Trillion Particles, 120,000 cores, and 350 TBs: Lessons Learned from a Hero I/O Run on Hopper

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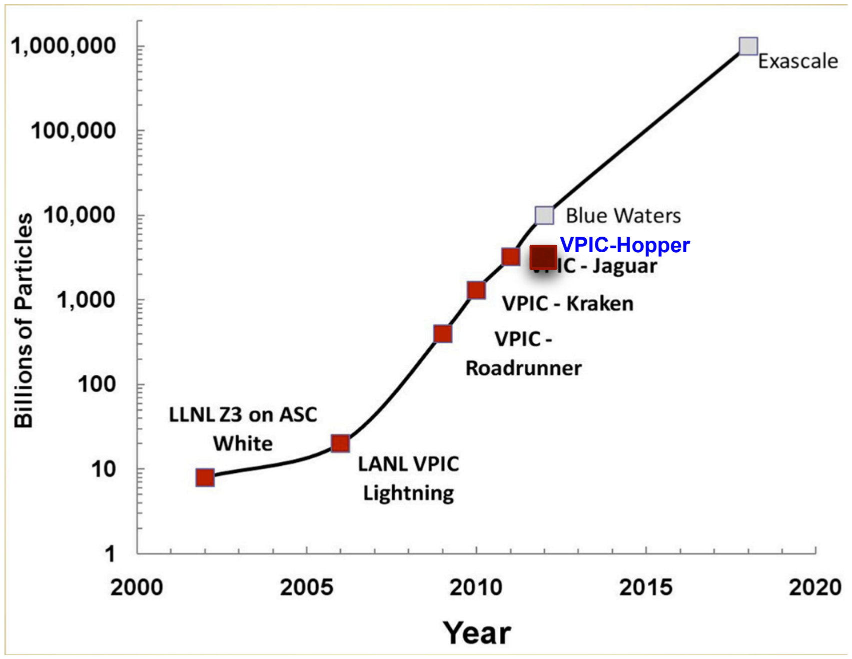
The application: Vector Particle-in-Cell (VPIC) Simulation

- ✧ A state-of-the-art 3D electromagnetic relativistic PIC plasma physics simulation
- ✧ It is an exascale problem and scales well on large systems
- ✧ An open boundary VPIC simulation of magnetic reconnection (Space weather)

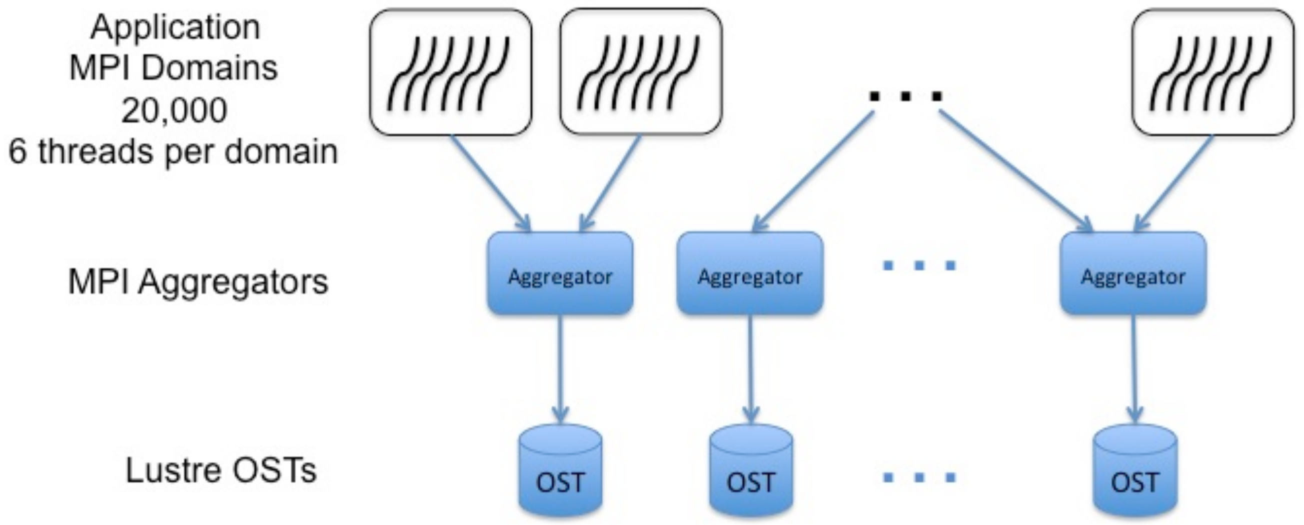


- ✧ NERSC Hopper Supercomputer
  - ○ 6,384 compute nodes; 2 twelve-core AMD 'MagnyCours' 2.1-GHz processors per node; 32 GB DDR3 1333-MHz memory per node; Interconnect with a 3D torus topology
  - ○ Lustre parallel file system with 156 OSTs at a peak BW of 35 GB/s

The application: Vector Particle-in-Cell (VPIC) Simulation

- March 1989: A power blackout in Canada affected 6 million people.
- October-November 2003: Solar panels fail on the $450 million Midori 2 research satellite, and astronauts take cover in the International Space Station.
- June 2011: Airlines report disruption of high-frequency radio communications near the Arctic.

