Extreme I/O on HPC for HEP using the Burst Buffer at NERSC

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HEP Centre for Computing Excellence
Outline

• Introduction to NERSC and our ‘Burst Buffer’
  – Hardware and Software Architecture

• HEP Use Cases
  – ALICE
  – ATLAS
  – Tractor (DESI)
  – H5Boss

• Conclusions
NERSC and Cori

• NERSC at LBL, production HPC center for US Dept. of Energy
  – >7000 diverse users across science domains including many outside HEP

• Cori – NERSCs Newest Supercomputer – Cray XC40
  – Phase 1 (available Nov 2015): 1630 Intel Haswell dual 16-core nodes 128 GB
  – Phase 2 (becoming available now): >9,300 Intel Knights Landing nodes

• Cray Aries high-speed “dragonfly” topology interconnect

• Lustre Filesystem: 27 PB; 248 OSTs; 700 GB/s peak performance.
Burst Buffer Concepts

- HDD performance not increasing sufficiently
  - HPC centers buying large capacity parallel filesystems to get bandwidth
  - Huge POSIX filesystems don’t scale
  - Actual bandwidth demands comes in ‘bursts’
  - For bandwidth SSD is cheaper than HDD
- Some applications (including experimental HEP) have I/O patterns that better match SSD than disk
- Use NVRAM-based ‘Burst Buffer’ (BB) as intermediate layer
  - Handle I/O spikes without a huge PFS (stage to PFS asynchronously)
  - Underlying media supports challenging I/O
  - Software for filesystems- on-demand - scales better than large POSIX PFS
Nersc Burst Buffer Architecture

Blade = 2x Burst Buffer Node: 4 Intel P3608 3.2 TB SSDs

I/O Node (2x InfiniBand HCA)

Phase 1:
920TB on 144 BB nodes
Now being doubled for Phase 2

Burst Buffer Blade:

Aries High-Speed Network

InfiniBand Fabric

Storage Fabric (InfiniBand)

Storage Servers

Lustre OSSs/OSTs
Software

- Cray *DataWarp* software (integrated with SLURM WLM) allocates storage to users per-job (or ‘persistent’ for multiple jobs)
- Users see a POSIX filesystem on-demand, striped across nodes
- Can specify data to stage in/out from Lustre while job is in queue
- Benchmark Results with IOR - 140 BB Nodes
  - 1120 Compute nodes: 4 ranks/node
  - Bandwidth: 8 GB block-size 1MB transfers
  - IOPS tests: 1M blocks 4k transfer

<table>
<thead>
<tr>
<th>IOR Posix FPP</th>
<th>IOPS</th>
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<tbody>
<tr>
<td>Read</td>
<td>Write</td>
</tr>
<tr>
<td>Peak</td>
<td>905 GB/s</td>
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HEP Use Cases

See also Cray Users Group Paper for more use-cases beyond HEP
ALICE

• I/O intensive analysis:
  – Running on ESDs: Events after reconstruction
  – Minimal compute – fill histograms
  – Serial application

• Data: “Pb-Pb 2015 full reco pass”, 1 run
  – ~10 TB data, 16k files
  – 10 files per compute core

• 26TB BB – 126 servers

• CPU time/wall time > 90%
• CPU ‘idle time’ = wall – cpu
• Effective average ‘bandwidth’ data read / idle time per process

Markus Fasel, Jeff Porter
• **ATLAS now making use of HPC resources**
  – Running simulation – not I/O intensive workloads
  – Test here I/O heavy ‘derivation’ and analysis
• ‘Derivation’: filtering ‘xAOD’ ROOT-based format to analysis-specific files
  – Run in ATLAS ‘AthenaMP’ framework
• BB allocation 2TB to 20TB
• Faster read times on BB
  – ‘Bandwidth’ = data read / IO time measured via xAOD::ReadStats (TVirtualPerfStats)
Atlas Analysis

• ‘QuickAna’ ROOT/python app
• Initial study to improve read I/O
  – Poor initial BB performance
  – Increase ROOT ‘TTreeCache’ - 100M
  – Less reads -> 17x boost on BB
  – Also use ‘branch access’ and ‘learning pre-fill’
• Scales well to larger job sizes
  – 50TB dataset: 143 node BB allocation
Tractor and DESI

- Tractor: make 3D map of distribution of galaxies
  - Optical images ~1/3 of night sky. Telescopes at Kitt Peak, AZ and Cerro Tololo, Chile
  - Astro sources classified $\chi^2$-fit between models and images
  - Combined with source spectra from DESI to infer redshift and distance (2D -> 3D Map (2D image + distance using spectra))

- Python application
- Files in FITS format
- Runs 1 process / node with 32 threads
- 32 TB BB used in tests shown here
Tractor

• Detailed profiling:
  — strace, ipm and custom code
  — Plot here data moved by application via freads and fwrites
  — Actual I/O is greater due to prefetching by glibc

• I/O time dominated by metadata (inc. python loads)

