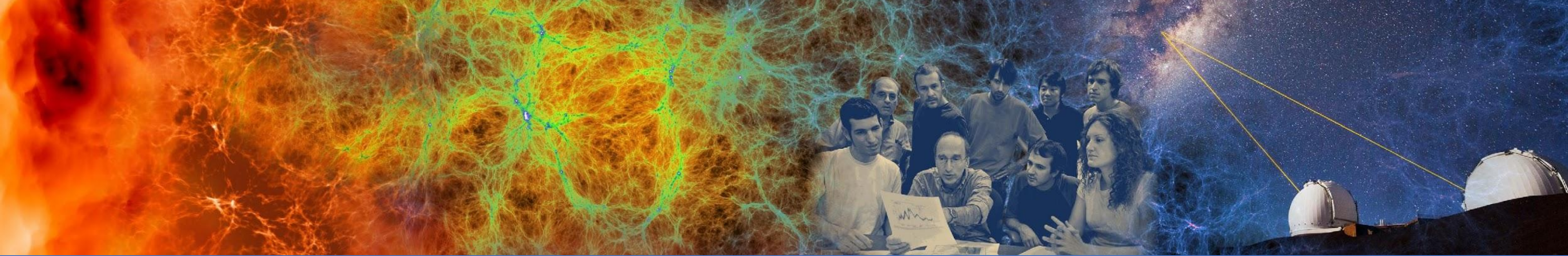
- Can I move on to the next sample?



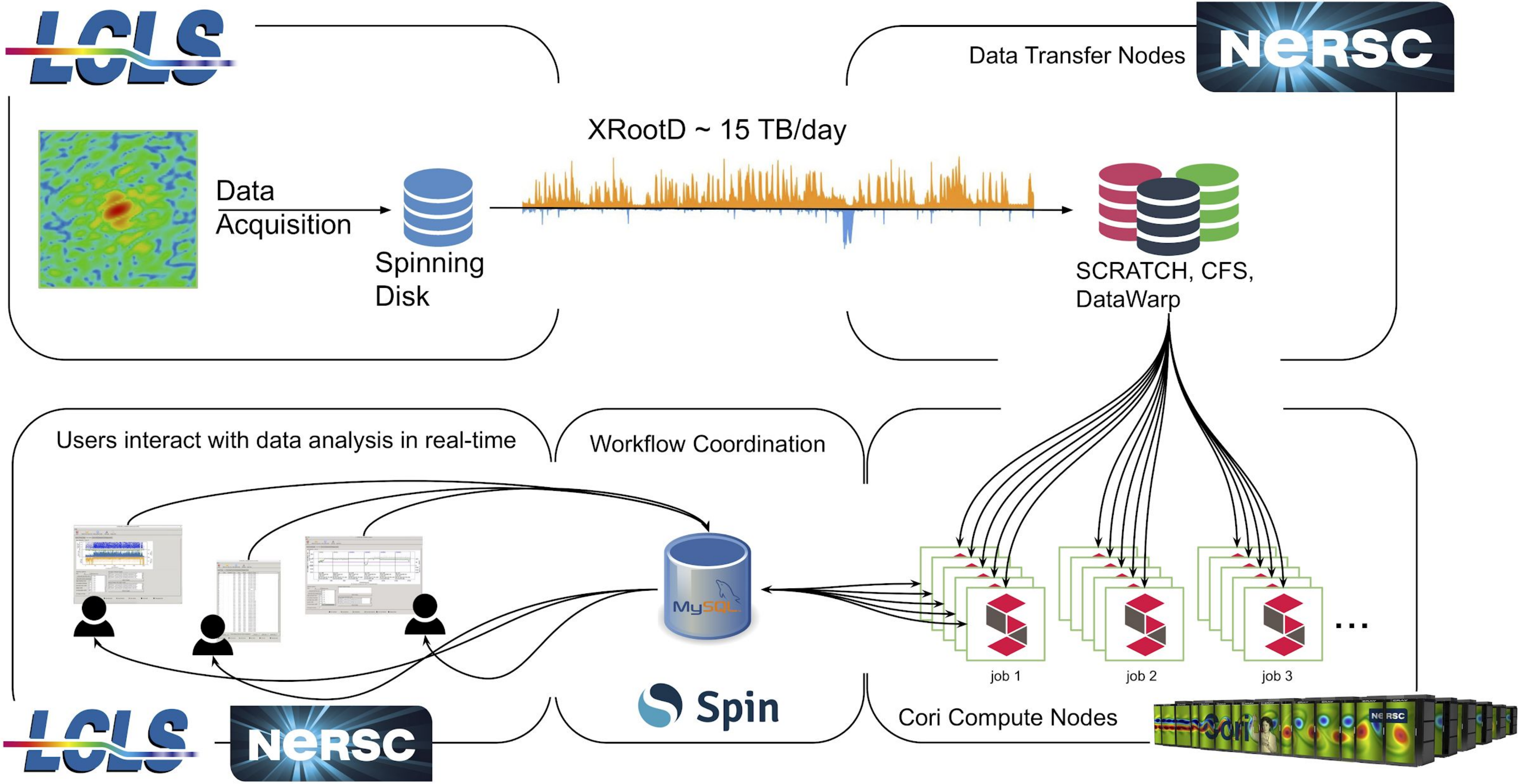
Experimentalists Are In The Driver's Seat

Live Data Analysis for Experiments in 2020, and Beyond!

