Physics Data Production on HPC: Experience to be efficiently running at scale

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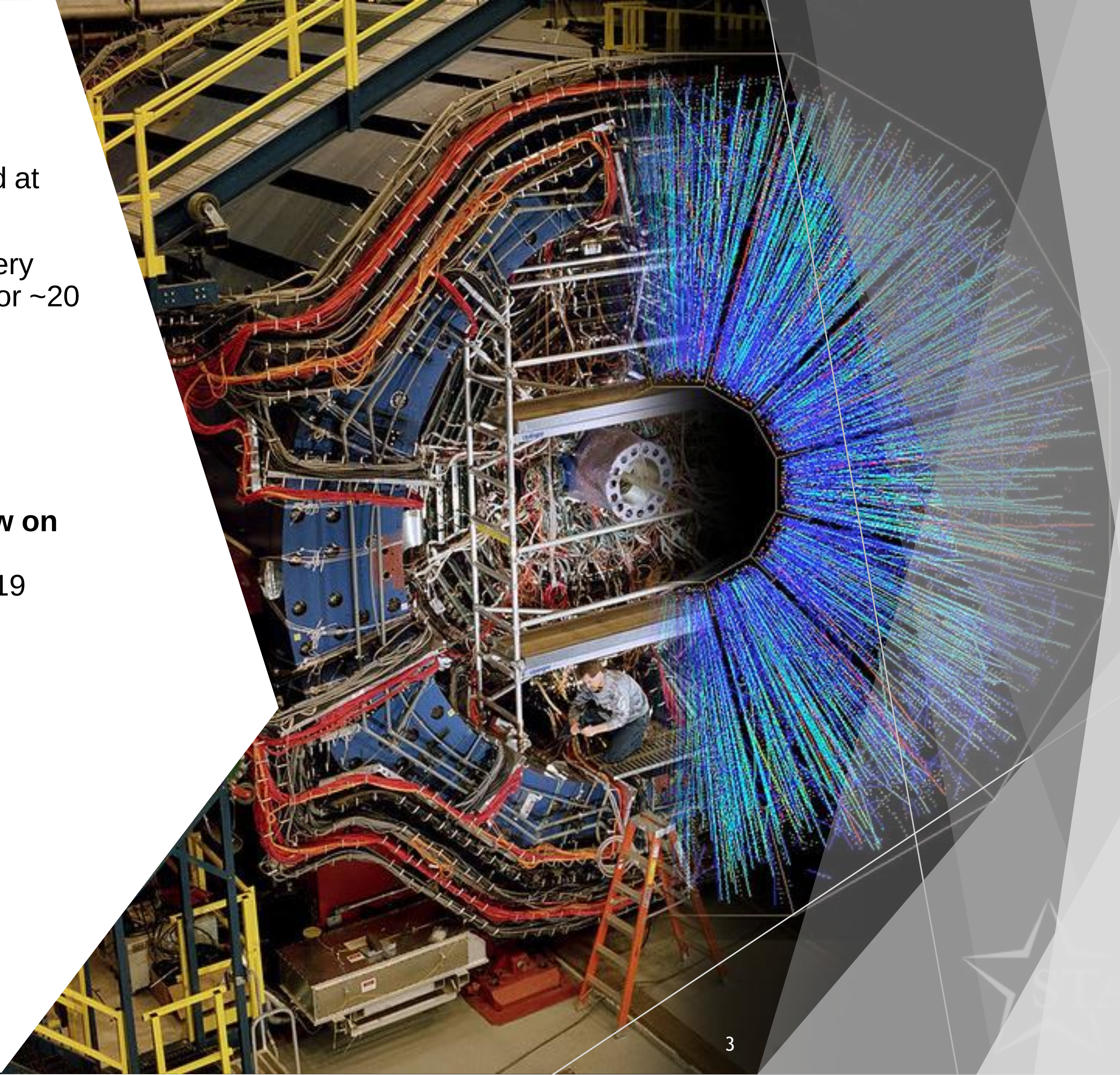
Outline

- Introduction
- Containers & CVMFS
- STAR Data Production Workflow
- Database Access
- Efficiency & Throughput Considerations
- Conclusion

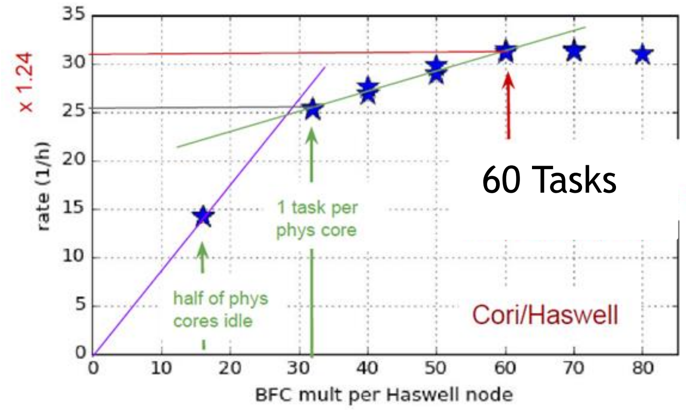
Introduction

- The Relativistic Heavy Ion Collider (RHIC) is located at Brookhaven National Lab (BNL) in Upton, NY
- The STAR detector at RHIC produces 10s of PB every year and ran its data production on NERSC/PDSF for ~20 years
- PDSF’s is EOL -> migrated to NERSC/Cori
- Our previous work focused on the scalability of CVMFS serving STAR Software on Cori
  - ACAT 2019 “**STAR Data Production Workflow on HPC: Lessons Learned & Best Practice**”, M.D. Poat *et al* 2019
- **Current Focus:**
  - Workflow
  - MySQL Database access
  - Efficiency

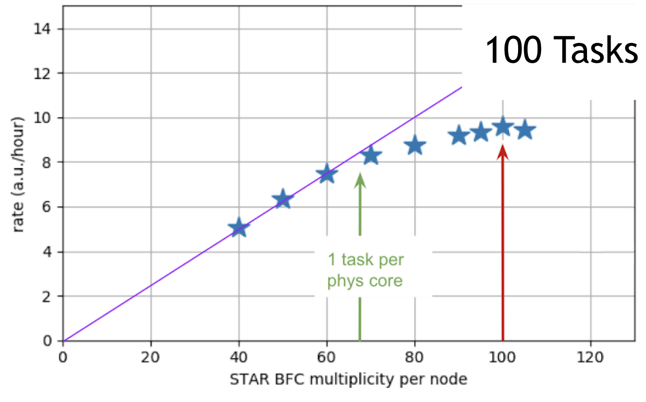


NERSC – ‘Cori’ Cray XC-40 Supercomputer

- 20 TB $SCRATCH/user (Luster FS)
- 2388 Xeon "Haswell" nodes
  - 32 Cores (64 vCores, 2-way HT)
  - 120 GB RAM (~ 1.8 GB / vCore, plenty for STAR)
- 9688 Xeon Phi "Knights Landing" nodes (KNL)
  - 68 Cores (272 vCores, 4-way HT)
  - 96 GB RAM (0.35 GB / vCore or 1.4 GB / core)