• Variation on Lustre - maybe due to other user impact

Kaylan Burleigh, Chris Daley, Peter Nugent

32-node Lustre I/O call times
H5Boss

• BOSS Baryon Oscillation Spectroscopic Survey – from SDSS
• Perform typical randomly generated query to extract small amount of stars/galaxies from millions
• Workflows involve 1000s of file open/close and random and small read/write I/O
• Run on final release of SDSS-III complete BOSS dataset
  – 2393 HDF5 files - total ~3.2TB

• 4.4 TB Burst Buffer - 22 nodes
• Lower I/O times on Burst Buffer
• 5.5x speedup for entire workflow
Conclusions

• Burst Buffer – A new approach to dynamically allocate filesystems striped across high-performance SSDs
  – Now in production at NERSC

• Demonstrated here for experimental HEP Workflows
  – Substantially improves I/O over comparable Lustre filesystem
  – Variety of use-cases from NP, HEP, Cosmology

• I/O is not (now) a significant barrier to these projects
  – Can run their most I/O intensive workflows on Cori

• Further improvements to performance and usability of NERSC Burst Buffer coming soon...
Extra slides: for those who just can’t get enough
Coming performance improvements

1. DVS client-side caching
   • Lustre has client-side caching, currently DVS (used for BB) does not
   • Essential for small sequential Read/Write transfers and re-reads
   • Expected later this year

2. Smaller granularity
   • Amount of space allocated on each BB node
     – Previously couldn’t be less than 200G
     – Users had to request larger space to get striped performance
     – Now have the ability to reduce this – testing lower values

3. Transparent caching
   • Allows user to specify directory in Lustre and blocks are cached as used
   • Software now available - but undergoing testing

4. Twice as much Burst Buffer! (and therefore ~2x bandwidth!)

Working with Cray to improve BB performance out-of-the-box for all use-cases
Burst Buffer Blade = 2xNodes

3.2 TB Intel P3608 SSD
3.2 TB Intel P3608 SSD
3.2 TB Intel P3608 SSD
3.2 TB Intel P3608 SSD

PCle Gen3 8x
PCle Gen3 8x
PCle Gen3 8x
PCle Gen3 8x

Xeon E5 v1
Xeon E5 v1

Aries

To HSN
DataWarp Filesystem layers

• Logical Volume Manager (LVM) group SSDs into one block device
• An XFS file system that is created for every Burst Buffer allocation
• Cray Data Virtualization Service (DVS), for communication between DWFS and the compute nodes.
• File written from compute node ends up as (configurable) 8MB chunks, laid out across the three (configurable) substripes on the Burst Buffer node.
Integrated with SLURM WLM

#!/bin/bash
#SBATCH -p regular -N 10 -t 00:10:00
#DW jobdw capacity=1000GB access_mode=striped type=scratch
#DW stage_in source=/lustre/inputs destination=$DW_JOB_STRIPED/inputs type=directory
#DW stage_in source=/lustre/file.dat destination=$DW_JOB_STRIPED/ type=file
#DW stage_out source=$DW_JOB_STRIPED/outputs destination=/lustre/outputs type=directory
srun my.x --indir=$DW_JOB_STRIPED/inputs --infile=$DW_JOB_STRIPED/file.dat \
   --outdir=$DW_JOB_STRIPED/outputs

Example illustrates:

– ‘type=scratch’ duration just for compute job (not ‘persistent’)
– ‘access_mode=striped’ – visible to all compute nodes (not ‘private’) and striped across multiple BB nodes
  • Actual distribution across BB Nodes is in units of (configurable) granularity (currently 218 GB at NERSC so 1000 GB would normally be placed on 5 BB nodes)
– Data stage_in before job start and out after
Burst Buffer Software

Non-recurring Engineering (NRE) arrangement with Cray (and SchedMD for SLURM WLM integration). Software in Stages:

Stage 0

Static mapping of compute to BB node, manual data migration

Stage 1

Striping, per-job and persistent allocations; staging; WLM Integration

Stage 2

Transparent caching mode

Stage 3

In-transit processing and filtering

we are here
• Nyx cosmological simulation code based on a widely-used adaptive mesh refinement (AMR) library, BoxLib
• Large data files ("plotfiles") written at certain time steps; checkpoint files also written
• Burst Buffer offers I/O
Nyx/Boxlib – Single BB Node

• Need larger transfer size for good performance
  – Less of an issue on Lustre
  – No client-side cache in DVS/DataWarp
Nyx/Boxlib – Single BB Node

- Need larger transfer size for good performance
- More MPI writers (~16) to approach 4 GB/s
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• Maximize bandwidth per compute node by adding more BB nodes until 1/1 CN/BB ratio
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• 32 CN nodes starts to outperform Lustre
ATLAS: Simulation Payload

- Initial scaling on BB poor
- Increase ROOT ‘basket size’ from 2k to 512k to increase transaction size
- Keep log files on Lustre
- Then scales to >300 nodes
H5Boss

• Typically produce a single FITS data file per object observed
  – Millions of files now -> Hundreds of millions in future

• This project uses instead a HDF5 data structure:
  – Improve small file metadata problems
  – Allow parallel access via HDF5 IO libraries.

• H5boss – python package: parses query, opens source HDF5 files, uses ‘subset’ function to create single shared output HDF5 file
  – Perform two independent copies – whole fiber including wavelength and exposures; only specific two in catalog