VPIC Trillion Particle Simulation setup



- 20,000 MPI processes (MPI domains) using 120,000 cores
- Each MPI process writes ~51 Million (±15%) particles
- Each particle has 8 variables
- Lustre-aware MPI-IO implementation
  - ✓ MPI collective buffer size is equal to the stripe size
  - ✓ Number of MPI aggregators is equal to the stripe count
- **Particle dataset size varies (30TB to 43TB) per time step – A total of 350 TB data + 150 TB checkpoint data**

Data Challenges

- ✧ What is a scalable I/O strategy for storing massive particle data output?
  - o In situ analysis works well when analysis tasks are known *a priori*
  - o Many scientific applications require to store data for exploratory analysis
- ✧ What is a scalable strategy for conducting analysis on these datasets?
  - o Sift through large amounts of data looking for useful information
- ✧ What is the visualization strategy for examining the datasets?
  - o Display information that makes sense

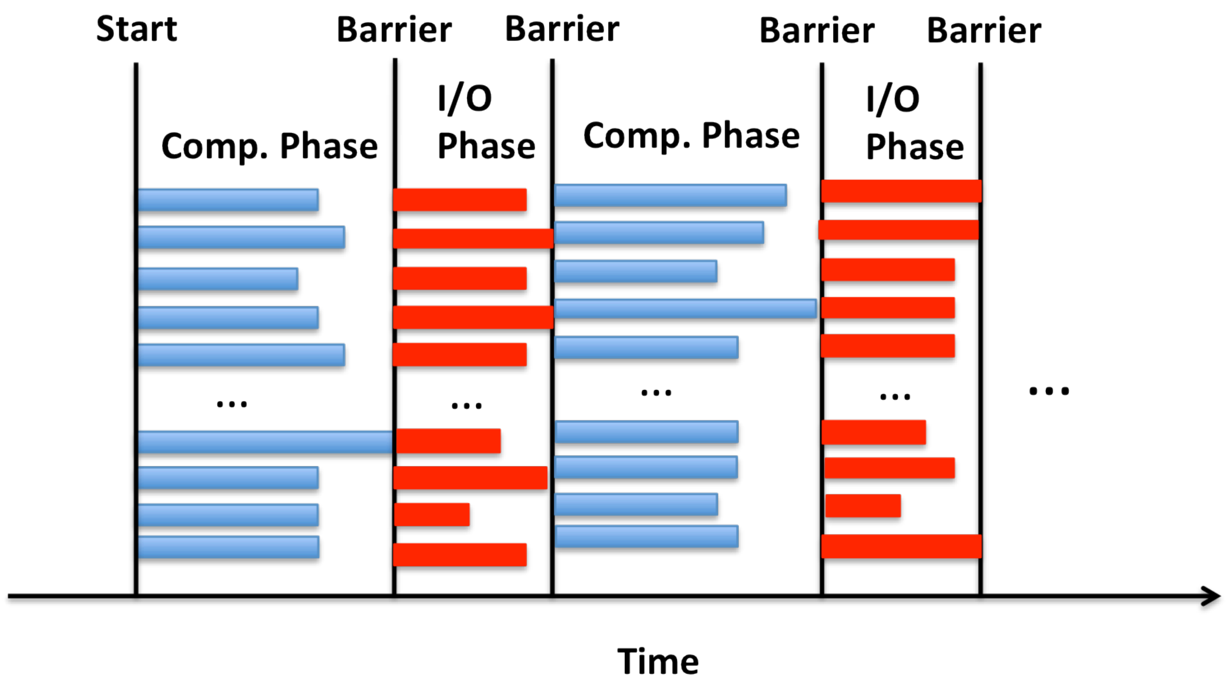
Expected challenges in running the application

- Scheduling a large job that would take ~80% of compute nodes
  - Queue time may be longer
  - Thanks to reg_xbig queue, which is turned on at 9PM on Fridays
- Lustre file system may be stressed due to large volume of data produced
- But…
  - There were a few more lessons we learned

Lessons Learned

1. Collective writes to a single shared HDF5 file can work as well as file-per-process writes
2. Tuning multiple layers of parallel I/O subsystem is a challenging task
3. Advance verification of file system hardware is important for obtaining peak performance
4. Advance verification of available resources for memory-intensive applications is important
5. Scalable tools are required for diagnosing software and hardware problems before running applications using 100k cores