Haswell



KNL

Balewski, J., Porter, J., Rath, G., Lee, R., Quan, T. (2018) PDSF - Status & Migration to Cori *HEPiX Fall 2018, Barcelona*

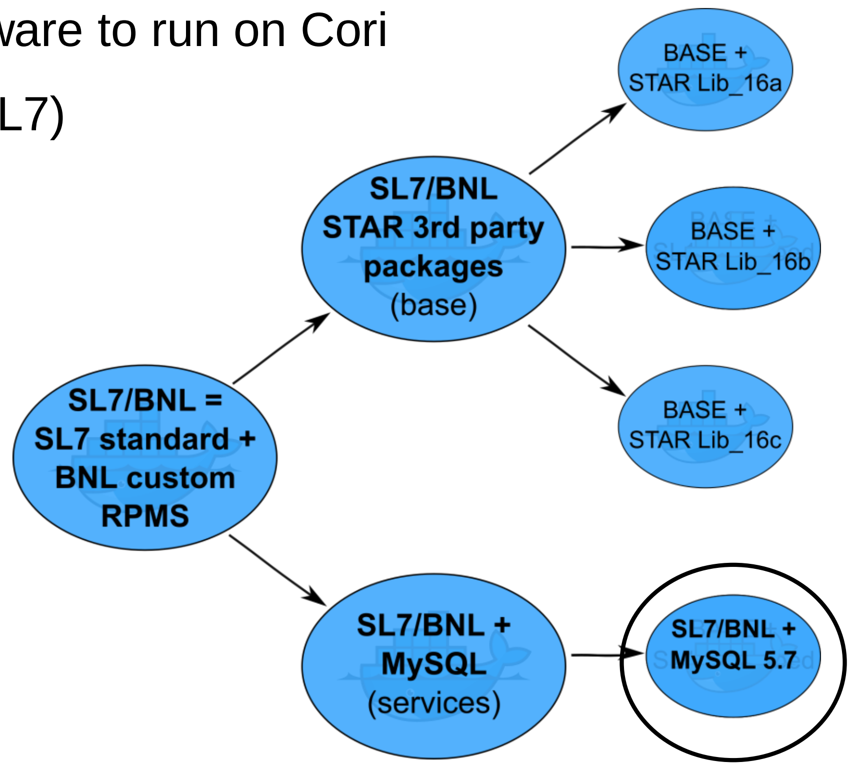
STAR Task Density

- Evaluated KNL & Haswell maximum utilization with STAR tasks
- STAR SW requires ~1 GB RAM
- Haswell: Supports 60 STAR tasks per/node
- KNL: Supports 100 STAR task per/node

STAR Software in Containers

- Docker/Shifter containers are required to enable the STAR Software to run on Cori
- STAR Docker containers are built based on Scientific Linux 7 (SL7)
  - SL7 + RPM (650 MB)
  - SL7 + RPM + STAR SW (3 GB)
  - SL7 + RPM + STAR SW + 1 STAR Library (4 GB)

- Cons: If we have to update the Base image, all images will need to be updated -> maintenance nightmare
- Pros: All Software and libraries packed in 1 container
- **Decision (standard practice):** Use CVMFS for all Experiment stack related software -> standard way for software provisioning

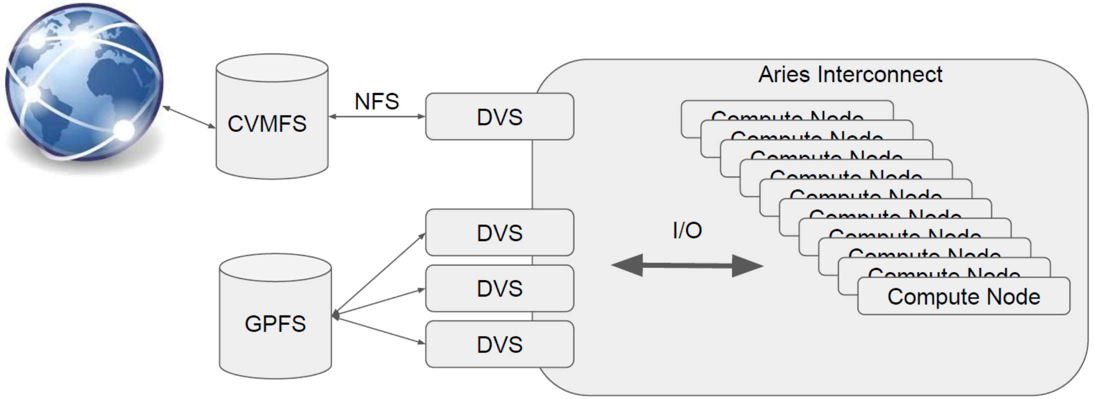


Container Maintenance Tree

CVMFS on Cori

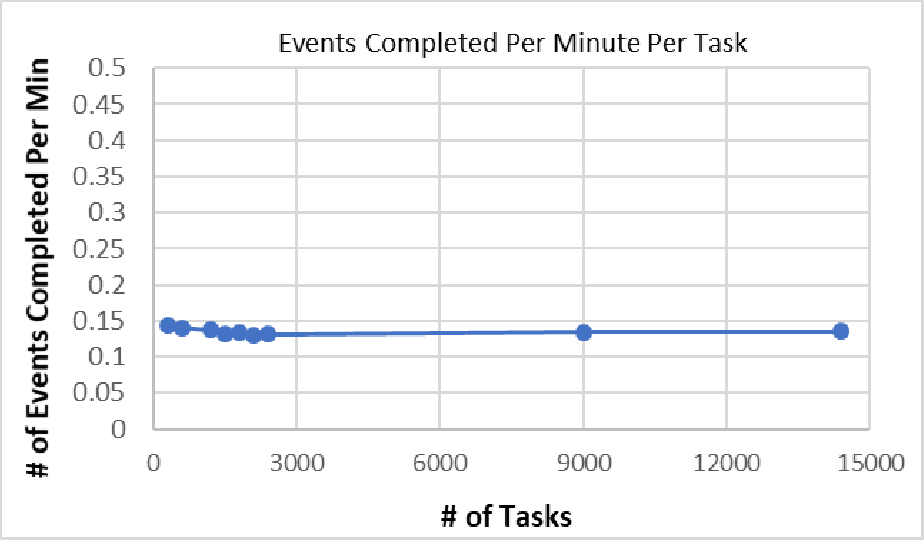
CVMFS on Cori

- CVMFS requires FUSE kernel module to mount natively
- Fuse restriction on Cori (No Kernel access on worker nodes)
- NERSC provides Cori with Data Virtualization Service (DVS) servers
  - Used for I/O Forwarding and data caching
- Cori has 32 DVS Servers, 4 dedicated to forwarding CVMFS I/O
- **DVS servers forward I/O well, but do not support metadata lookups (requires lookup to real CVMFS backend -> latency)**

