

# STAR Data Reconstruction at NERSC/Cori, an adaptable Docker container approach for HPC

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**Abstract.** As HPC facilities grow their resources, adaptation of classic HEP/NP workflows becomes a need. Linux containers may very well offer a way to lower the bar to exploiting such resources and at the time, help collaboration to reach vast elastic resources on such facilities and address their massive current and future data processing challenges.

In this proceeding, we showcase STAR data reconstruction workflow at Cori HPC system at NERSC. STAR software is packaged in a Docker image and runs at Cori in Shifter containers. We highlight two of the typical end-to-end optimization challenges for such pipelines: 1) data transfer rate which was carried over ESnet after optimizing end points and 2) scalable deployment of conditions database in an HPC environment. Our tests demonstrate equally efficient data processing workflows on Cori/HPC, comparable to standard Linux clusters.

## 1. Introduction

The expected growth in High Performance Computers (HPC) capacity over the next decade makes such resources attractive for meeting future computing needs of High Energy and Nuclear Physics (HEP/NP) experiments [1], especially as their cost is becoming comparable to traditional clusters. However, HPC facilities rely on features like specialized operating systems and hardware to enhance performance that make them difficult to be used without significant changes to data processing workflows. Containerized software environment running on HPC systems may very well be an ideal scalable solution to leverage those resources and a promising candidate to replace the outgrown traditional solutions employed at different computing centers.

While STAR data real-data reconstruction has been carried at remote sites before in a sustainable and geographically distributed manner [2], the HPC environment provided a new set of unique challenges. In this proceeding we report on the first test of STAR real-data reconstruction utilizing Docker [3] containers on the data partition of the Cori supercomputer at NERSC<sup>1</sup>. The target dataset was recorded by the STAR experiment at RHIC in 2016 and is estimated to require ~50 M core-hours for full processing. To ensure validity and reproducibility, STAR data processing is restricted to a vetted computing environment defined by system architecture, Linux OS, compiler and external libraries versions. Furthermore, each data processing task requires certain STAR software release and database timestamp. In short, STAR data processing workflow represents a typical embarrassingly parallel HEP/NP computing task.

<sup>1</sup> <http://www.nersc.gov/users/computational-systems/cori/>

Thus, it is an ideal candidate to test the suitability of running containerized software, normalized to run on a shared HPC systems instead of its traditional dedicated off-the-shelf clusters. This direction, if successful, could address current and future experiments’ computing needs. We report on the different opportunities and challenges of running in such an environment. We also present the modifications needed to the workflow in order to optimize Cori resource utilization and streamline the process in this and future productions as well as performance metrics.

Section 2 outlines some of the technical aspects of our pipeline and discusses conditions database location in an HPC environment. In section 3, we show performance results from an extended test that uses +120k core-hours. Summary and outlook are provided in section 4.

