STAR Data Production at NERSC/Cori
An adaptable Docker container approach for HPC

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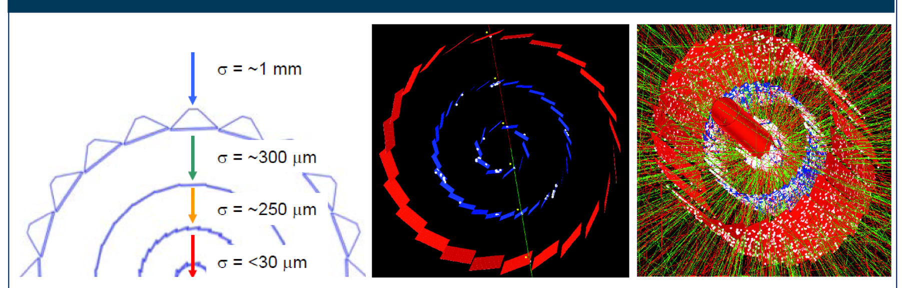
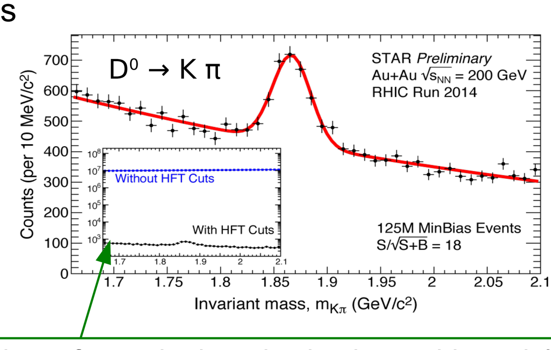
Heavy Flavor Tracker



Tracking inward with gradually improved resolution | Cosmic ray event | Au+Au event

- Quark Gluon Plasma is the expected state of nuclear matter under extreme temperature and pressure. It is the state of all the matter in the universe a few micro-seconds after the big bang before it proceeds to be confined in protons and neutrons as we know it now.
- Measurements of D mesons flow help us understand the degree of thermalization of the Quark Gluon Plasma and to constrain its transport parameters.
- Heavy Flavor Tracker with State of the art MAPS Pixel sensors technology, allows for ~20μm resolution on secondary decay vertices
- Installed at STAR in year 2014 and collected 3B Au+Au events



+4 orders of magnitude reduction in combinatorial background

- For the first time we can study charm hadron chemistry in heavy-ion collisions (D^0/D^{*+}, D_s, Λ_c)

Motivation & Idea

Challenge: the increasing sizes of data collected by HEP/NP experiments lead to an increasing demand on computing capacity that is challenging to meet by scaling the conventional clusters solution.

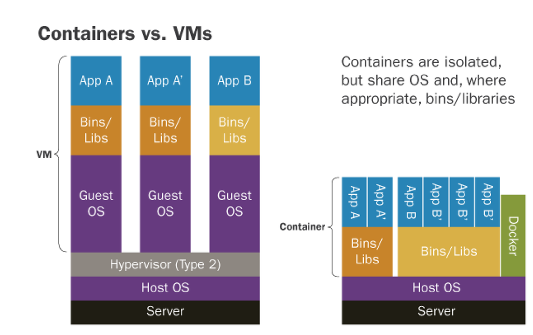
Cori, second generation exa-scale facility at NERSC

Opportunity: new generation HPC facilities provide vast computing resources with adequate memory and network connectivity for data intensive application. These facilities can allow for on-demand expansion of HEP/NP data production capacity that significantly shorten the time needed to get physics ready data and thus accelerate the pace of scientific discovery.

Idea: Linux containers enabled HPC systems can provide the right virtual environment for experiments to run their customized software stack, ensuring reproducibility and high walltime efficiency.

In this poster: we report on the first test of STAR real-data production utilizing Docker/Shifter containers on Cori Phase I supercomputer at NERSC.

Docker/Shifter



- HPC systems provide vast resources for computation and data intensive applications. However, for technical and logistic reasons, their software is not readily customizable for specific project needs.
- With a Docker enabled system we can push STAR software/environment with the job to the computing node.
- **Shifter** [1] is a NERSC project to bring docker-like virtualization functionality on cray compute nodes to allow custom software stack deployment.