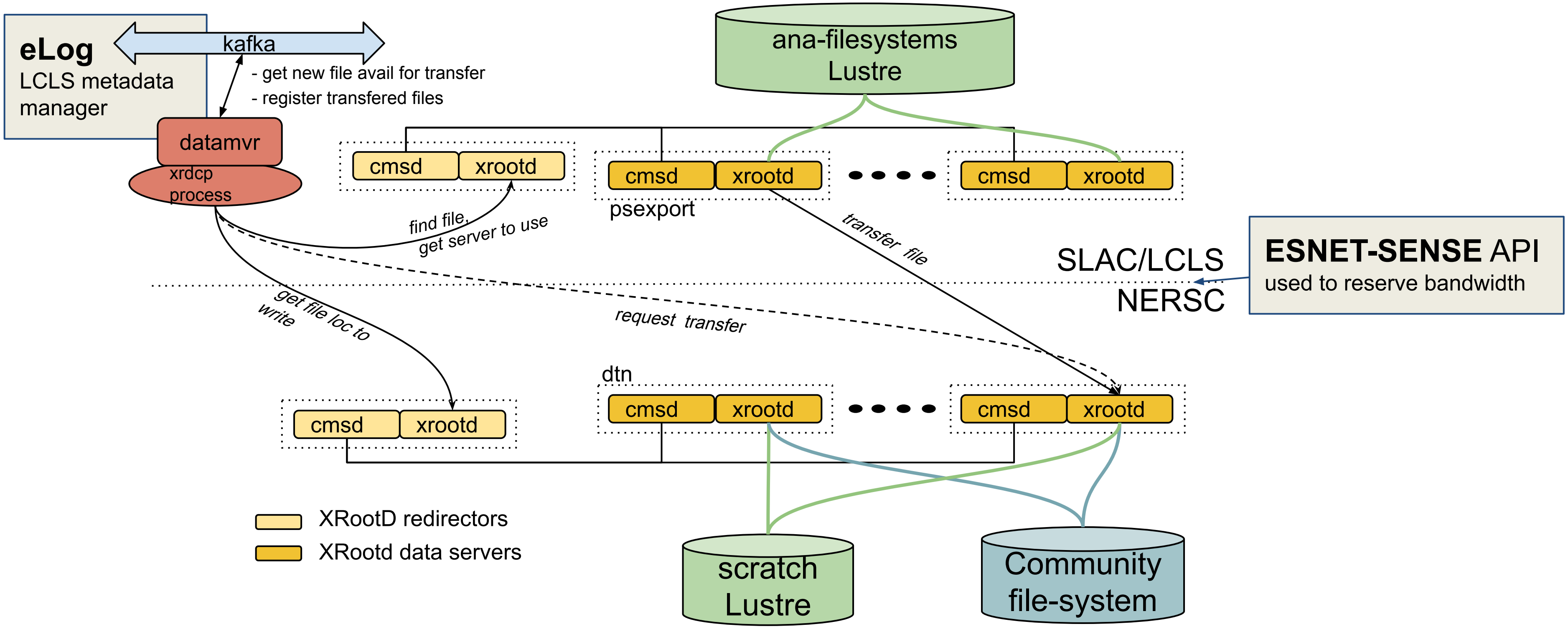
Click anywhere on this screen to play video



Deploying CCTBX at NERSC

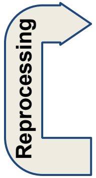

LCLS
Data Transfer Nodes
NERSC
XRootD ~ 15 TB/day
Data Acquisition
Spinning Disk
SCRATCH, CFS, DataWarp
Users interact with data analysis in real-time
Workflow Coordination
MySQL
job 1
job 2
job 3
...
LCLS
NERSC
Spin
Cori Compute Nodes

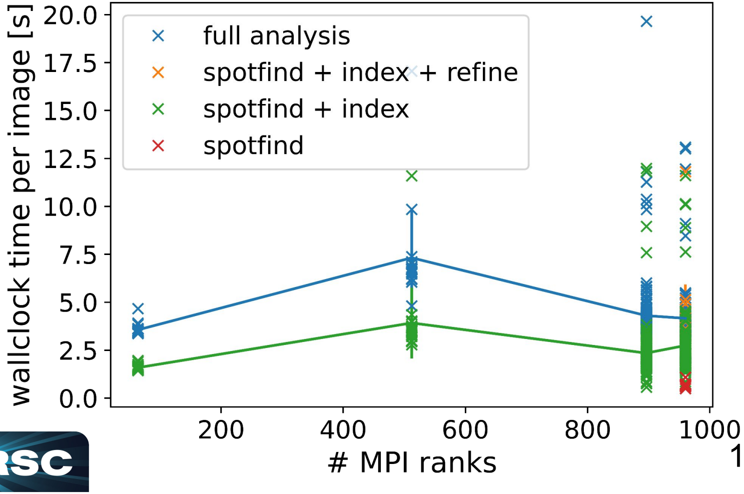
Data Movement XRootD clusters

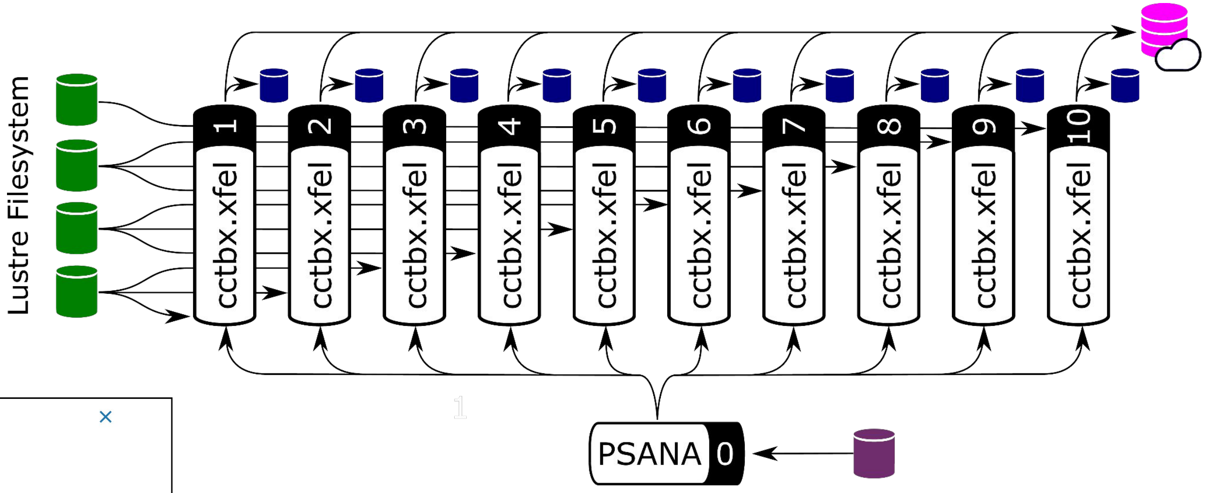


Data Analysis

- Data analysis follows sequential stages:
  - spotfinding
  - indexing Bragg spots
  - model refinement
  - integrating Bragg spots







How’s the Computation Weather Today?

