Analyzing IO Usage Patterns of User Jobs to Improve Overall HPC System Efficiency

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SDSC SAN DIEGO SUPERCOMPUTER CENTER

UNIVERSITY OF CALIFORNIA

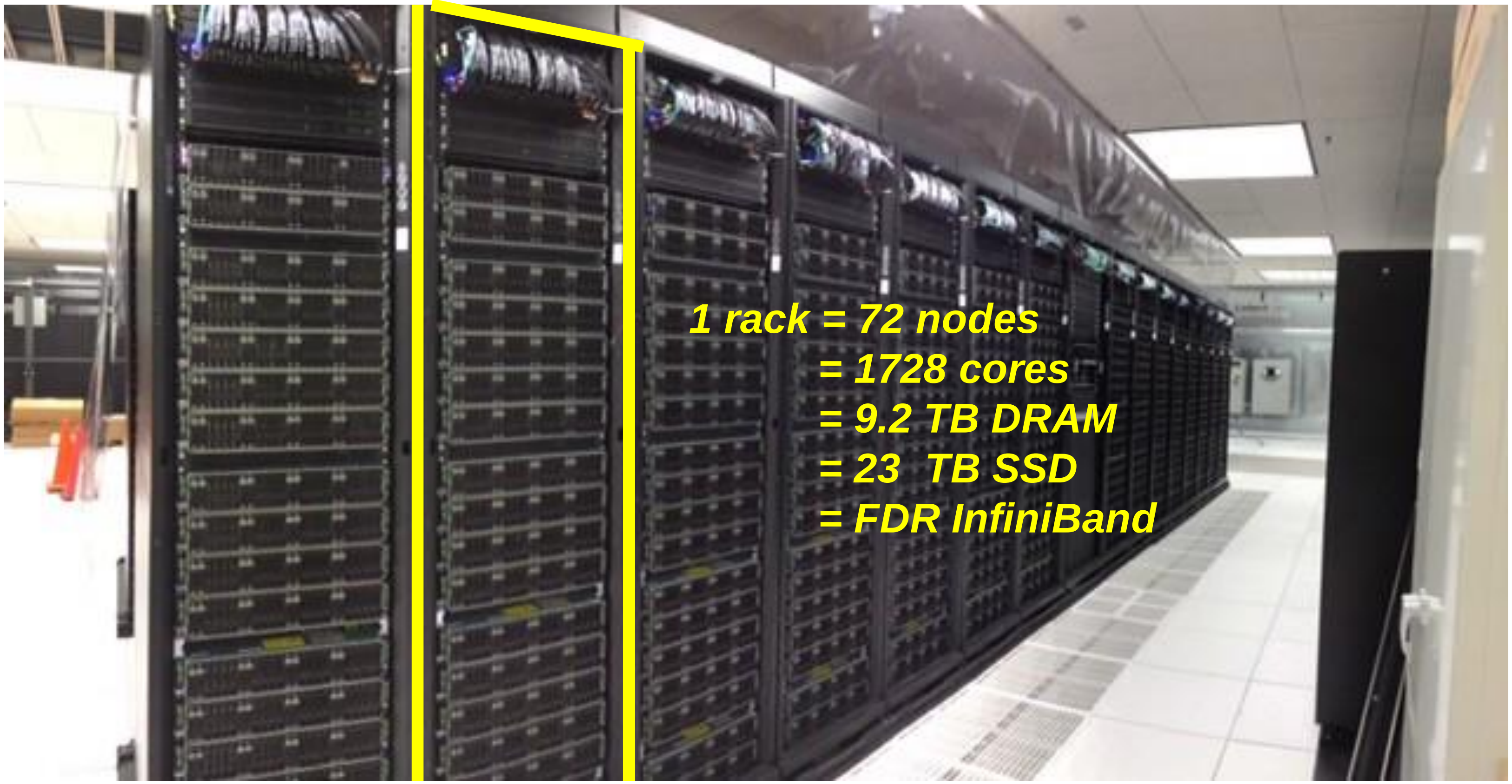
Comet
“HPC for the long tail of science”