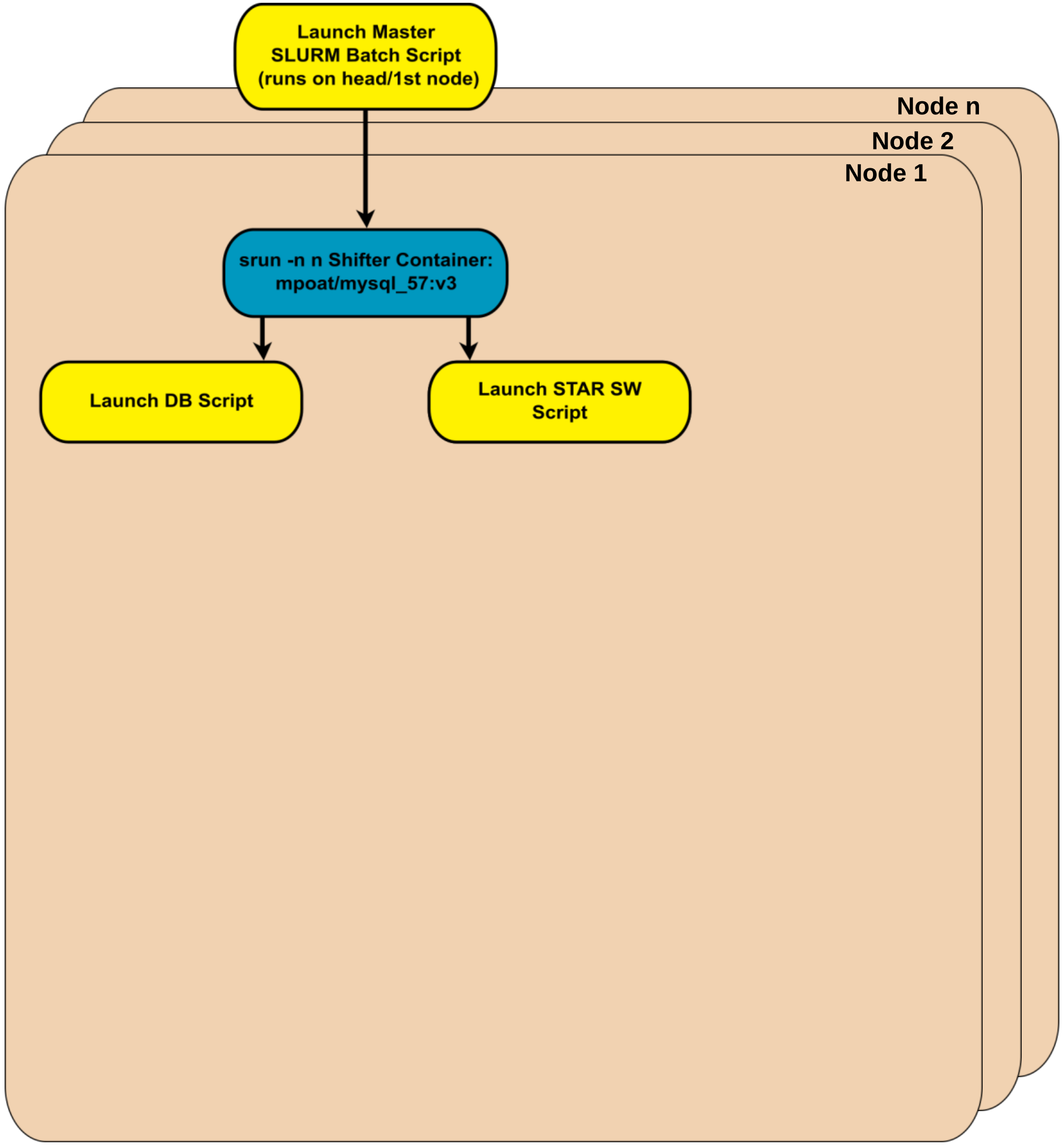


Throughput Maximization for CVMFS

- Looked at average of events produced min/“task”
- Scaled from 1 – 240 nodes
- Drops by ~10-12% at first but we still gain in “events min/node”
- Curve remains flat afterward up to our max @15,000 tasks on 240 nodes
- **In order to achieve this we needed to modify our workflow with time delays…**