- Computational Weatherplot:
  - Each line shows work done by one MPI rank
  - There is no “*the* `cctbx.xfel` workload”

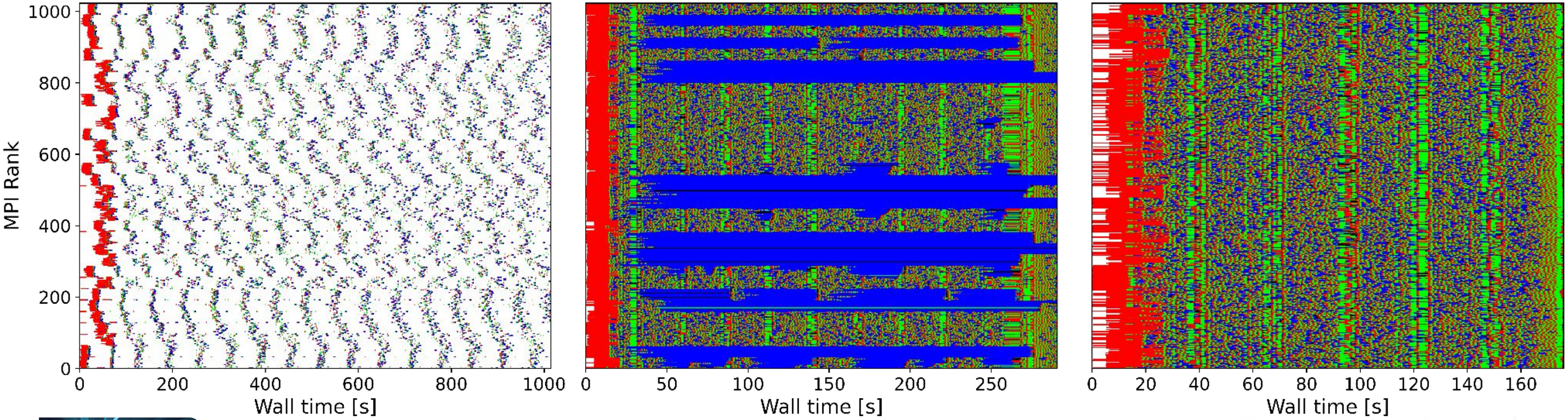
🟥 Start-Up and I/O (PSANA)

🟩 Spot Detection (DIALS)

🟦 Indexing (DIALS)

▨ Refinement (DIALS)

⬛ Integrating (DIALS)



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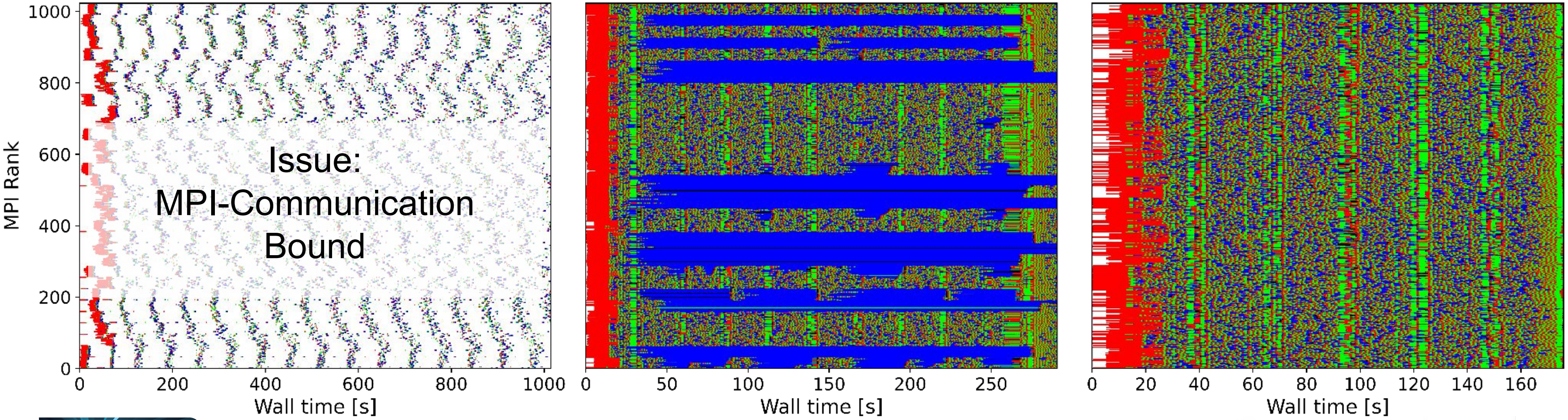
Refinement (DIALS) ▨

Integrating (DIALS) ⬛


Issue: MPI-Communication Bound

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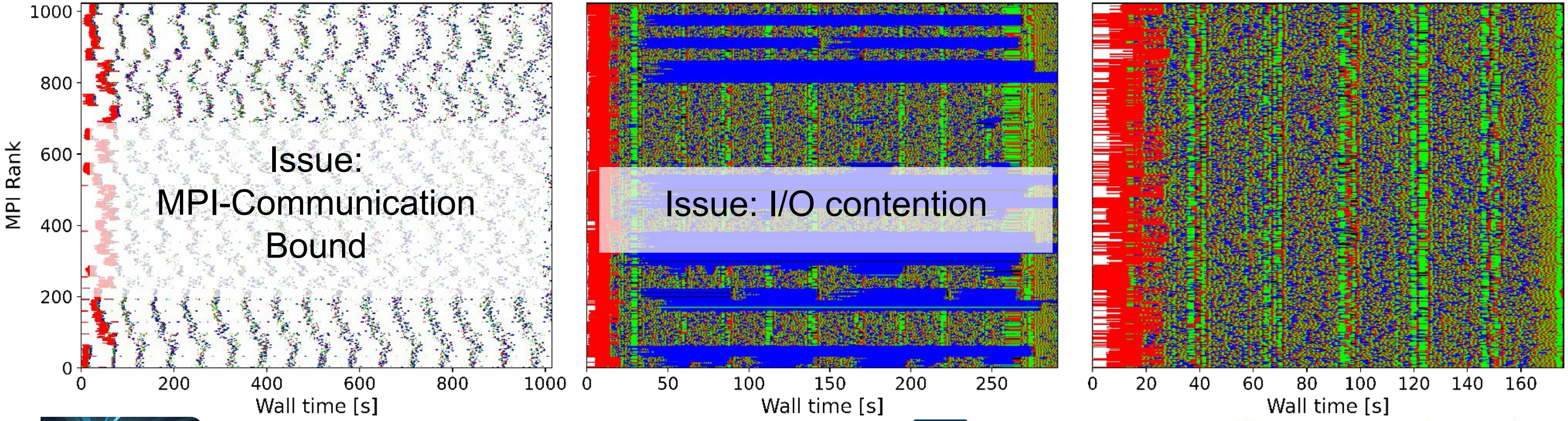