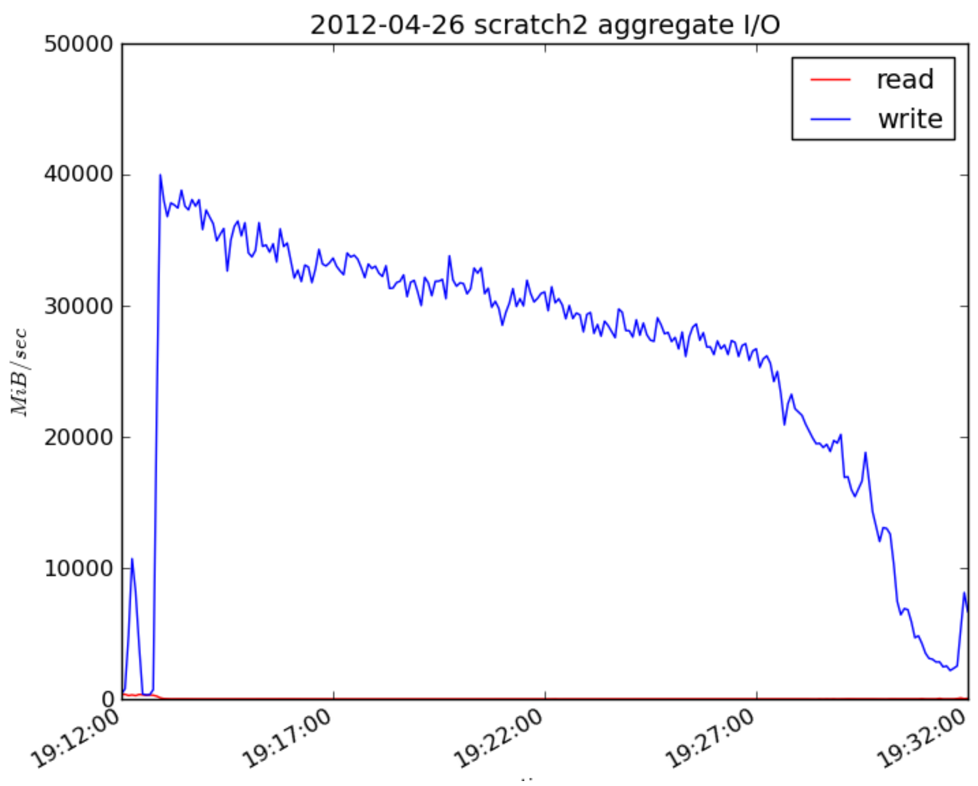
Lesson 1: Parallel HDF5 works – I/O pattern



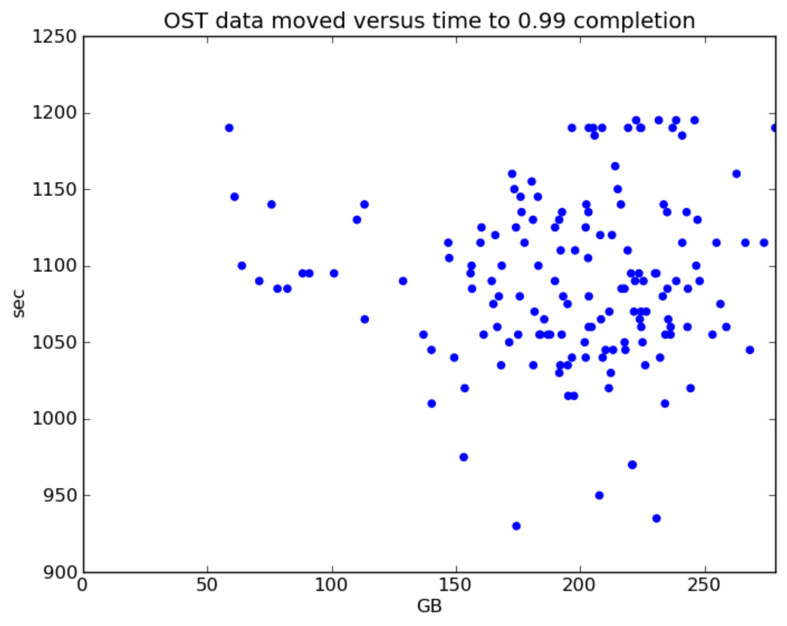
- I/O of VPIC follows a banded pattern
- Two file writing strategies
  - File per process model
  - Shared file with HDF5 and H5Part

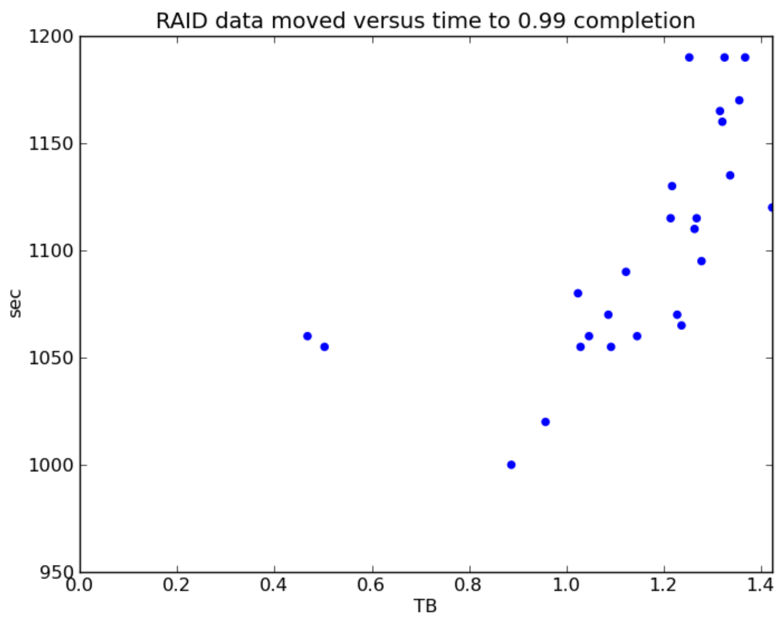
Lesson 1: Parallel HDF5 works – File-per-process