iPhone panorama photograph of 1 of 2 server rows

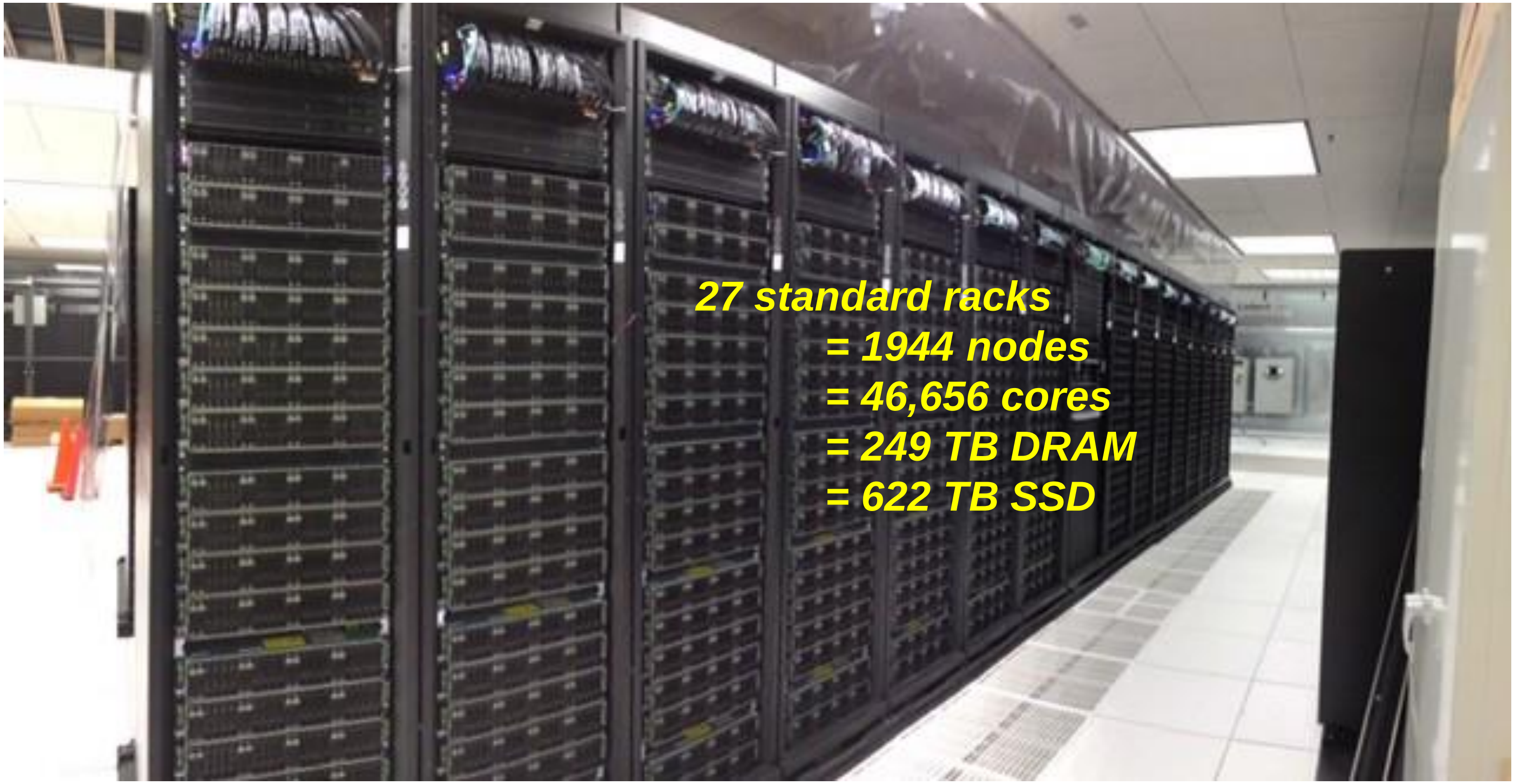
Comet: System Characteristics

- ***Total peak flops ~2.1 PF***
- ***Dell primary integrator***
  - *Intel Haswell processors w/ AVX2*
  - *Mellanox FDR InfiniBand*
- ***1,944 standard compute nodes (46,656 cores)***
  - *Dual CPUs, each 12-core, 2.5 GHz*
  - *128 GB DDR4 2133 MHz DRAM*
  - *2*160GB GB SSDs (local disk)*
- ***72 GPU nodes***
  - *36 nodes same as standard nodes plus Two NVIDIA K80 cards, each with dual Kepler3 GPUs*
  - *36 nodes with 2 14-core Intel Broadwell CPUs plus 4 NVIDIA P100 GPUs*
- ***4 large-memory nodes***
  - *1.5 TB DDR4 1866 MHz DRAM*
  - *Four Haswell processors/node*
  - *64 cores/node*
- ***Hybrid fat-tree topology***
  - *FDR (56 Gbps) InfiniBand*
  - *Rack-level (72 nodes, 1,728 cores) full bisection bandwidth*
  - *4:1 oversubscription cross-rack*
- ***Performance Storage (Aeon)***
  - *7.6 PB, 200 GB/s; Lustre*
  - *Scratch & Persistent Storage segments*
- ***Durable Storage (Aeon)***
  - *6 PB, 100 GB/s; Lustre*
  - *Automatic backups of critical data*
- ***Home directory storage***
- ***Gateway hosting nodes***
- ***Virtual image repository***
- ***100 Gbps external connectivity to Internet2 & ESNet***