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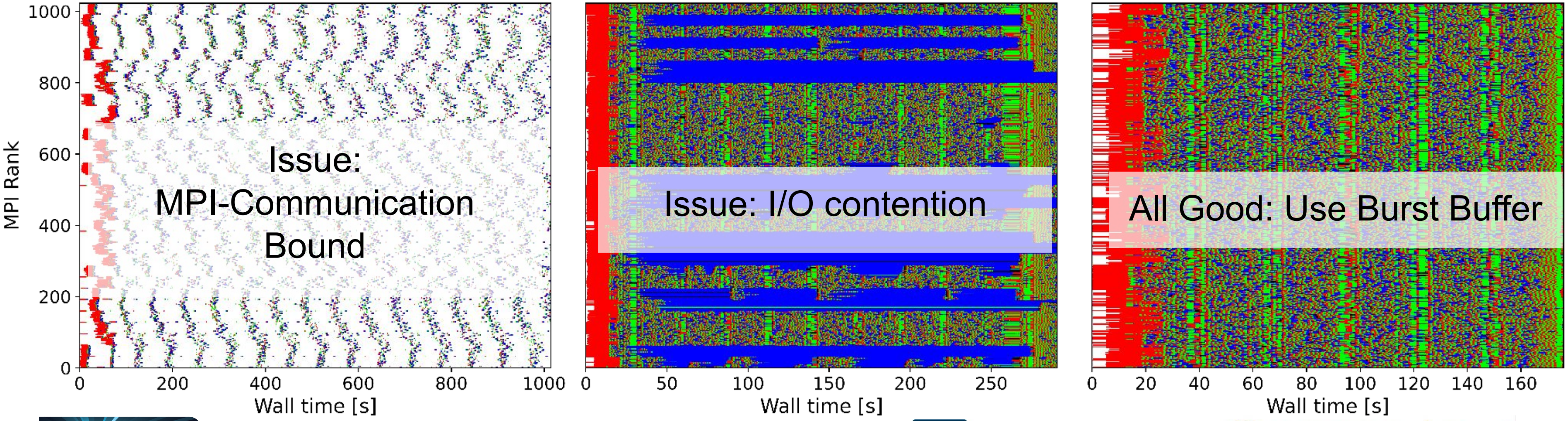
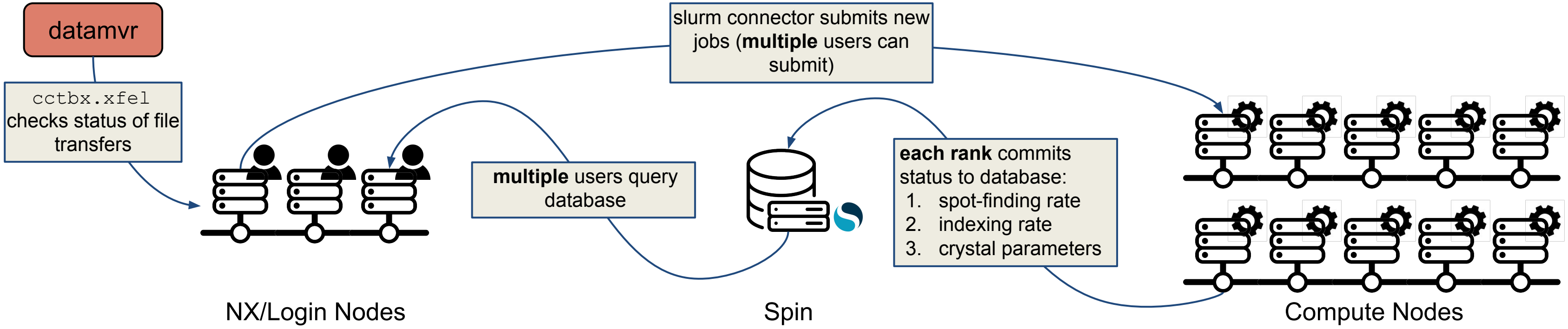

Issue: MPI-Communication Bound

Issue: I/O contention

All Good: Use Burst Buffer

Workflow Coordination using NERSC Spin

- Home-grown workflow manager `cctbx.xfel`
  - mySQL database hosted on Spin (NERSC microservice platform)
  - Each worker commits progress to DB
  - `cctbx.xfel` determines new analysis runs and “assembles” jobs (input files, job scripts, ...)
  - `cctbx.xfel` monitors slurm and DB, reporting live progress



datamvr

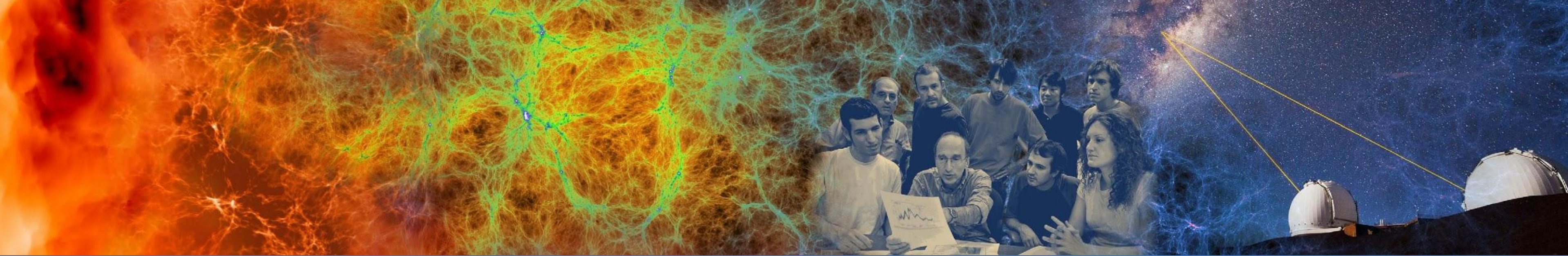
`cctbx.xfel` checks status of file transfers

slurm connector submits new jobs (**multiple** users can submit)

multiple users query database

each rank commits status to database:

1. spot-finding rate
2. indexing rate
3. crystal parameters



XFEL as a Proxy for HPC Data Analysis

Why is XFEL relevant to other "Data Analysis for Science" projects?