STAR Workflow on Cori



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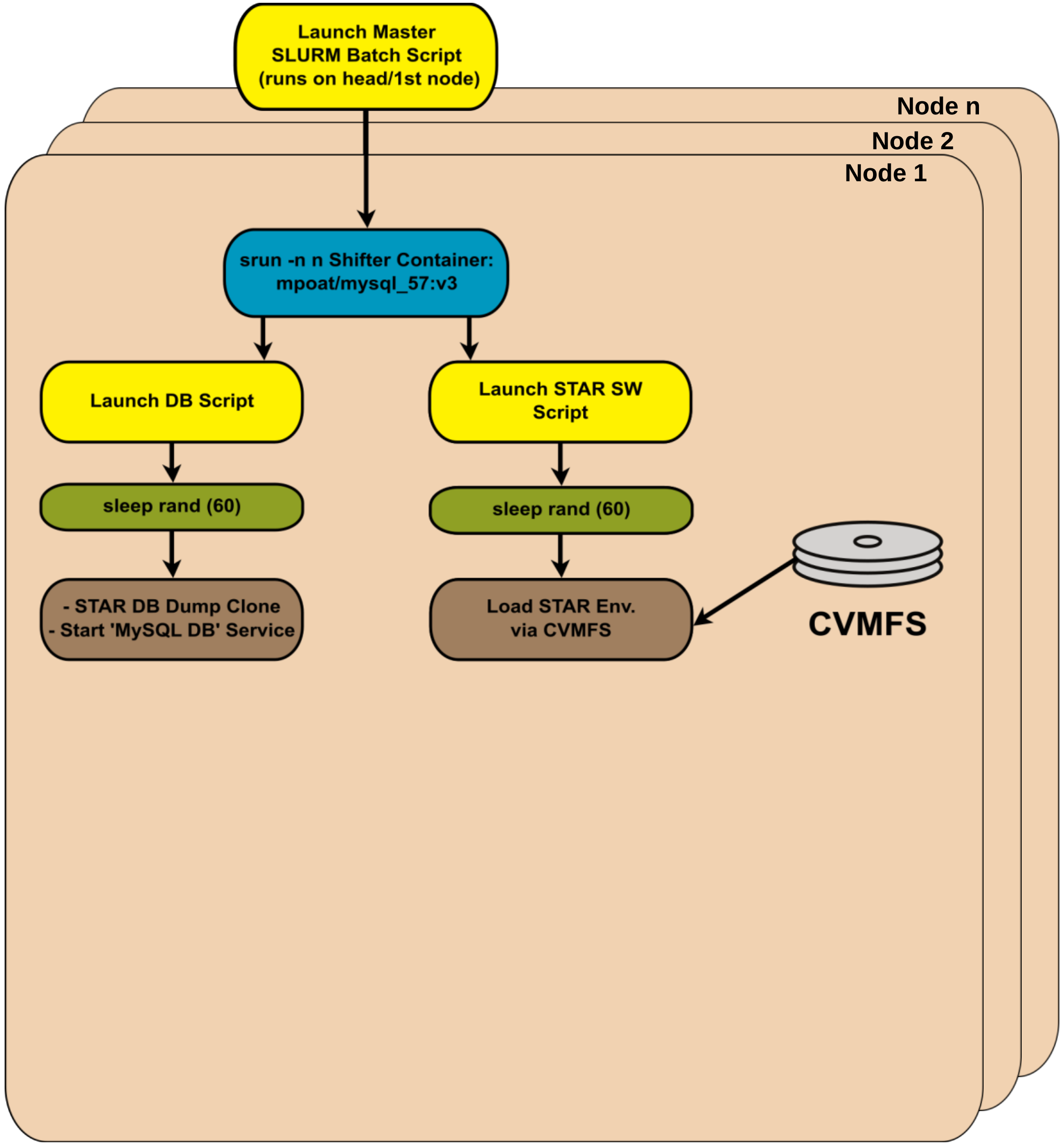

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- Runs ‘Load DB’ & STAR SW scripts in parallel

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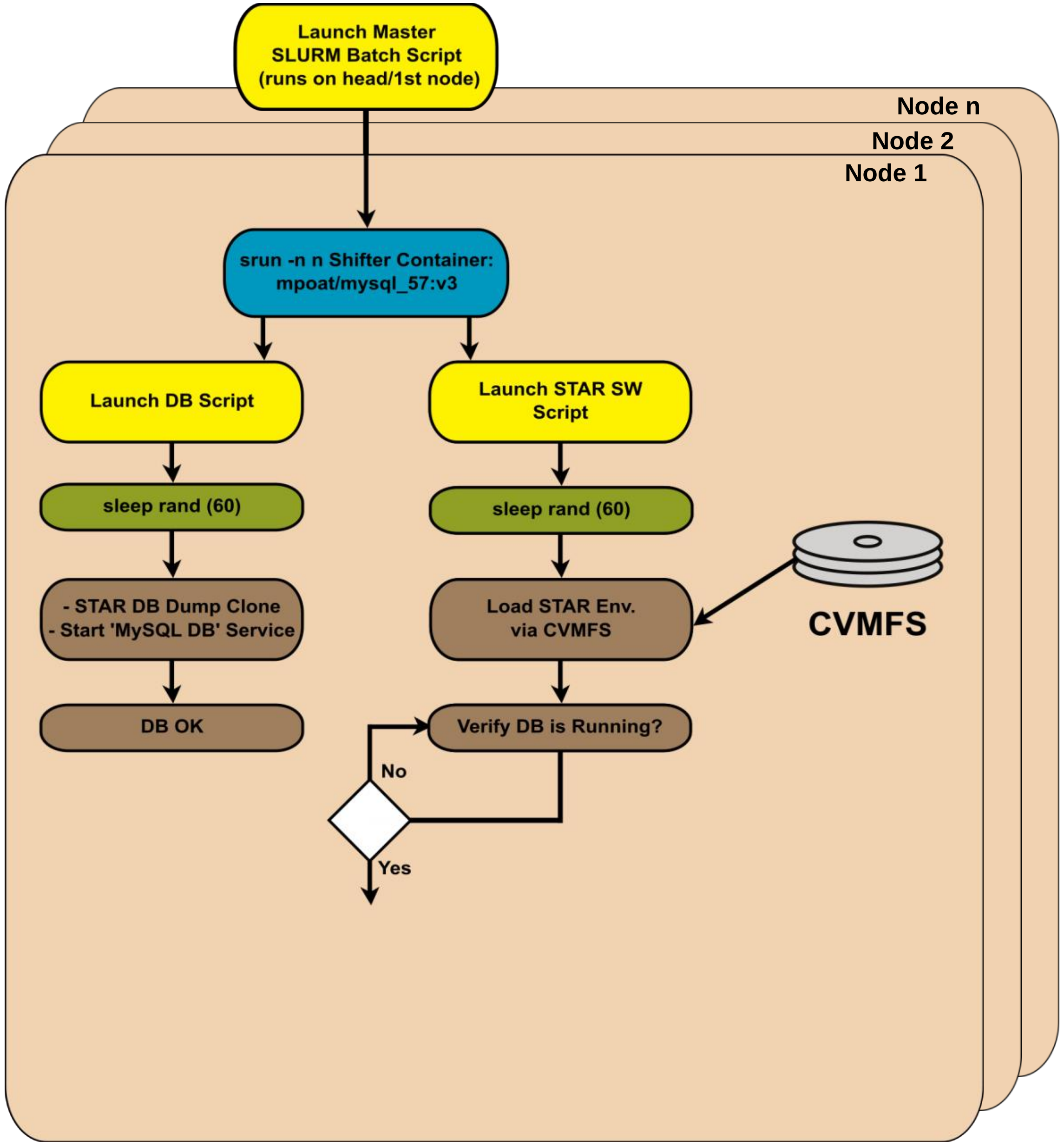