- Performance of 20,000 files with a combined size of ~30TB
- Lustre Monitoring Tool
- Load imbalance and the last OST finishing writing dictate performance
- I/O rate: 27,007 MB/s



Lesson 1: Parallel HDF5 works – File-per-process





- Uneven load leads to uneven completion times
- Problems with file per process model
  - Too many files – 20,000 files per time step in our case
  - Dictates the concurrency of subsequent stages in the analysis pipeline
  - Many data management and visualization tools only support standard data formats, such as HDF5 and NetCDF

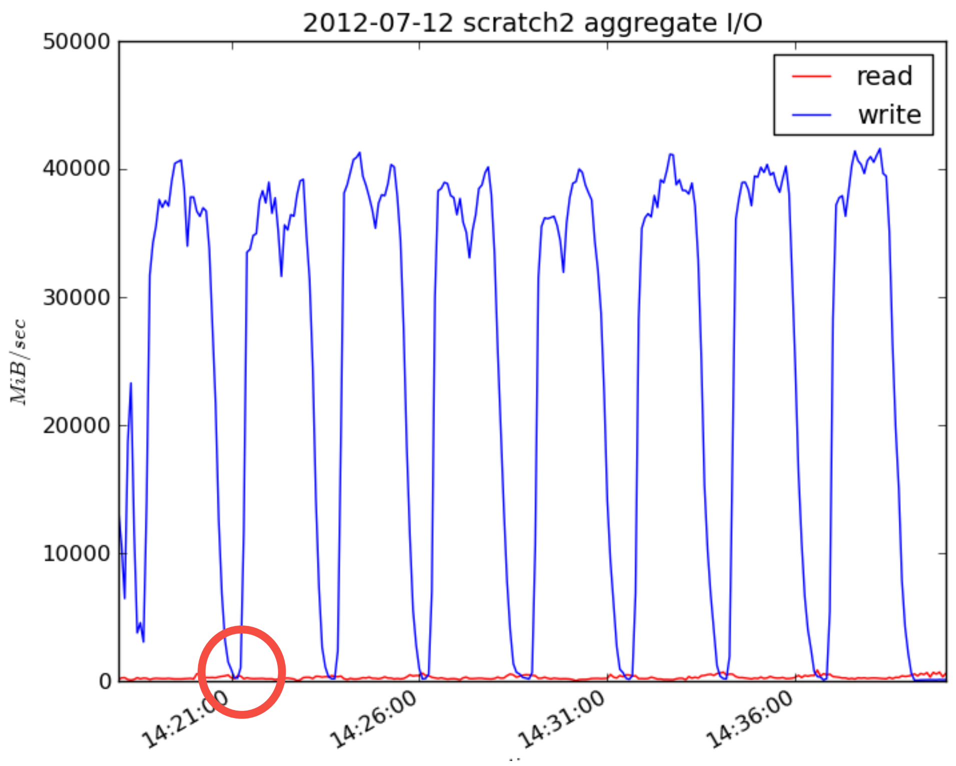
Lesson 1: Parallel HDF5 works – HDF5 and H5Part

```
h5pf = H5PartOpenFileParallel (fname, H5PART_WRITE |
                         H5PART_FS_LUSTRE, MPI_COMM_WORLD);
H5PartSetStep (h5pf, step);
H5PartSetNumParticlesStrided (h5pf, np_local, 8);

H5PartWriteDataFloat32 (h5pf, "dX", Pf);
H5PartWriteDataFloat32 (h5pf, "dY", Pf+1);
H5PartWriteDataFloat32 (h5pf, "dZ", Pf+2);
H5PartWriteDataInt32   (h5pf, "i",  Pi+3);
H5PartWriteDataFloat32 (h5pf, "Ux", Pf+4);
H5PartWriteDataFloat32 (h5pf, "Uy", Pf+5);
H5PartWriteDataFloat32 (h5pf, "Uz", Pf+6);
H5PartWriteDataFloat32 (h5pf, "q", Pf+7);

H5PartCloseFile (h5pf);
```