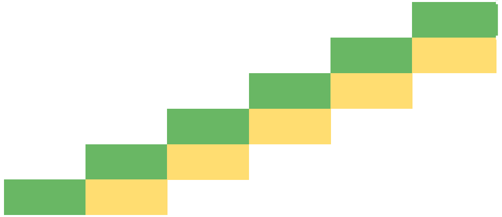
Challenge 1: Urgent Computing Resources

🟩 : collecting/transferring

🟨 : processing

⬚ : no live results

Reservation with 3 nodes, each run takes 1 unit of time to collect and process ⇒ can only process 3 yellow squares at once



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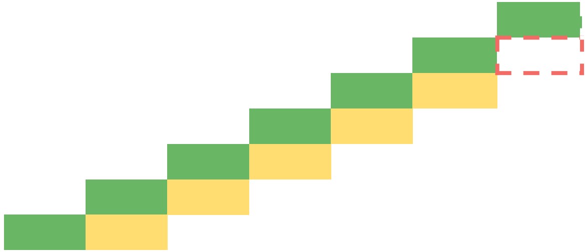

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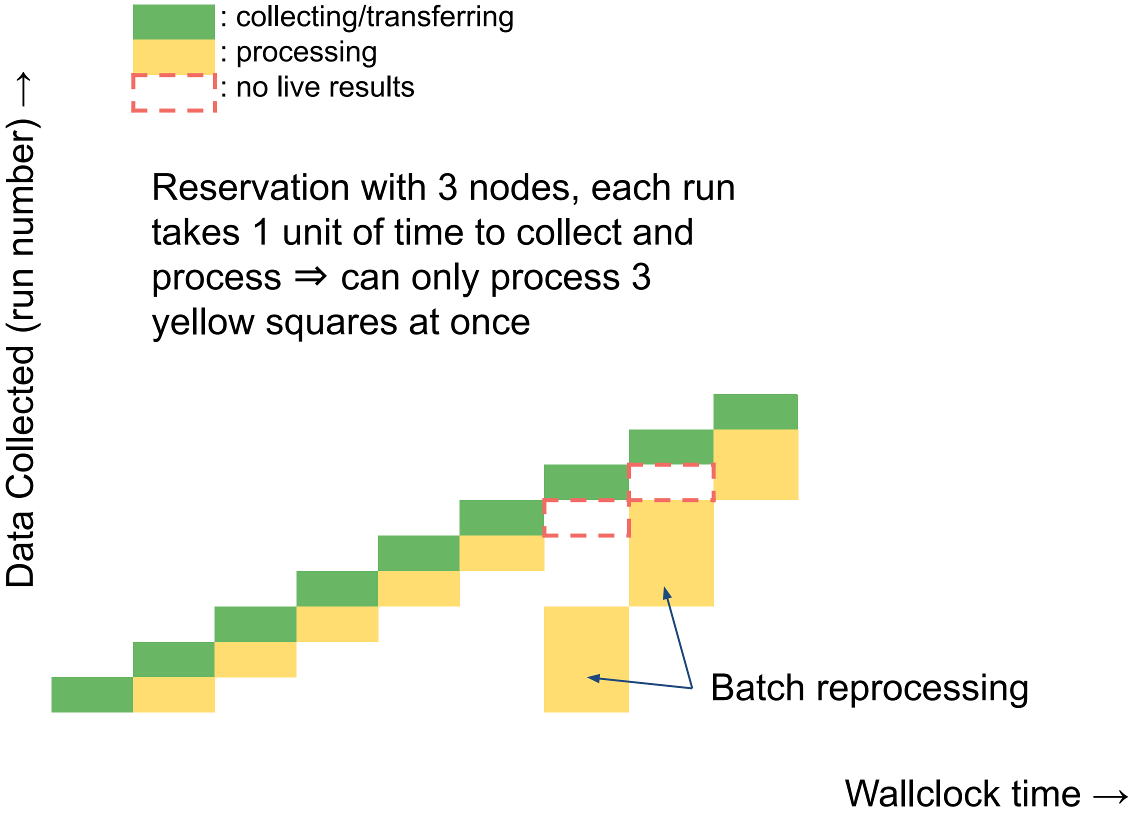

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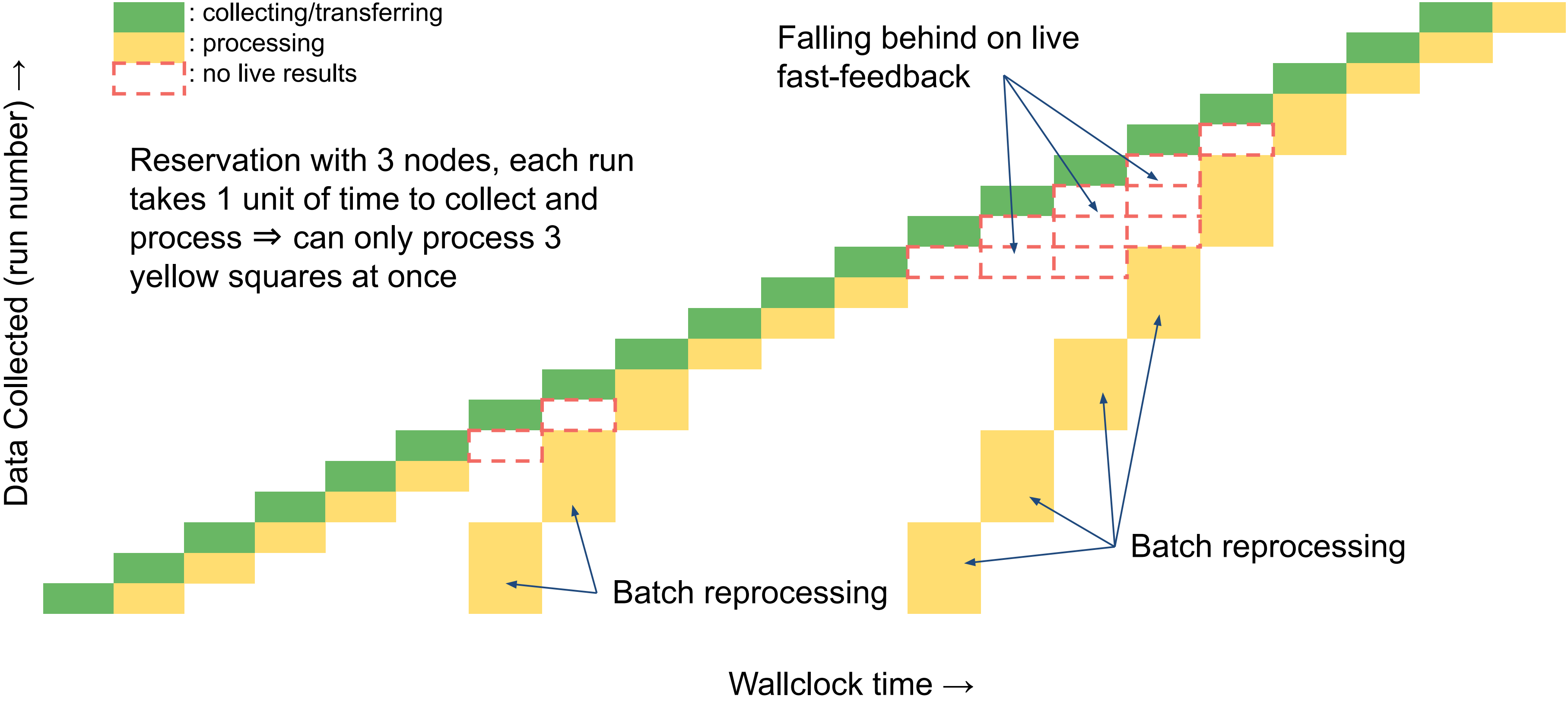