## 2. Implementation

### 2.1. Docker/Shifter

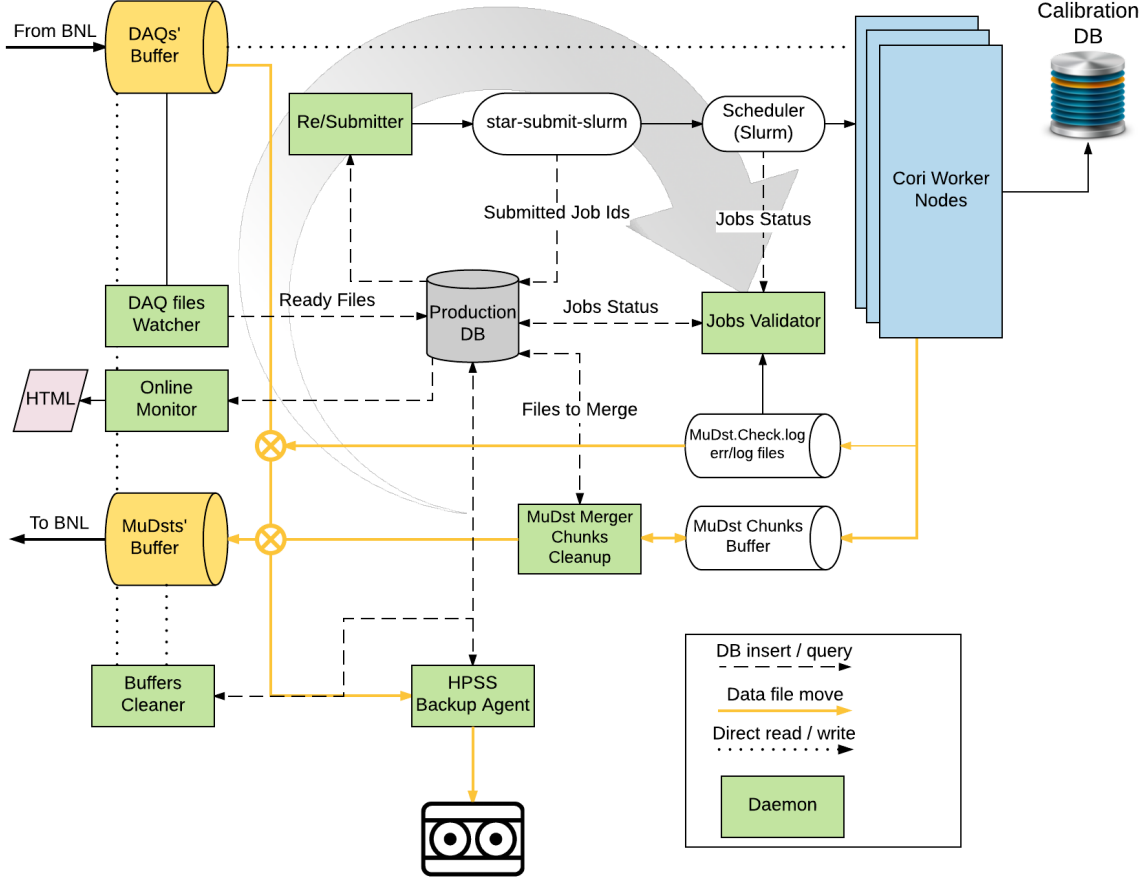
HPC systems provide vast resources for computation and data intensive applications. However, for technical and logistic reasons, their software is not readily customizable for specific project needs. With a Docker enabled system, experiments can run their operating system of choice and a customized software stack in Linux containers. The ability to ”push” the software image with the job to the computing nodes makes any computing environment, e.g. HPC or Cloud, very versatile. Shifter [4] is a NERSC project created to allow easy custom software stack deployment by bringing the functionality of Linux containers to Cray compute nodes along with the tool to convert Docker images into Shifter images for running on NERSC HPC systems.

We base our STAR Docker image on Scientific Linux 6.4. ROOT [5] and STAR software are baked into the image from pre-compiled binaries. MySQL server and OpenMPI are the only components in the Docker image that are different from the STAR software environment used on traditional clusters. The MySQL server providing conditions DB is launched locally on the compute node. MPI is used to fan-out jobs to process sections of the same input data file by as many data reconstruction chains as available number of processors (or threads) on the node. This is complete data parallelism without any message passing between threads.

### 2.2. Pipeline

A schematic of the pipeline we built for reconstruction of STAR data at Cori is shown in Figure 1. To carry a months long data processing campaign at an HPC facility requires a high level of pipeline fault-tolerance. In addition, HPC systems are known for their more frequent maintenance downtimes, thus the pipeline needs to demonstrate cold-start capability. For these reasons and to facilitate end-to-end optimization we opted for a modular multi-threaded design (12 daemon threads) as opposed to a monolithic design. Our pipeline is designed for a target throughput of 10,000 cpu-cores continuously running to process raw data in the order of 100 TB per week. The entire campaign is expected to use 25 M core-hours. The pipeline handles 1) transfer of raw data files (DAQ’s) from BNL to NERSC over ESnet and checking for integrity (md5sum) 2) submitting jobs to the queue; one file can be processed using 1 to 32 processors depending on queue partition availability and input file size. The output of the different processors are later merged into one file (MuDST) and 3) perform quality assurance on the output of the jobs and transfer successfully produced data back to BNL.