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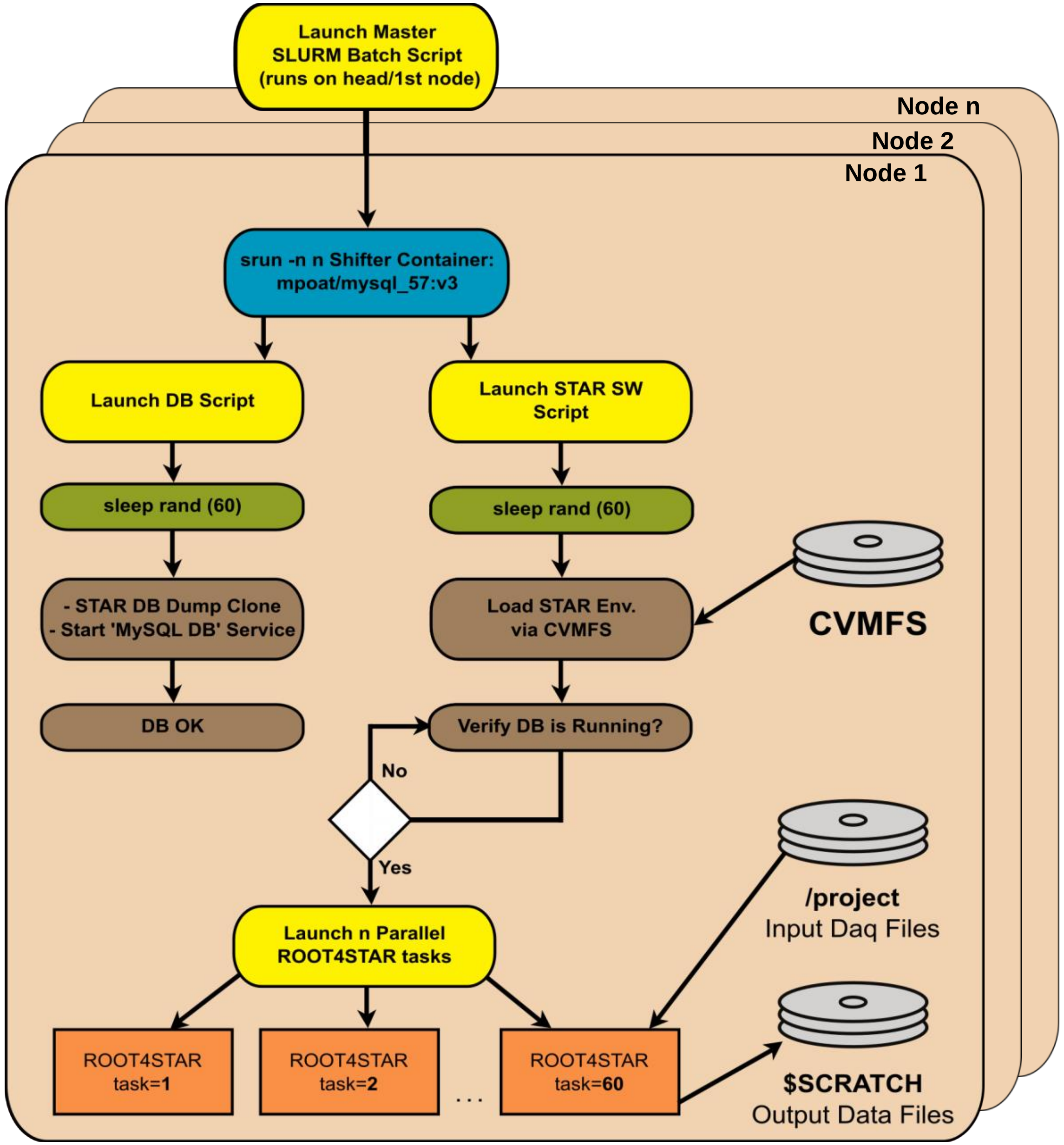