See "Using Shifter to Bring Containerized CVMFS to HPC", Lisa Gerhardt, Wed., 12 Oct 2016, 12:30, id: 293.

[1] D. M. Jacobsen and R. S. Canon, "Contain This, Unleashing Docker for HPC", Cray User Group 2015, April 23, 2015.

Scalable Access to Database

STAR data production software uses a MySQL service for detector online running parameters and calibrations. The location of this DB is critical for scaling the number of jobs to the throughput planned at Cori.

For a large scale production STAR can place the DB as:

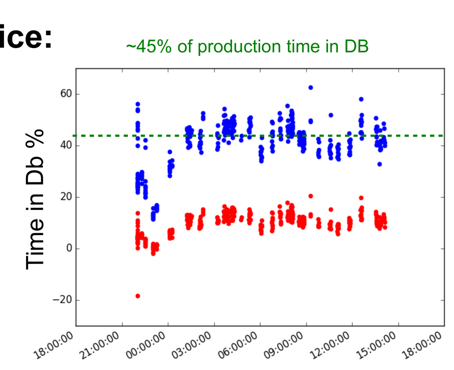
1) A network isolated DB service
2) A snapshot local DB server at the computing node
3) Full payload local DB server at the computing node

Each approach comes with its own advantages. The location of the DB is an important part of the end-to-end workflow optimization.

Network isolated DB service:

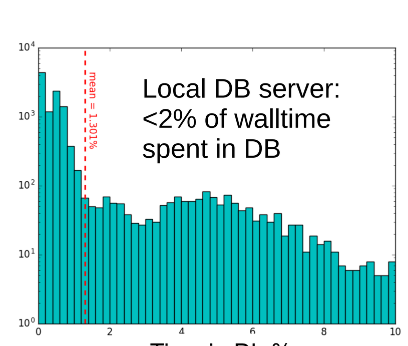
Unpredictable network conditions → Not easy to scale to projected throughput.

An example of a bad incident: 45% of walltime spent in DB



Local DB server at the compute node:

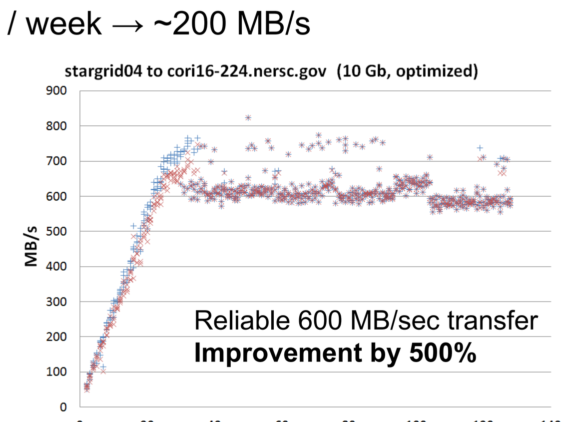
Pros:
- No network routing → trivial scalability with number of jobs



Cons:
- Have to start the server from scratch for every job
  - Some tables take a long time to cache (a particular table makes ~30k queries) → solved with perCacheNode feature of shifter (XFS file)
- Time taken to copy payload at the beginning of the job
- Consumes cpu allocation