~67 TF supercomputer in a rack

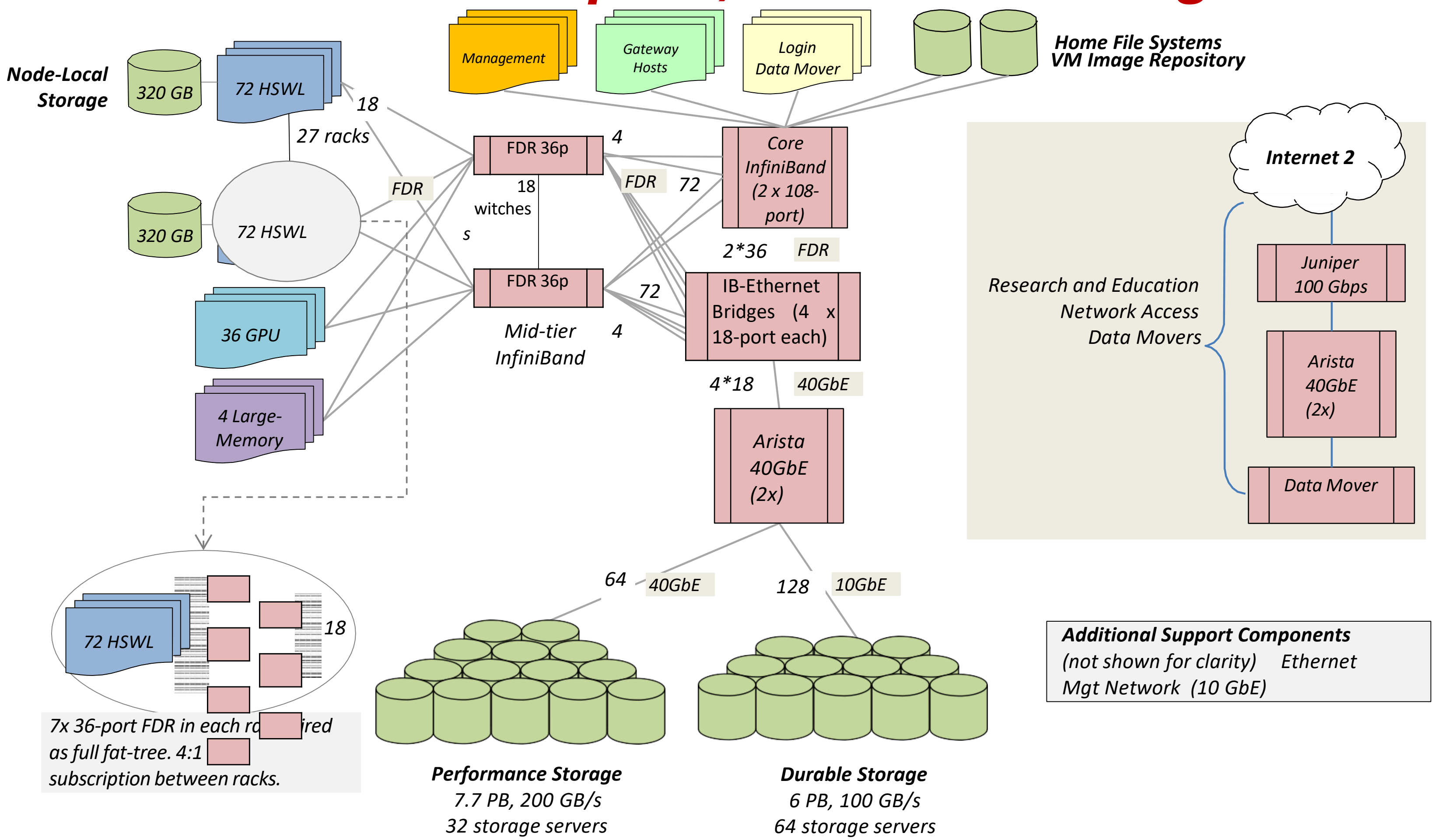


And 27 single-rack supercomputers



Comet Network Architecture

InfiniBand compute, Ethernet Storage



Comet: Filesystems

- ***Lustre filesystems – Good for scalable large block I/O***
  - *Accessible from all compute and GPU nodes.*
  - */oasis/scratch/comet - 2.5PB, peak performance: 100GB/s. Good location for storing large scale scratch data during a job.*
  - */oasis/projects/nsf - 2.5PB, peak performance: 100 GB/s. Long term storage.*
  - ***Not good for lots of small files or small block I/O**.*
- ***SSD filesystems***
  - */scratch local to each native compute node – 210GB on regular compute nodes, 285GB on GPU, large memory nodes, 1.4TB on selected compute nodes.*