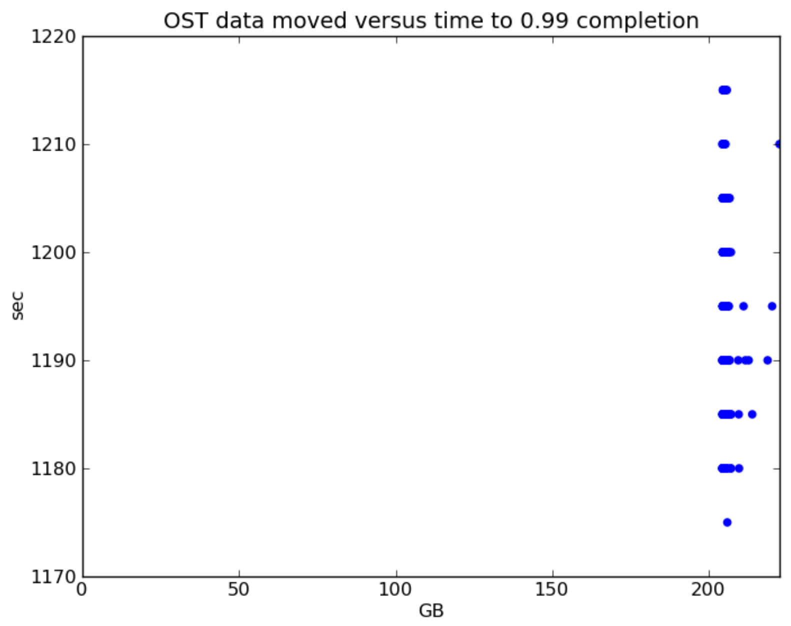
http://vis.lbl.gov/Research/H5Part/

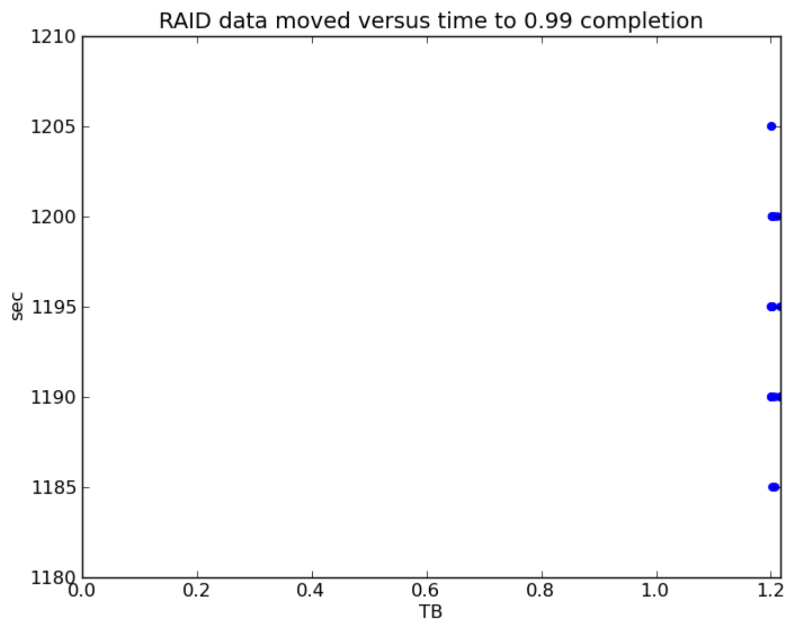
Lesson 1: Parallel HDF5 works – HDF5 and H5Part

- Performance of writing one ~31 TB particle file
- I/O rate: 27,035 MB/s
- Need for rendezvous after writing each variable, due to H5Part and HDF5 interactions



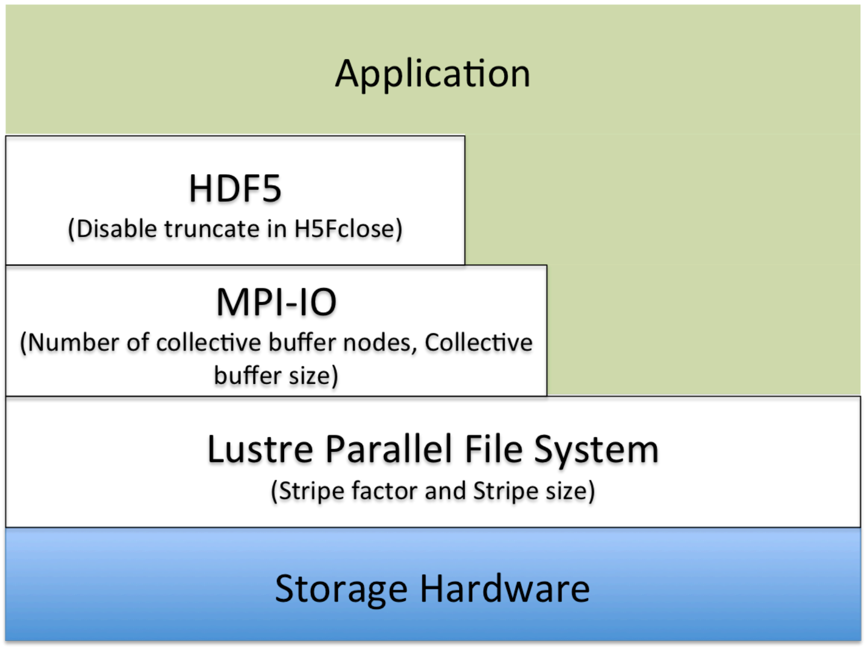
Lesson 1: Parallel HDF5 works – Load balance