Central to our design is the production database to which all the states of the different stages of input file processing, daemons states (heartbeats) and summary statistics are logged. The daemons themselves are internally stateless and no communications between daemons happen except through the database, this provides 1) persistent storage of all pipeline states 2) daemon failure tolerance; daemons can be individually restarted and they pickup from where they left off 3) continuous collection and monitoring of pipeline states and statistics is easily done by



**Figure 1.** A schematic of STAR data reconstruction pipeline at Cori, NERSC. The raw data input files (DAQ's) are transferred from BNL to NERSC over ESnet. The reconstructed data (MuDST's) are pulled back from BNL side.

querying the database. We rely on Slurm<sup>2</sup> [6] to monitor jobs states and resource utilization on the compute node, i.e. no heartbeats directly from the job to the production DB.

In addition to the core tasks, Figure 1 also shows some auxiliary daemons, such as HPSS backup agent and the buffers cleaner. A Python Flask app running on NERSC web-portal responds to web-base users queries to production DB and generates aggregate statistics plots showing progress of the production. This allows the operators of the production campaign to catch failures of the systems that are not automatically handled by the pipeline daemons.

### 2.3. Conditions database

STAR data processing software uses a MySQL service for detector online running conditions and calibration parameters. The location of this DB is critical for scaling the number of jobs to the planned throughput of the pipeline. Given Cori layout and STAR framework capabilities we had a couple of options for this DB: 1) a network isolated DB service, i.e. a DB server on a machine outside the Cori network or 2) full or minimal snapshot payload DB server local to the compute node. Other options such as launching DB servers in separate jobs to serve a collection

<sup>2</sup> Slurm Workload Manager is the scheduler used by many supercomputers as well as Cori

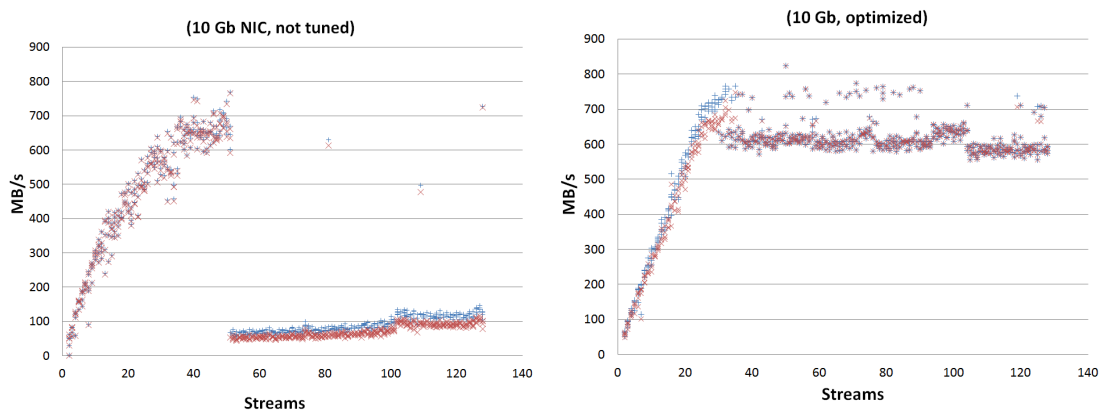
of compute nodes were entertained but deemed to pose unnecessary technical challenges.

We found that network isolated DB service suffers from unpredictable network conditions, in particular network throughput relies on other users' traffic and other not easily foreseen conditions. For example, during our stress tests of the pipeline the network was under performing which made the jobs spend 45% of their walltime waiting for the DB. Jobs usually spend less than 2% of their walltime in the DB. This incident lasted for more than 24hrs. At this point it was clear that we have to move the DB server closer to the jobs.