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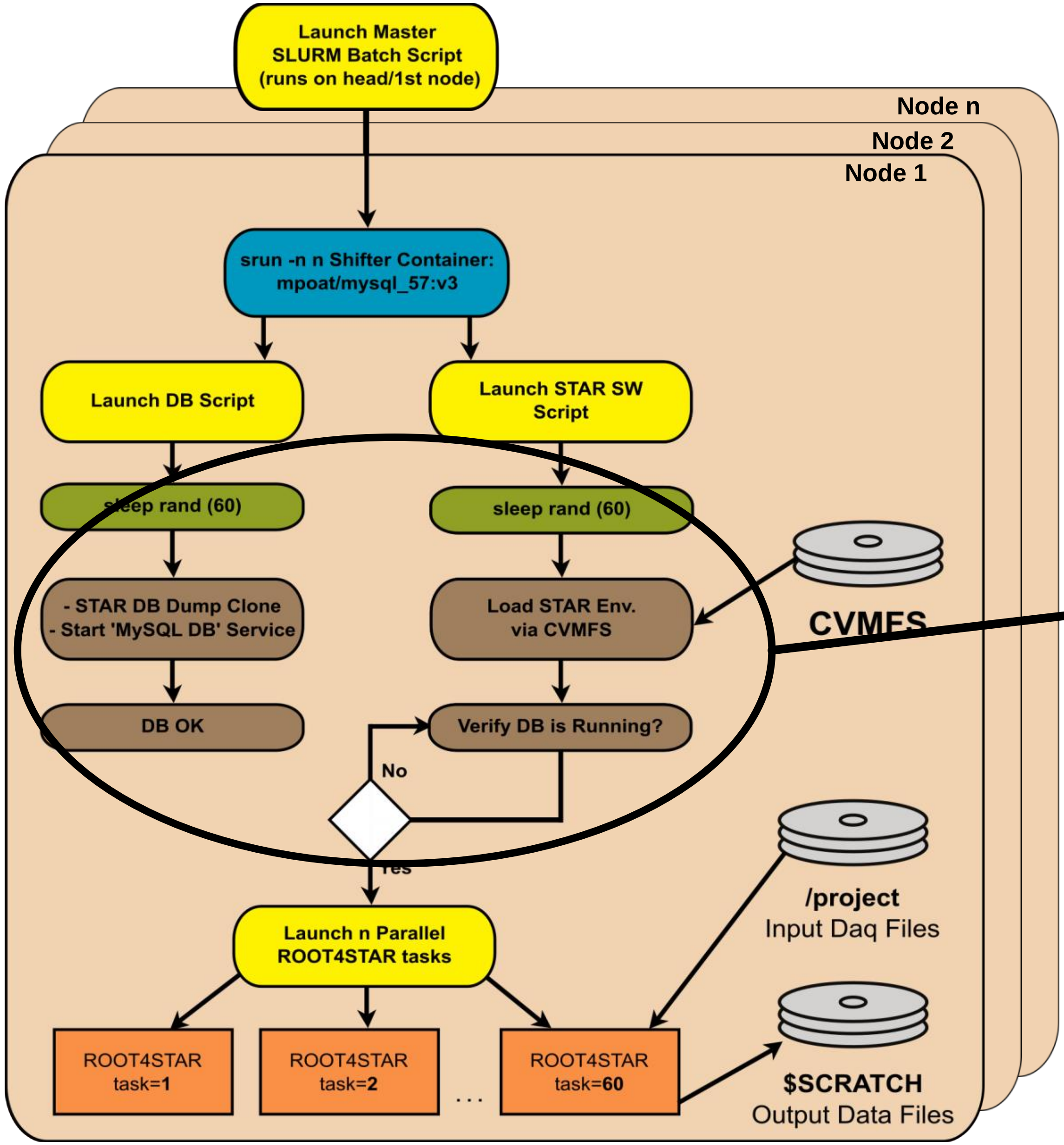
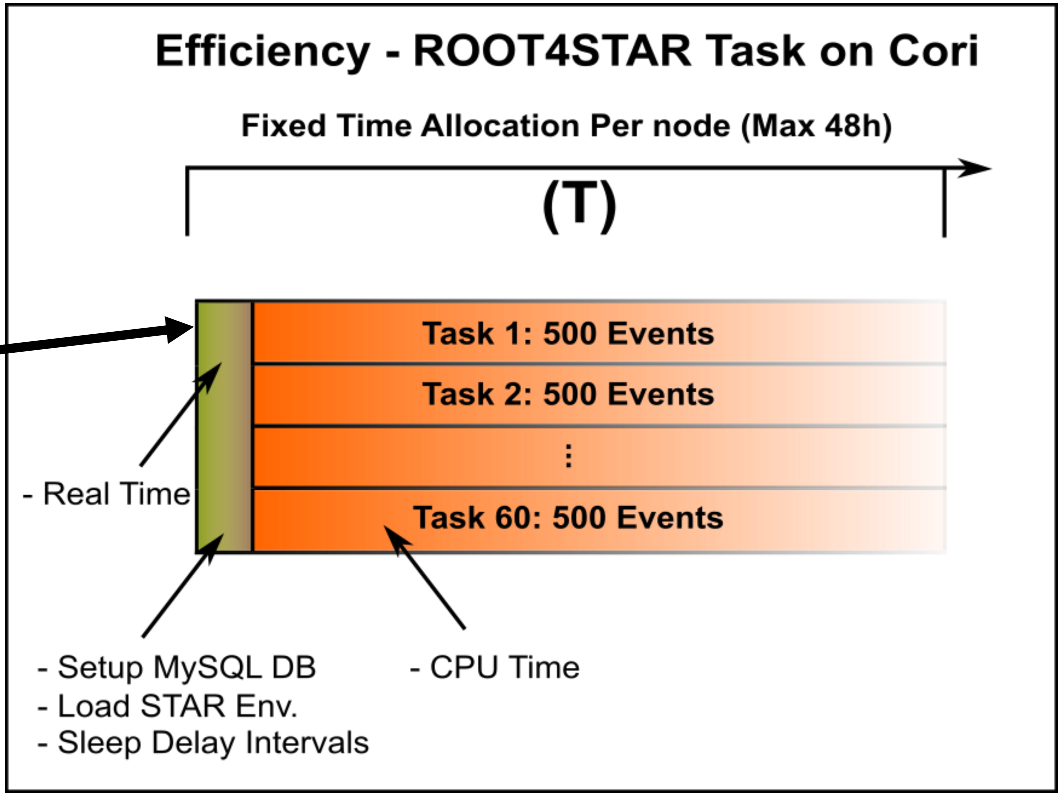
- Node(s) will launch 'n' Parallel ROOT4STAR tasks



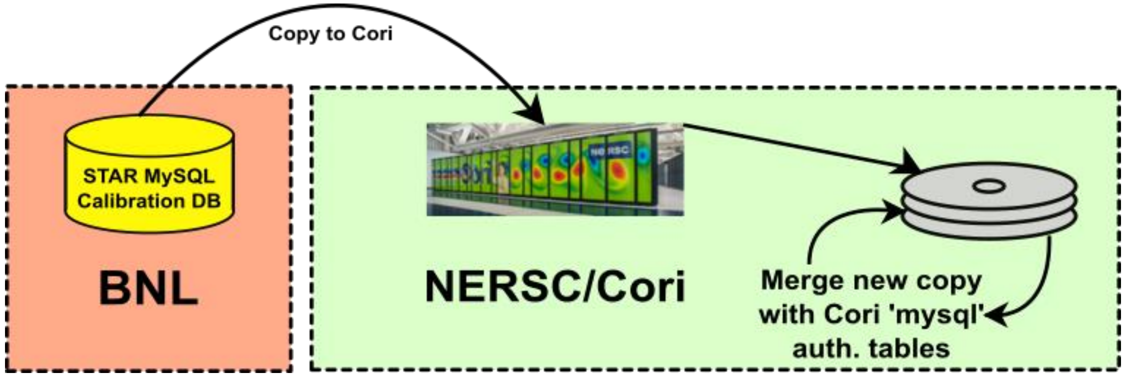
Job start efficiency loss



Database Server on Cori Batch Nodes

MySQL Database Access is required for the STAR Software to run

- STAR does have public facing DB servers that do scale, but Cori worker nodes are on an internal network.
- Hours old snapshots of the DB can be copied to run locally on Cori at anytime
- Once copied, a Cori authentication table is merged with the new DB and we are ready to run



STAR DB copied from BNL to NERSC/CORI

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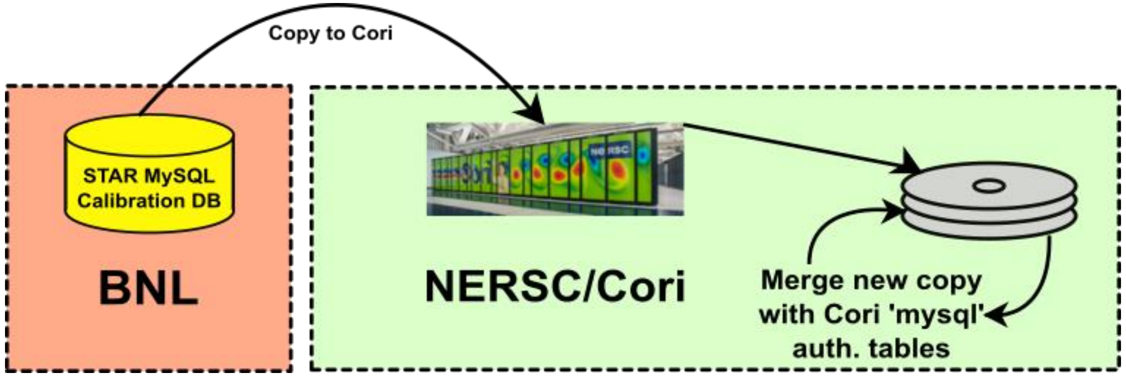