NY-CA Data Transfer over ESnet

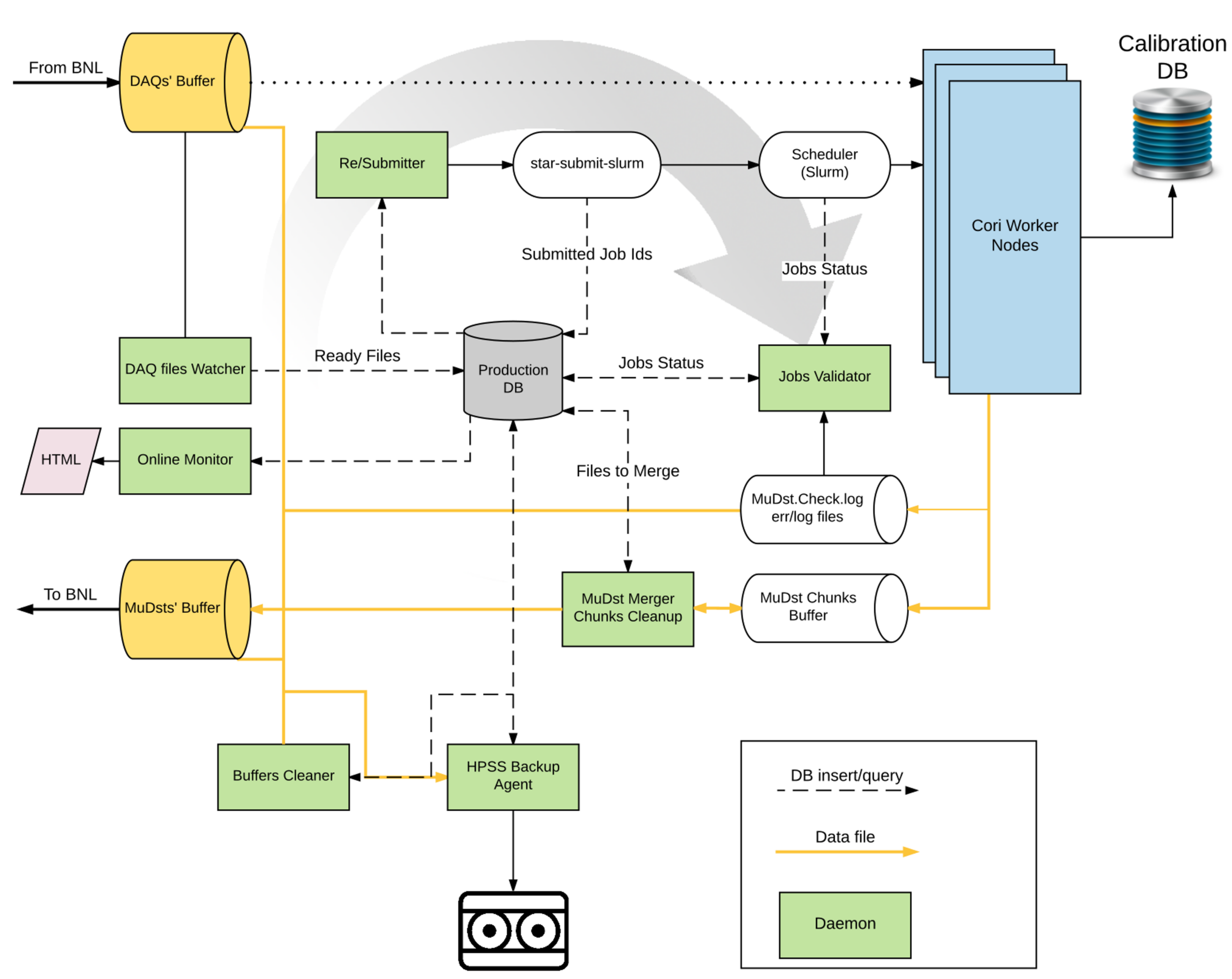
- For best utilization of CPU resources we need a reliable data transfer between BNL and NERSC → 100TB / 10k CPUs / week → ~200 MB/s



- ESnet + optimized end points and transfer protocol provides 600 MB/s transfer rate, a 5x improvement over the vanilla system rate of ~120 MB/s
- Large scale test is on way to ensure reliability of the connection at this rate

Production Pipeline

Pipeline design objectives:
- Modularity to enable end-to-end optimization
- Need to be ready for all Cori downtime scenarios
  - Jobs cold start capability
  - daemons failure tolerance
- Continuous monitoring
- To handle a target throughput ~10k cores / week → ~100TB / week transferred over ESnet
- Archive input and output files to HPSS