Relying on DB servers local to each computing node comes at a cost. In particular, as with many HPC systems, Cori nodes do not have local disks. The MySQL DB payload has to be placed on a globally mounted Lustre filesystem. The Lustre filesystem is not designed for the database transactional workloads that do a lot of metadata lookups. This is particularly problematic; the need to start a MySQL server with a fresh cache at the beginning of each job causes many queries to Lustre metadata to build up the data in-memory. As a result, long delays were observed during the start of each job due to this inefficient use of the filesystem. For example, a particular table requires  $\sim 30k$  queries to build, building such a table takes more than 30 minutes with the payload on Lustre.

Shifter provided a solution to the problem of slow startup times due to building the DB cache on Lustre with its perNodeCache feature. This allows for the creation of a write-able XFS file which is loopback mounted on the compute node and acts as a local file system for the container. While the loopback mounted file is placed on Lustre, the metadata can be safely cached in the compute node's memory since it is private to the node. We opted for a solution where every job starts by copying the MySQL payload into its own perNodeCache then launches the MySQL server. To simplify the workflow we copy the entire STAR DB payload as opposed to a single year's snapshot, copying the 30 GB payload takes 1-2 minutes. This solution dramatically changed the DB performance. For example, caching the  $\sim 30k$  queries table dropped from +30 minutes to a few seconds. We launch one DB server per compute node which serves all the reconstruction chains on that node, 1-32 chains on Cori Haswell nodes. We found that over-committing the node cores has not decreased the aggregated events throughput per core per walltime. So we run 1 MySQL server + N reconstruction chains on N cpu-cores. The local DB server strategy avoids the network routing bottlenecks altogether and trivially scales to our projected pipeline throughput.

#### 2.4. NY-CA data transfer

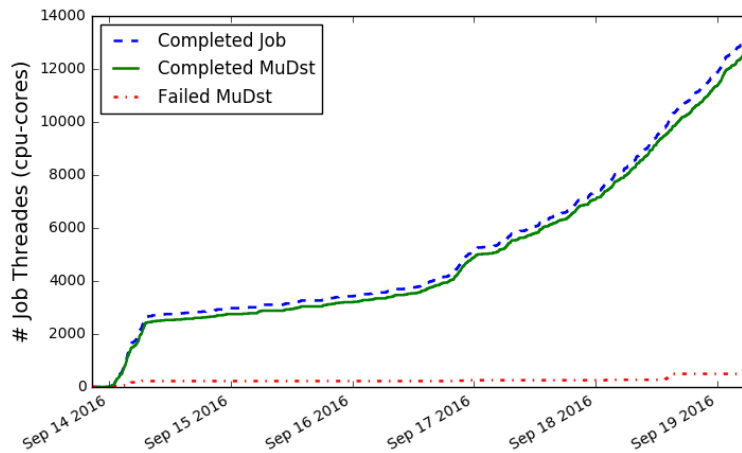


**Figure 2.** Transfer rates over ESnet before (after) end-points and transfer protocols optimization, left (right), 5x improvement over the vanilla setup

For best utilization of CPU resources we need reliable data transfer between BNL and NERSC. Projected throughput requires the transfer of  $\sim 100$  TB/week and  $\sim 15$  TB/week of reconstructed data back to BNL or approximately a continuous transfer rate of 200 MB/s in steady state production. The data is transferred over the Energy Sciences Network (ESnet)<sup>3</sup>.

Our initial setup was composed of two active-passive data transfer nodes connected at 2x1 Gb speeds behind a firewall. This did not fulfill our minimal requirement of 200 MB/sec. We started by upgrading the interface to 10 Gb network interface cards (NIC) and migrated the transfer nodes to BNL's Science DMZ which connects each node at 2x10Gb (LACP). Our initial testing of the performance is showed on Figure 2 (left). The network transfer pattern, showing a bimodal feature, is a clear indication and a sign of transfer collapse due to congestion and transfer buffer size - following the basic tuning instructions available on [7], we obtained and confirmed stable data transfers with a plateau at 600 MB/sec. The most relevant tuning were the change to the congestion control from bic to htcp and modifying the rmem/wmem parameters as suggested (Fig. 2, right).