STAR DB copied from BNL to NERSC/CORI

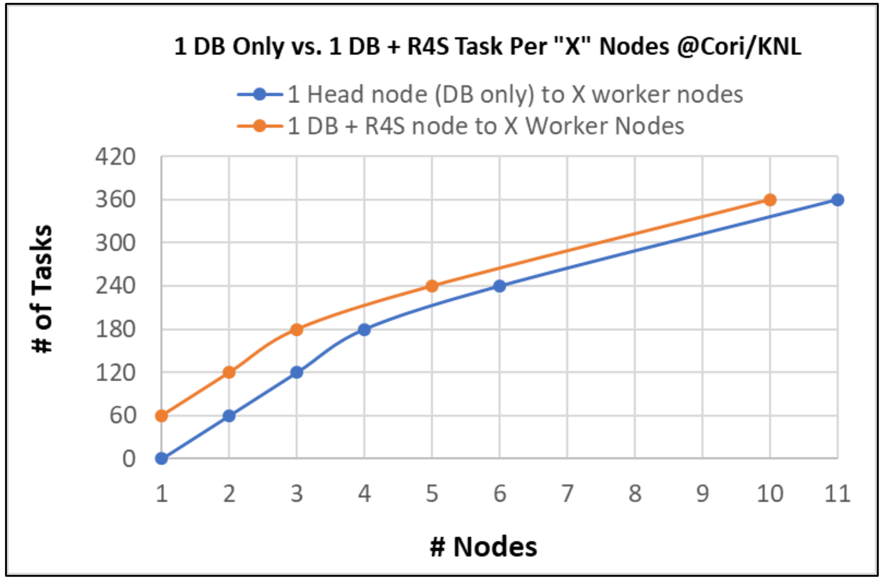
How we run the DB

- In the past, we would dedicate 1 head node on Cori to run the STAR Database serving **X** worker nodes
- We now have our ‘mysqld’ DB server installed in the same docker container running the STAR Software on Cori -> each node serving itself

Can worker node running DB + R4S tasks serve DB to itself & other worker nodes?

- With configuration tuning a worker node can run DB + R4S tasks to serve itself & 10s of other worker nodes
  - Default configuration DB could only handle 150 connections
- ‘Head node’ model sacrifices an entire node

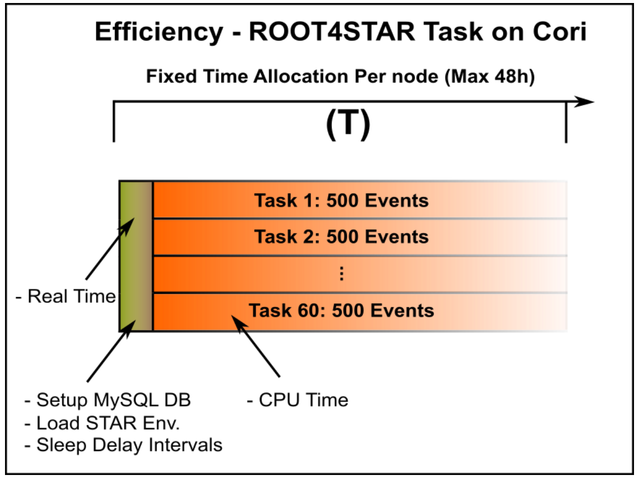
How does this affect our efficiency…?



Efficiency on Cori

Efficiency on Cori

- **<u>Job Start Efficiency</u>:** Real time to copy/start DB, load env., sleep delays **(E1)**
- **<u>Event Efficiency</u>:** CPU/Real time ratio for STAR event data reconstruction **(E2)**
- **<u>Total Efficiency</u>:** SLURM job Start ->Last Task Finished (NodesUsed/NodesUnused) * E1 * E2



Efficiency on Cori

Goal: Maximize (event per sec. / per $)

- NERSC charges the same for KNL or Haswell
- Dedicating 1 head node as DB only to serve 10 worker nodes (1-to-11) **VS.** (1-to 1) model (each worker node self-serves DB)
  - 1-to-1 model: Total Eff. 99.30%
  - 1-to-11 model: Total Eff. 89.44%
  - **Better to self-serve DB**
- Job Start Efficiency: we lose ~.05%
- Event Efficiency: ~98-99%
  big job = highest value
- Total Efficiency on 1-to-1 KNL/Haswell, and BNL BCF: ~98-99%
- Total vCore Utilization:
  - Haswell: 87% @ 60 task + 1 DB
  - KNL: 36.9% @ 100 task + 1 DB
  - Cannot maximize CPU util. due to memory limit -> **Best to focus on packing best # of tasks per/node & Total Efficiency**

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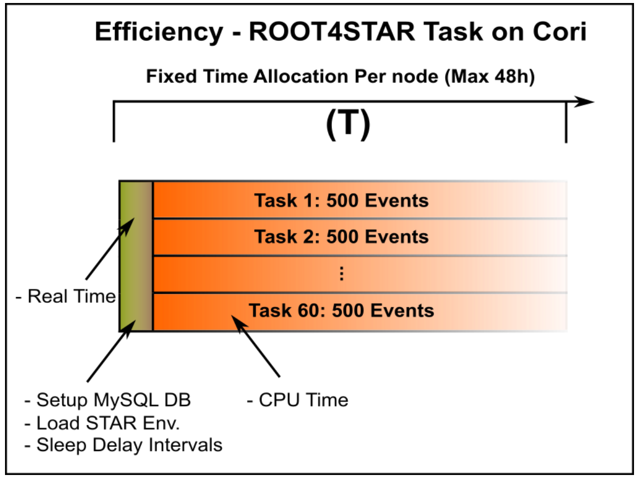
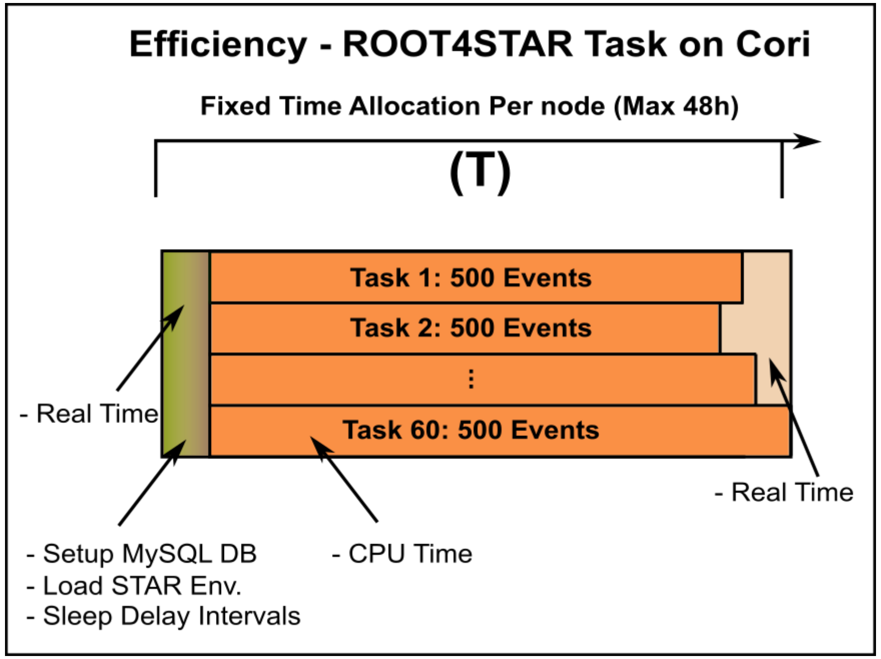