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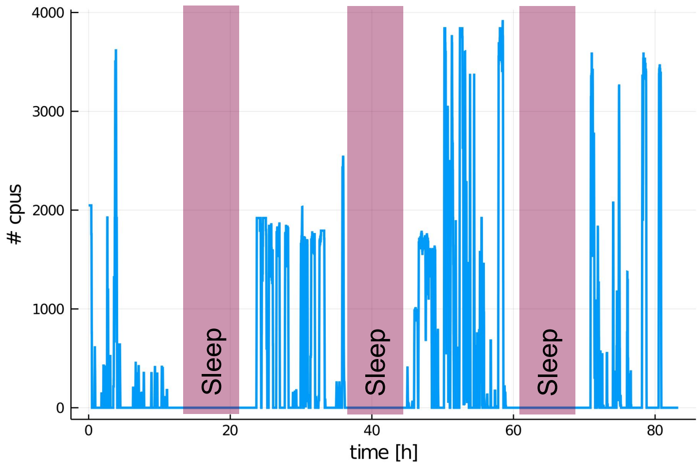
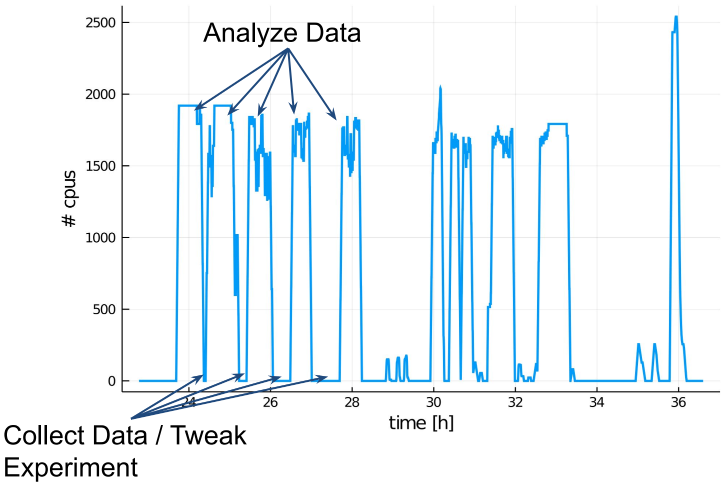
Falling behind on live fast-feedback

Batch reprocessing

Batch reprocessing

Challenge 1: Urgent Computing Resources





Analyze Data

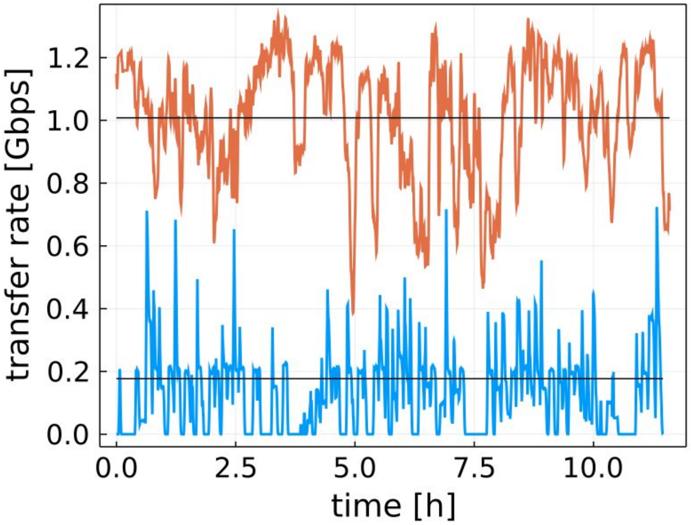
Collect Data / Tweak Experiment

- Reservation:
  - 32 - 64 Haswell nodes for live data processing
  - Can be used for preemptible jobs in the future (avoid idle nodes)

- Realtime QOS:
  - Flexibly add up to 20 Haswell nodes for reprocessing

Challenge 2: High-Speed Data (Network and I/O)

- In data analysis workflows, file systems and network can become bottlenecks
- I/O Optimization:
  - Optimize python logger for high-frequency parallel I/O
  - Write logs to Burst Buffer
- Experience:
  - Transfers ran smoothly, can switch redirect destination
  - **FS performance limited the transfer rate**
- Improvements:
  - Use SSD storage at LCLS to speed up transfers
  - Improve write performance at NERSC
  - Allow users to initiate the remote transfers
  - Better monitoring and alerting



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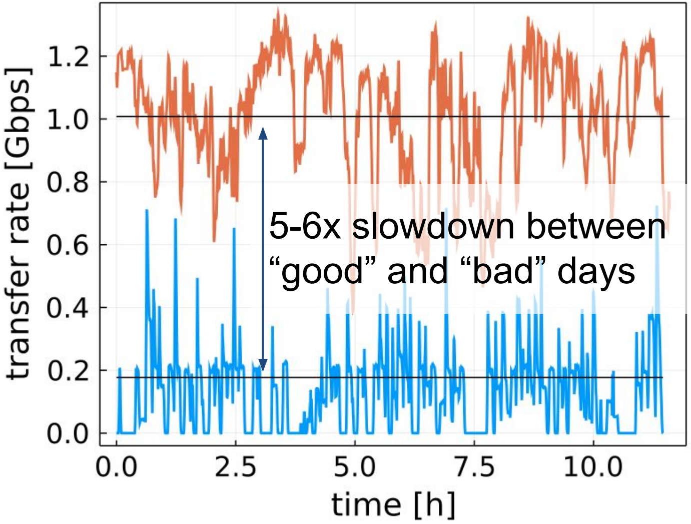