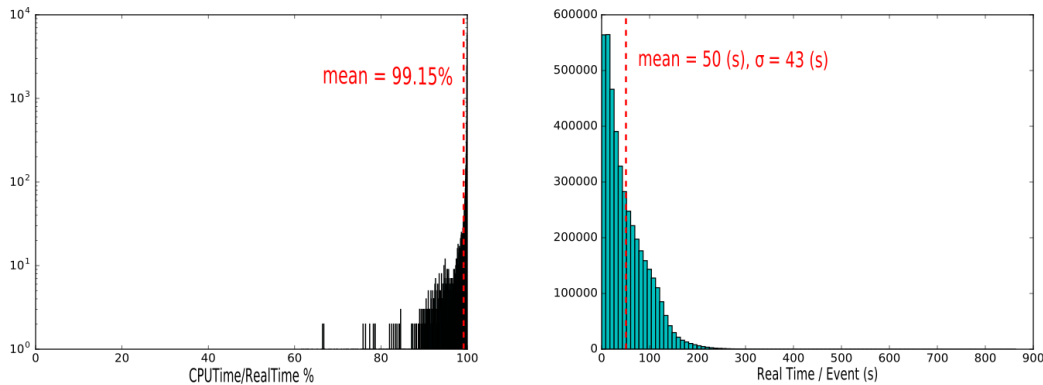
### 3. Performance test



**Figure 3.** An example of pipeline monitor plot showing aggregate statistics of successful and completed jobs during a test production. "Completed job" is for jobs which ran to completion. "Completed muDst" is for produced files which pass QA and +98% of events produced

We carried a real-data reconstruction test that used +120k core-hours to test the different pipeline units integration and calculate the overall success rate (SR). Our criteria for a successful output file is for the job to run to completion and for the file to have +98% of the data events reconstructed. Figure 3 shows job success/failure aggregate statistics during our test production which was carried over 6 days. The tests had a SR > 96% for reconstructed files that passed our QA. Generally, we require an SR > 95% to qualify the workflow and computing facility to be real-data processing quality. The failed  $\sim 4\%$  are mainly due to the failure of the local MySQL server. Solving this problem by making the server persistent will allow us to increase the SR to the +99% range.

<sup>3</sup> <https://www.es.net/>



**Figure 4.** (Left) CPU utilization efficiency CPUTime/WallTime (Right) Distribution of walltime to process one event

Finally, we examined the CPU utilization efficiency of the jobs. Each one of our test jobs was granted 16 cpu-cores, and ran 16 reconstruction chains + 1 MySQL server (overcommitting the cores). The CPU utilization efficiency is well above 99% for most jobs as shown on the left plot in Figure 4. Figure 4 right shows the distribution of walltime per event. The average time of 50s/Au+Au event is comparable to 48s without a local MySQL server.

#### 4. Summary & Outlook

In this proceeding we outlined STAR strategy for carrying HEP/NP real-data reconstruction on Cori HPC facility. Docker/Shifter-enabled Cori and Edison at NERSC have vast resources that can be used to run customized HEP/NP software stacks. Edge services availability, such as conditions database, are a traditional challenge for running in HPC environments. We showed that, in the database case, running a database server at the compute node with the DB payload in a Shifter perNodeCache is a highly scalable solution without much overhead on the CPU resources. ESnet enables the transfer of large amounts of data across the continent; however, we found that both network protocols and endpoint optimizations are essential components of steady-state end-to-end transfer operations. Finally, our test production shows +99% walltime with very high success rate (+95%), allowing us to deem the pipeline at Cori real-data processing quality. We plan to use the pipeline to process half of the 3Pb of Au+Au collision data recorded by the STAR experiment during RHIC run 2016 which will require  $\sim 25$  M core-hours.

#### 5. Acknowledgements

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