  - *SSD location is good for writing small files and temporary scratch files. Purged at the end of a job.*
- ***Home directories (/home/$USER)***
  - *Source trees, binaries, and small input files.*
  - ***Not good for large scale I/O.***

Motivation

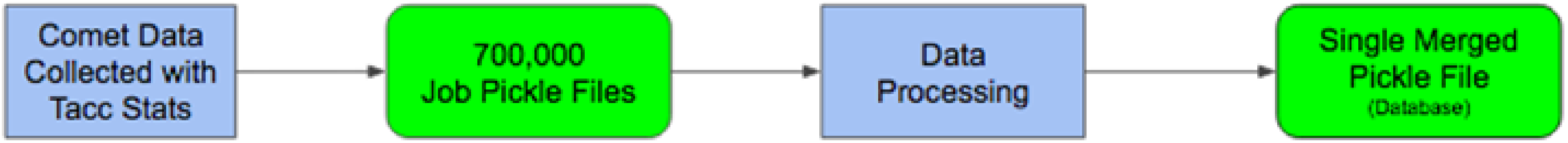
- **Currently HPC systems monitor/collect lots of data**
  - Network traffic, file system traffic (I/O), CPU utilization etc.
  - Analyzing users' job data can provide insight into static and dynamic loads on
    - File system
    - Network
    - Processors
- **How to analyze data, observe patterns, use those for improved system operation**
- **Analysis of I/O usage patterns of users' jobs**
  - Insight into which jobs to schedule together or not
  - System admins perform I/O work coordinating with specific user jobs etc.