Design and implementation:
- Automated finite state workflow → allows us to achieve high overall fidelity
- One input raw data file is mapped to multiple process at the node (a simple mapreduce pattern)
- Multi-threaded design (12 daemon threads). All daemons are configurable using json files
- Central production DB (MongoDb)
  - communicate/control system states
  - Provides persistent storage of pipeline states (all daemons are stateless)
- Slurm for job submission. Jobs resources utilization also gathered from slurm and log files to allow monitoring and further tuning (no heartbeat from jobs)
- Continuous online pipeline monitoring
  - Python Flask app running on portal-auth.ners.gov responds to web-base users queries to MongoDB
  - JavaScript runs in browser end renders numbers into either tables or graphs

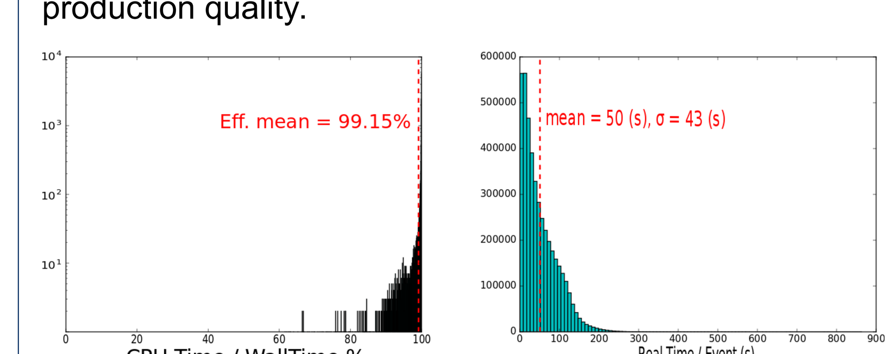
Performance

We carried a real job production test that used ~100k CPU hours to test the different units integration and calculate the overall success rate:

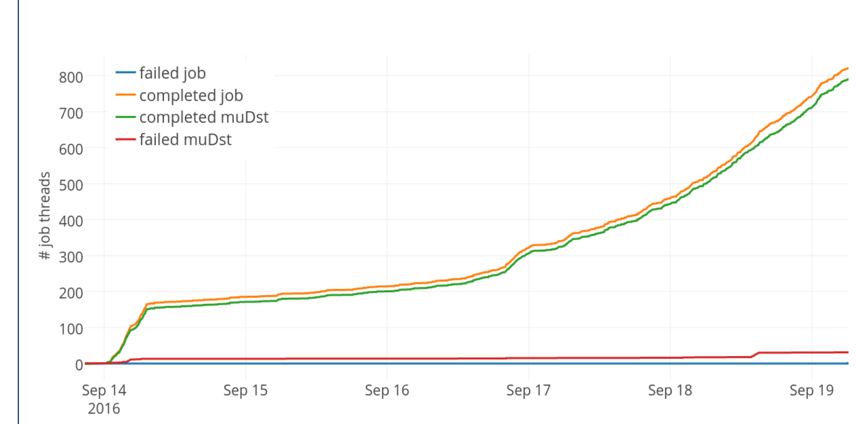
J = Successful job completion
O = Good output file with +98% of events produced

Success Rate (SR) = J * O

Generally, an SR > 95% is enough to qualify the workflow and computing facility to be real data production quality.



- 16 production processes + 1 MySQL server per 16 CPU cores → +99% walltime efficiency
- 50s / Au+Au event is comparable to 48s without a local MySQL CPU overhead



- < 4% failure → SR > 96%
- A solution has been identified to increase the SR to the +99% range
- Trivial DB scalability with a local MySQL server per job

Summary & Outlook

- Docker/Shifter + HPC can carry HEP/NP data production at a large scale
  - Shifter enabled Cori and Edison at NERSC offer such an opportunity
- Network bandwidth optimization is essential for end-to-end optimization: ESnet enables transfer of large amounts of data across the continent
- +99% walltime efficiency demonstrated

Production plan:
- STAR collected a 3Pb of Au+Au collision data during RHIC run 2016 → +50M CPU hours
- We requested to process 50% of the data at Cori
  - Transfer 1.5Pb into Cori, ~1Pb output data → ESnet
  - Use 25M CPU hours
- Full integration test with NY-CA transfer pipe