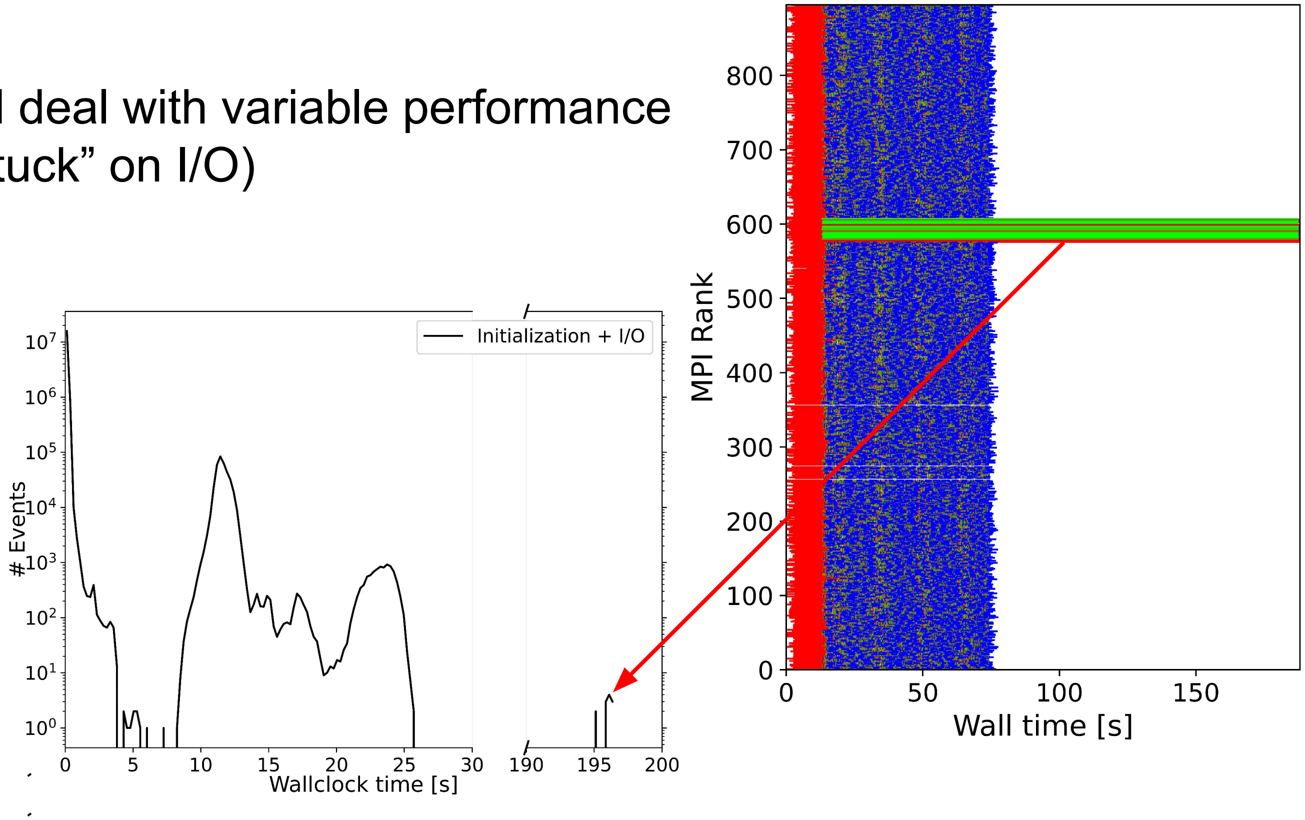
5-6x slowdown between "good" and "bad" days

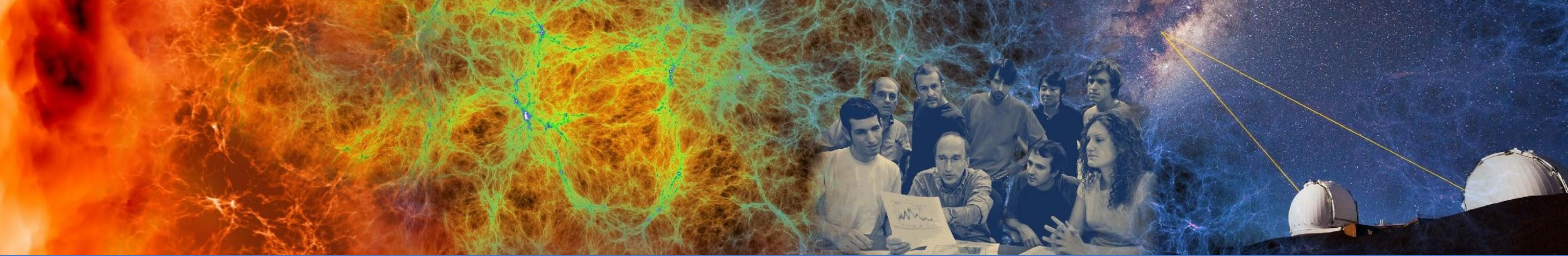
Challenge 3: Realtime Monitoring and Workflow Coordination

- Need to identify and deal with variable performance (e.g. rank getting “stuck” on I/O)

- Weatherplots good for identifying load imbalance

- Ongoing research: How to integrate with workflow manager? How to automate?