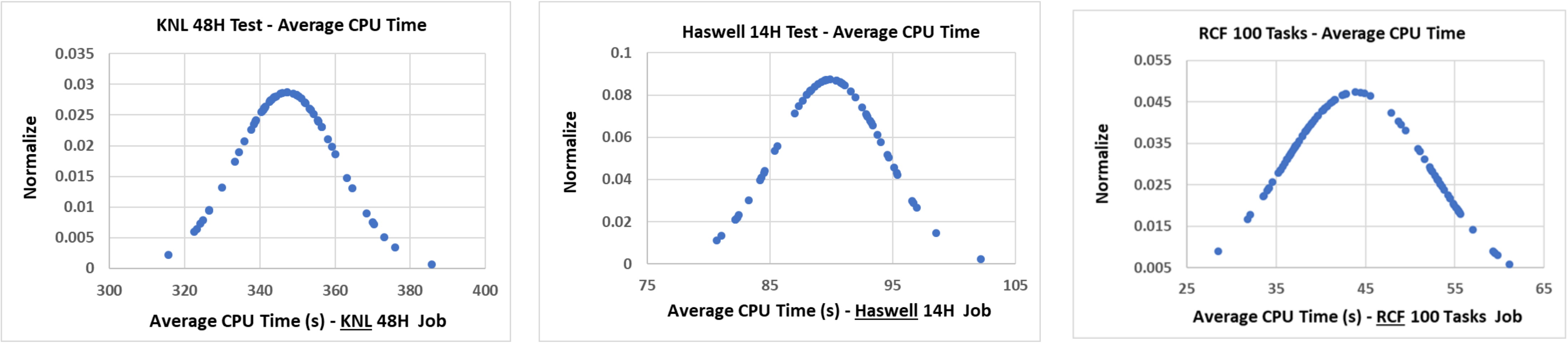
Job	(T) DB dump, Load Env., Rand (1-60s) delays	Job Start Efficiency (Total Job Time - (T))/Total Job Time (E1)	Event Efficiency All Events (E2)	Total Efficiency (NodesUsed/Nodes Unused) * E1 * E2
KNL 1 Node (Long Test - 60 task)	819 sec.	99.50%	99.79%	**99.30%**
KNL 11 Nodes 1 Node ded. DB server (60 task)	864 sec.	99.48%	99.90%	**89.44%**
Haswell 1 Node (Long Test - 60 task)	378 sec.	99.76%	99.04%	**98.80%**
BNL RCF Job - 100 tasks	1 sec.	99.99%	99.81%	**98.82%**

Idle CPU Problem

- When a job is submitted with multiple tasks, each task will finish at different times.
- If no new task is assigned, the CPU will sit idle
  - You pay for the total time of the longest running task
- If we push the tasks to run past the 48h time limit, **and** if it does not finish gracefully = Data not easily usable
- Average Idle CPU Loss at end of ~48h job
  - KNL: 0.02% CPU Time Loss
  - Haswell: 0.01% CPU Time Loss
- To Fix this "Problem" we need
  - A "Throughput Estimator" to estimate how long a job will take
  - "Signal Handling" to ensure a task can be "soft killed" properly with no data loss
  - An "Event Service" to launch new tasks
    - "Event Service" would also serve to launch new tasks with low events to maximize 48h time slot



Throughput Estimator



- Due to the ‘Job Start’ efficiency loss, it is best to run for the maximum amount of time (48h)
- By obtaining the average time events are processed per task, we can estimate how long a job will take
  - Multiple tests run on a single **KNL** node**,** a single **Haswell** node**,** & **BNL RCF (2.8GHz Intel)**
- The distribution and scaling is very predictable between the systems on any dataset
  - With the estimator, we only need to run a small batch of jobs on our BNL RCF farm to get estimate of total time on Cori KNL/Haswell
- **Provides starting point for “Event Service” to launch new tasks when one finishes**

Conclusion

- **Database:**
  - DB can be copied to NERSC on demand and remerged with authentication tables
  - On Cori: Worker node running 'mysqld' DB instance + R4S tasks to self-serve & serve DB connections to some worker nodes -> most efficient model
- **Workflow:**
  - Launch DB & environment scripts in parallel
  - DVS for CVMFS is a workable solution but required us to implement time delays (latency)
- **Efficiency:**
  - Events produced min/node:
    - **Haswell**: **40.55 total events per min** (60 tasks total)
    - **KNL: 13.7 total events per min** (100 task per node)
  - Head node model introduces biggest efficiency % loss
  - Haswell provides best CPU power / $ for us

Our next steps

- Ensure graceful termination of the tasks (use of "signal handling")
- Potential use of Burst Buffer to pre-stage DB content
- "Event Service" is coming soon
- Efficiency loss at start & end of job is minimal -> acceptable range

Thanks!

Summary Slide

- Docker/CVMFS
  - Containers are kept to minimum -> SL7 + RPM + mysqld
  - Software provisioned from CVMFS via DVS servers on Cori
- DB Access
  - STAR DB snapshot dumped at Cori, remerged with auth tables, then run in container to serve STAR tasks
  - Each node on Cori can run its own copy of DB + ROOT4STAR tasks & serve other worker nodes
  - Burst Buffer may be a solution to pre-stage DB copies before start of job
- Workflow: Maximize our “Job Start Efficiency” with parallel setup scripts
  - Delays for DB dump and loading software via CVMFS -> needed to not overload subsystems
- Efficiency: “Job Start Efficiency” and “Idle CPU Problem” have minimal impacts on “Total CPU/Real time Efficiency” if we run for maximize node allocation (48h)
- Places where we lose CPU time are understood – solutions underway
- Total CPU/Real time Efficiency on Cori with 1-to-1 DB model: **~98-99%**