This work - preliminary

- Looked at I/O traffic of users' job on Comet for three months – early phase of Comet: June – November 2015
- Analyze data and extract information
  - Monitor system operation
  - Improve system operation
- Aggregate I/O usage pattern of users' jobs
  - On NFS, Lustre and node-local SSDs
- Data science applied to tie I/O usage pattern to users' particular codes

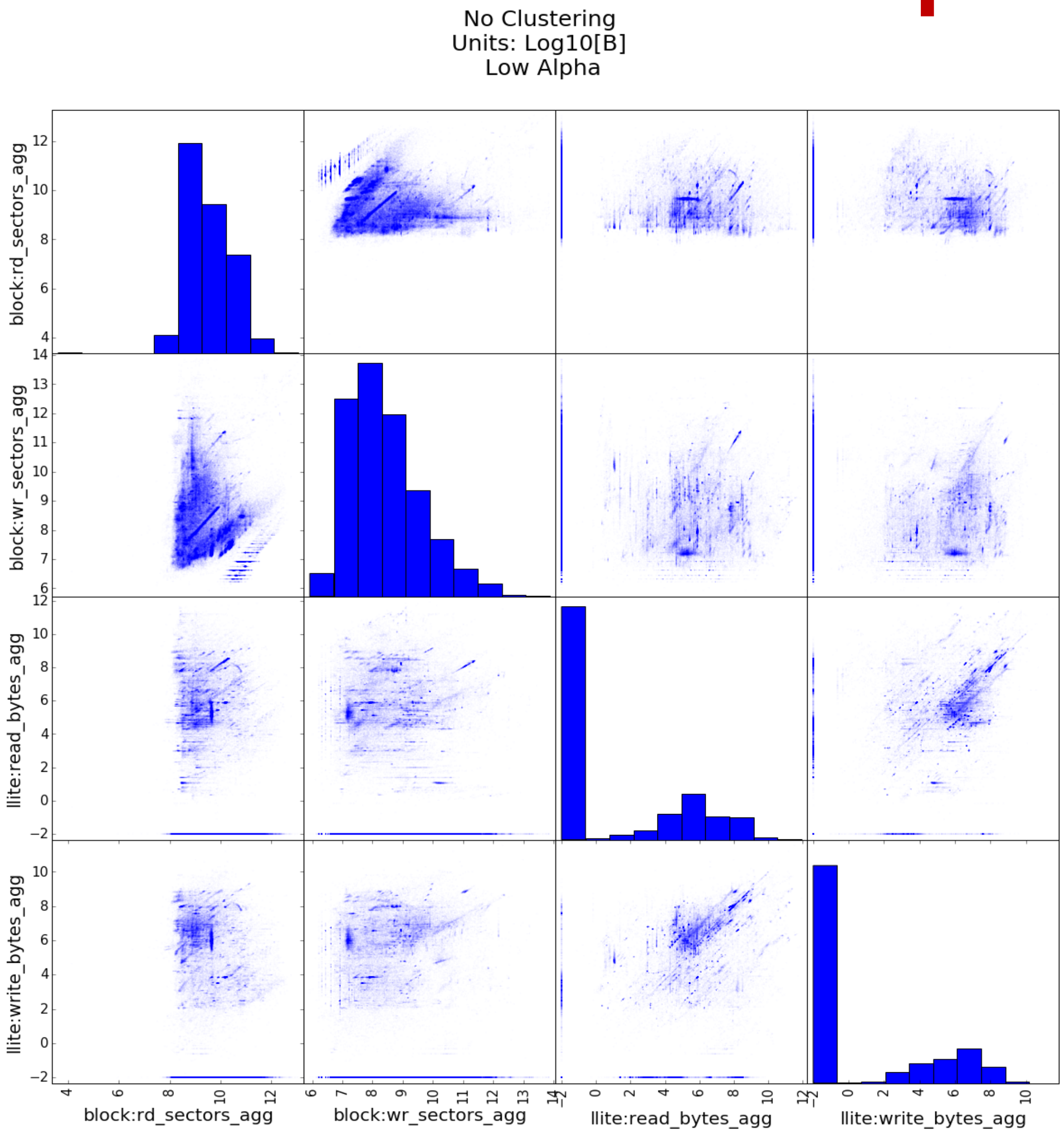
Data Analysis

- Data collected using TACC Stats (still being collected continuously)
- ~700,000 jobs that ran during the time period, and is around 500 GB in size