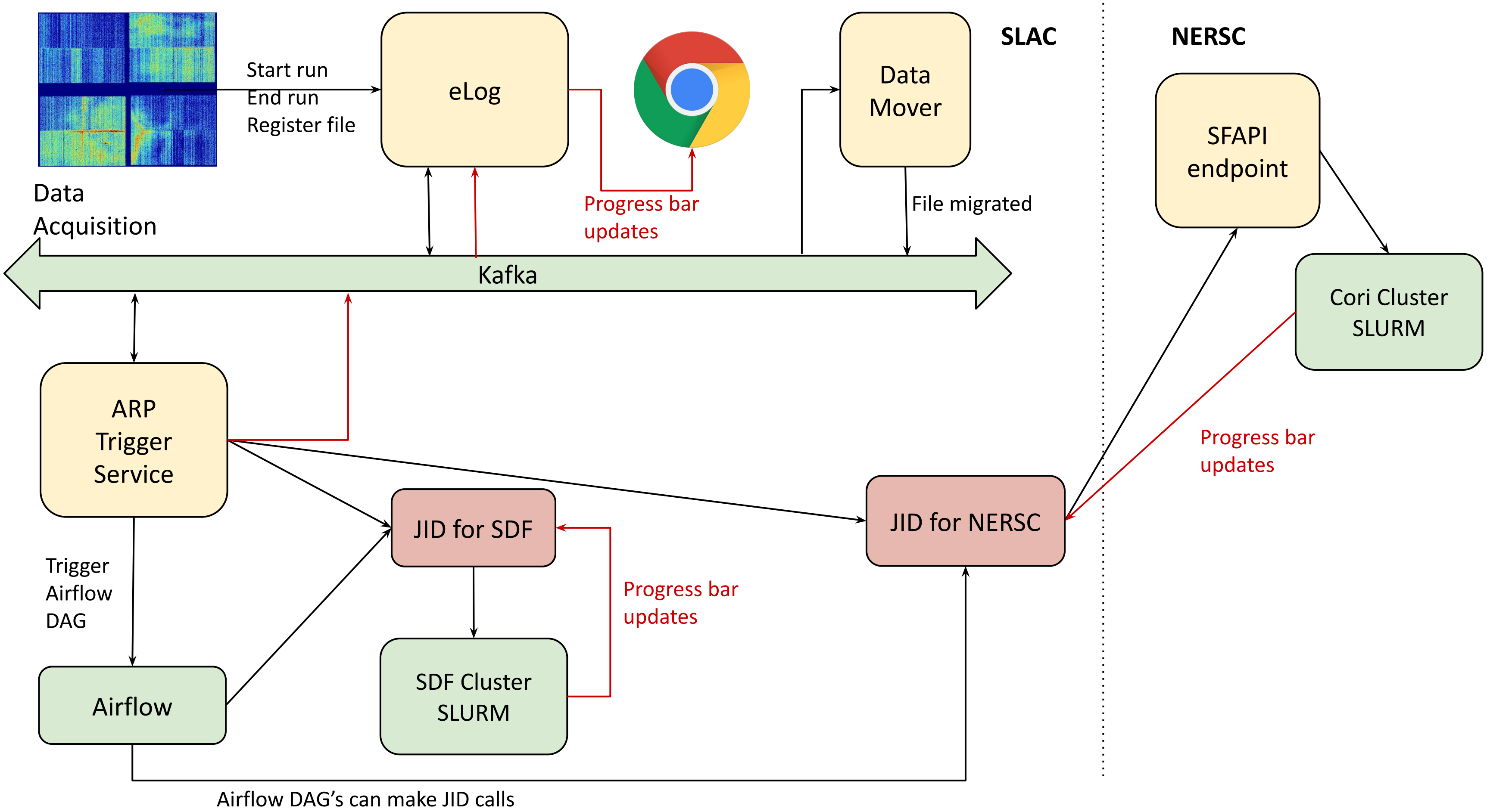
Looking Forward:
(Standardized) Facility APIs

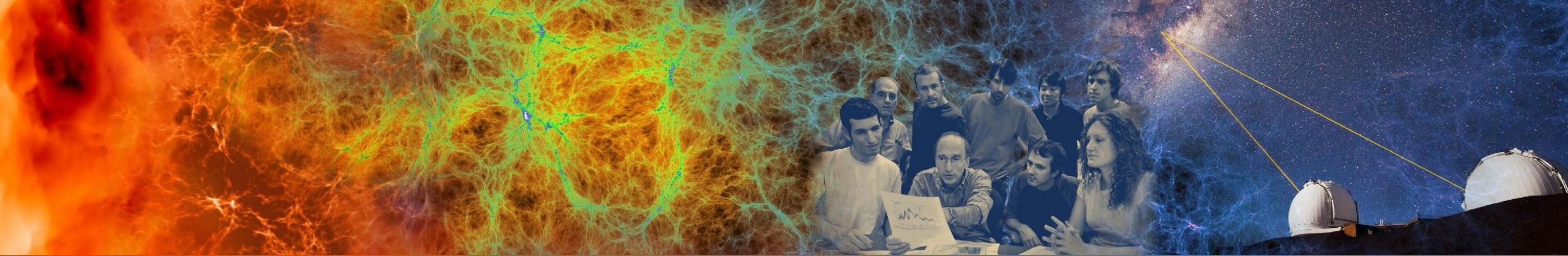
What can an API do?

Vision: all NERSC interactions are callable;
backend tools assist large or complex operations.

Endpoints prototyped or in prep:

`/account`	data about the user’s projects, roles, groups and usage information.
`/compute`	run batch jobs, query job and queue statuses on compute resources.
`/task`	get info about asynchronous tasks (eg. from `/compute` or `/storage`).
`/status`	query the status of NERSC component system health
`/storage`	move data with Globus or between NERSC storage tiers
`/reservations`	submit and manage future compute reservations (in prep)
`/utilities`	traverse the filesystem, upload and download small files, and execute commands on NERSC systems

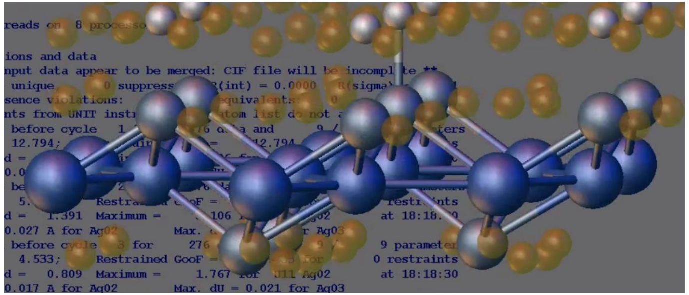

Start run
End run
Register file
eLog
Data Mover
SLAC
NERSC
SFAPI endpoint
Data Acquisition
Progress bar updates
File migrated
Kafka
Cori Cluster SLURM
ARP Trigger Service
Progress bar updates
JID for SDF
JID for NERSC
Trigger Airflow DAG
Progress bar updates
Airflow
SDF Cluster SLURM
Airflow DAG's can make JID calls



Conclusion

Successful Realtime Data Analysis at NERSC

- Live Feedback:
  - **10 mins from end of run to the molecular structures**
    - Enable real-time feedback to beamline staff
  - No babysitting from NERSC staff needed



Structure of Tethrene
(determined during LV95 beamtime)

- XFEL Flexes the following “HPC Muscles”:
  - Urgent Computing Resources
  - High-Speed Data (Network and I/O)
  - Realtime Monitoring and Workflow Coordination

- Beamtime is scarce! Fast feedback is critical! github.com/cctbx/cctbx_project
  - G. Winter *et al*. DIALS: implementation and evaluation of a new integration package. *Acta Crystallogr D Struct Biol* **74**, 85-97 (2018)