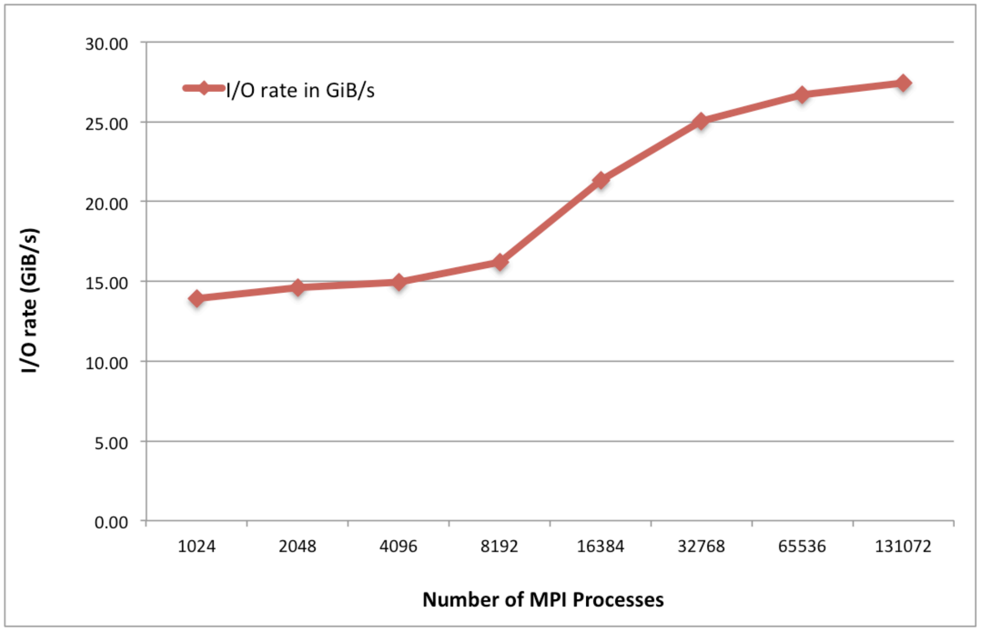
- Uniform load across the 156 OSTs and the RAIDs
- Some variability due to collective operations after each variable dump
- Overall, I/O performance of parallel HDF5 compares favorably with that of file-per-process
- HDF5 and Lustre performance was not automatic, but needed some tuning

Lesson 2: Tuning parallel I/O is a challenge, but not impossible – I/O Stack


Application
HDF5
(Disable truncate in H5Fclose)
MPI-IO
(Number of collective buffer nodes, Collective buffer size)
Lustre Parallel File System
(Stripe factor and Stripe size)
Storage Hardware

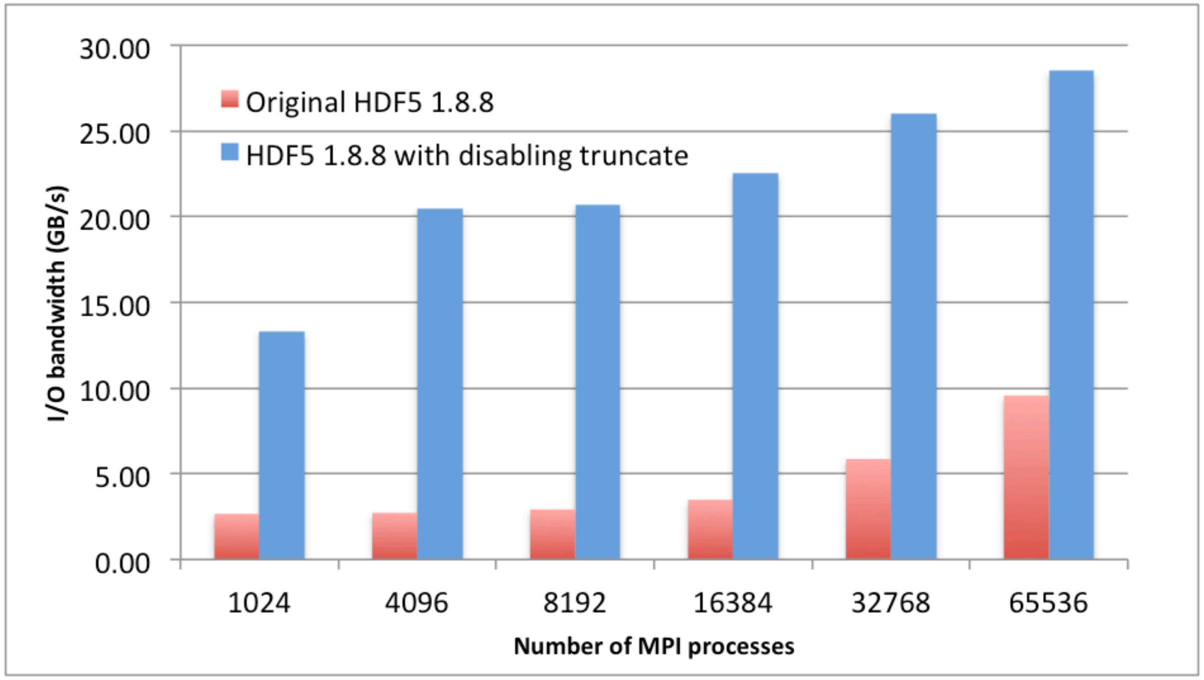
- Layers of parallel I/O software stack offer various tunable parameters
- Finding the right tunable parameters is a challenge
- To search the parameter space, we extracted the I/O kernel of VPIC
  - VPIC-IOBench
  - Two versions: Uniform and non-uniform writes from each process

Lesson 2: Tuning parallel I/O is a challenge, but not impossible – Lustre and MPI-IO tuning



- Lustre stripe count and stripe size
  - Varied stripe count from 64 to 156 and stripe size from 1MB to 1GB
  - Chose stripe count of 144 and stripe size of 64MB
- Lustre-aware MPI-IO collective buffering on Hopper uses CB2 algorithm
  - Number of collective buffering aggregator nodes is equal to the stripe count
  - Size of collective buffer is equal to the stripe size

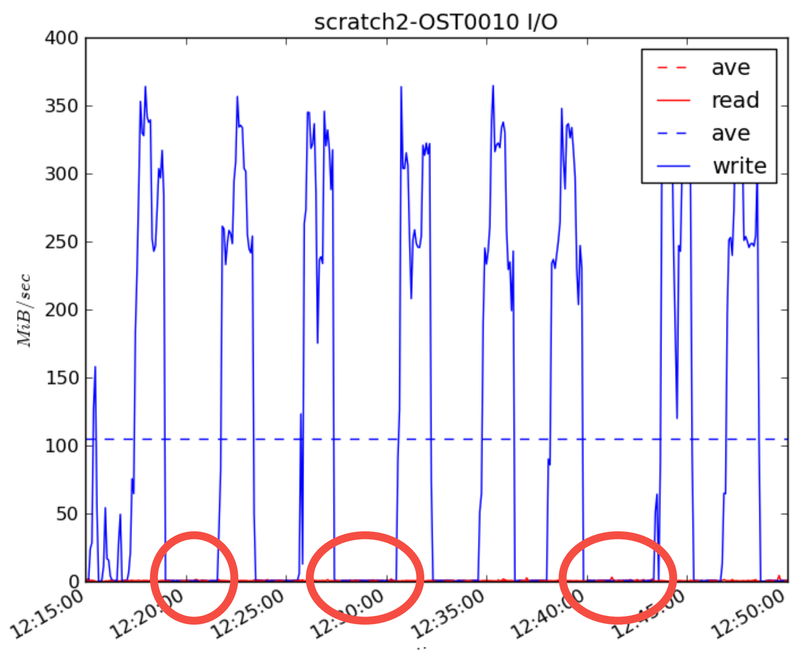
Lesson 2: Tuning parallel I/O is a challenge, but not impossible – HDF5 truncate

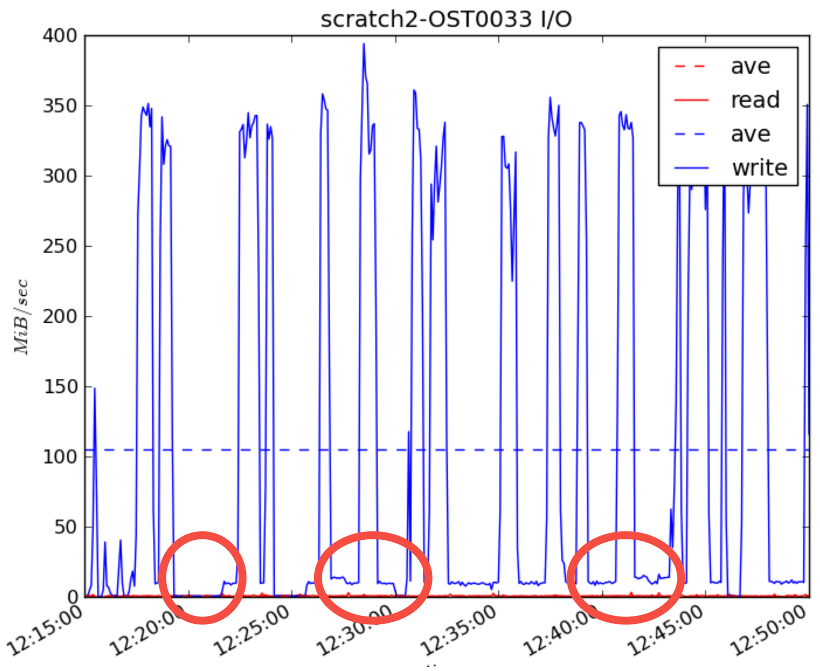


- HDF5 file close function verifies the size of the file matching with its allocated size to detect any external modification or corruption
- This is an expensive operation because of its collective nature
- Modified HDF5 to disable this "truncate" operation and achieved 3-5X performance improvement

Lesson 3: Advance verification of file system software is important – OSTs behaving badly

- Early runs obtained a 60% of peak bandwidth
- To achieve peak performance, each OST needs to be performing at 250 MB/s





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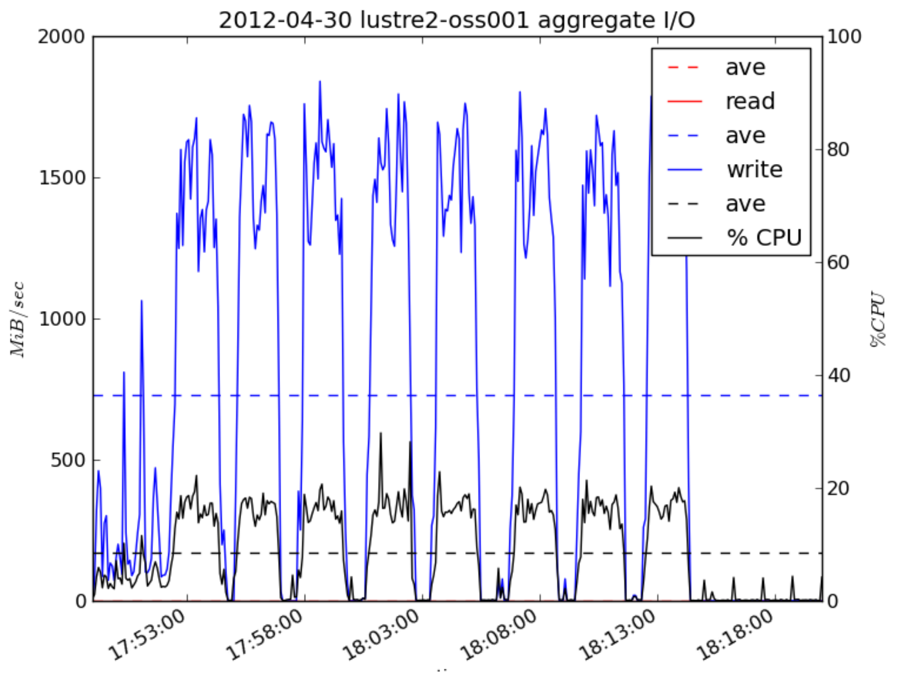

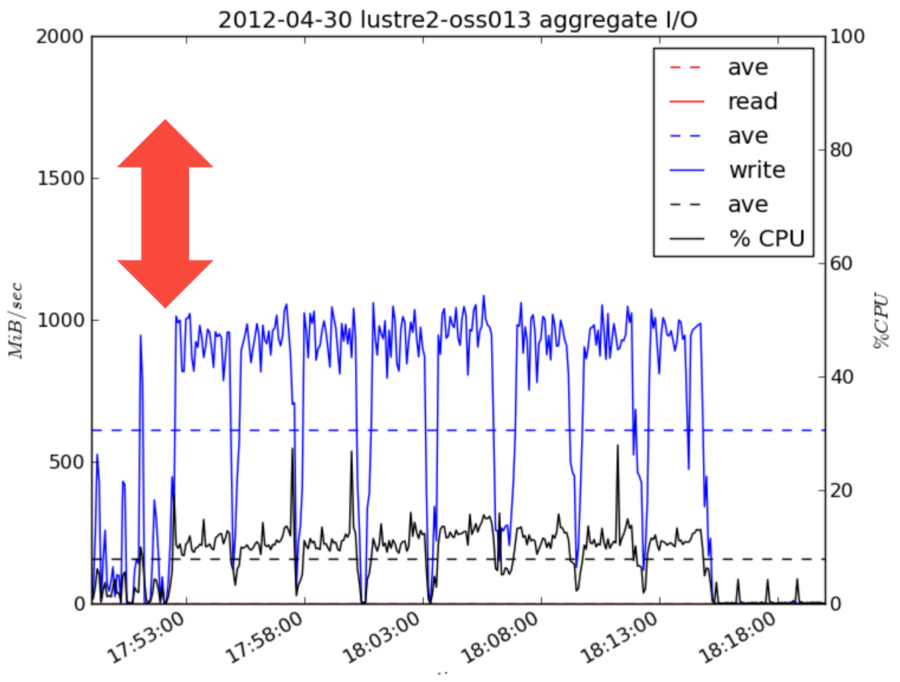

Lesson 4: Advance verification of resources for memory intensive apps is important

- On most nodes, Hopper has 32 GB memory
  - Some nodes have 64 GB
  - Total memory of 5,000 nodes: ~156 TB
- VPIC memory footprint is ~142 TB
  - Translates to ~29 TB on each node when the simulation uses 5,000 nodes
  - 90% of the memory on each node
- Considering some lightweight OS tasks running on the nodes, 90% of memory requirement puts significant pressure
- Experienced OOM error from one node crashing the application

Lesson 4: Advance verification of resources for memory intensive apps is important - Solution

- Used a combination of tools to verify memory availability before each run and after dumping large particle data
- Node Health Checker (NHC)
  - Free Memory Check to verify the available free memory
  - “Admindown” nodes with less than 29GB free memory
- Developed a Perl script that reads the free memory information from /proc/buddyinfo on all the nodes in allocation
  - Manually sorted and verified the free memory

Lesson 5: Scalable tools are required for diagnosing SW and HW problems

- It can be time consuming and tedious for a user to verify system health prior to a large run
- Scalable tools can help diagnosing the SW and HW problems
- Some tools exist, but need streamlining the process of verification
- Scalable computation and memory resource checker
  - With the help of Cray and NERSC staff, used NHC and “xtprocadmin” to verify the current status of nodes
  - Used NHC and local script to check memory status

Lesson 5: Scalable tools are required for diagnosing SW and HW problems

- Scalable I/O subsystem checker
  - Used manual I/O tuning to identify good set of optimization parameters
  - Our work in progress to identify tuned set of parameters at each layer of the parallel I/O stack
- Scalable Runtime I/O Monitor
  - Typically, many applications idle during I/O wasting CPU resources
  - Even one sluggish OST can increase the waste significantly
  - Lustre Monitoring Tool (LMT) was great; OSTs of bad behavior had to be found manually in postmortem – Any better and pro-active solutions??

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