  - Collects user job's I/O stats on file systems every 10 min interval
- Looked at Compute and GPU queue (not shared queue for first pass)
- Data can be quickly extracted as inputs for learning algorithms – NFS, Lustre, node local SSD I/O data



- Ran controlled IOR for validating the data processing pipeline

Scatter plot



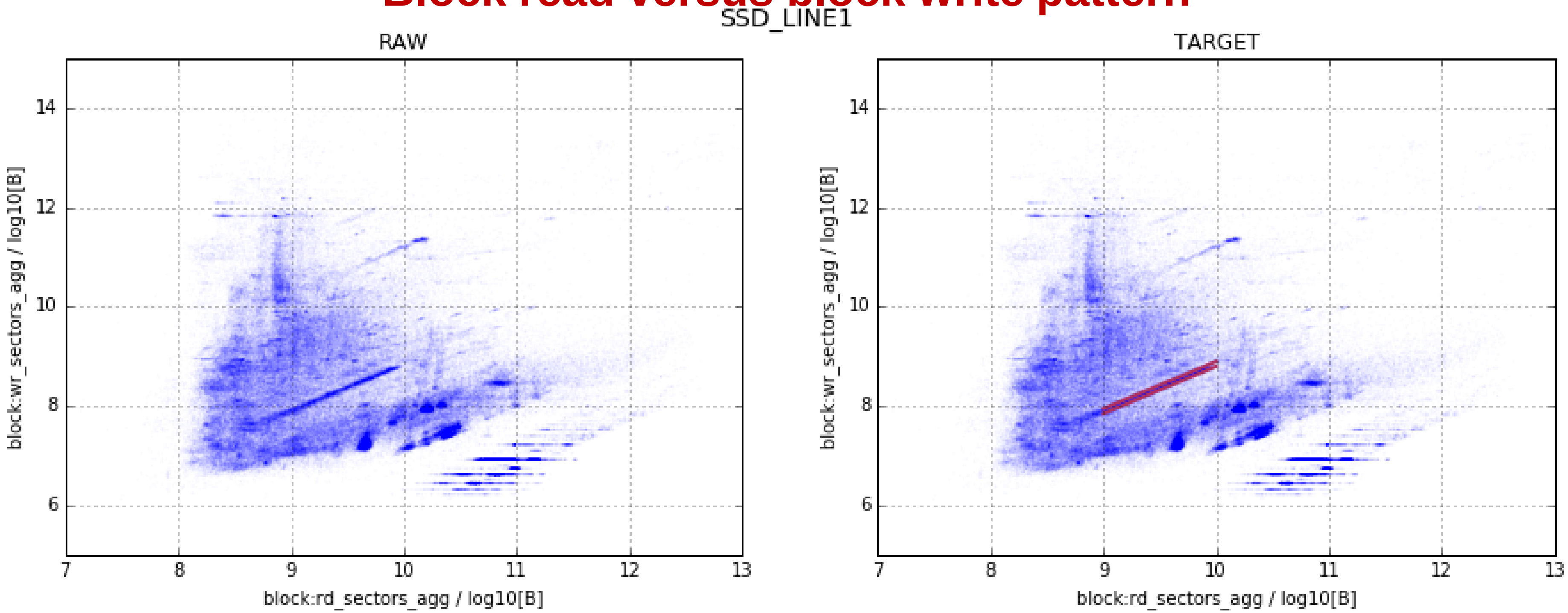
- *scatter matrix from Scikit-learn*

- Block refers to SSD
- llite refers to Lustre

- Analyzed the linear patterns
- Tried to tie to apps

Linear Pattern

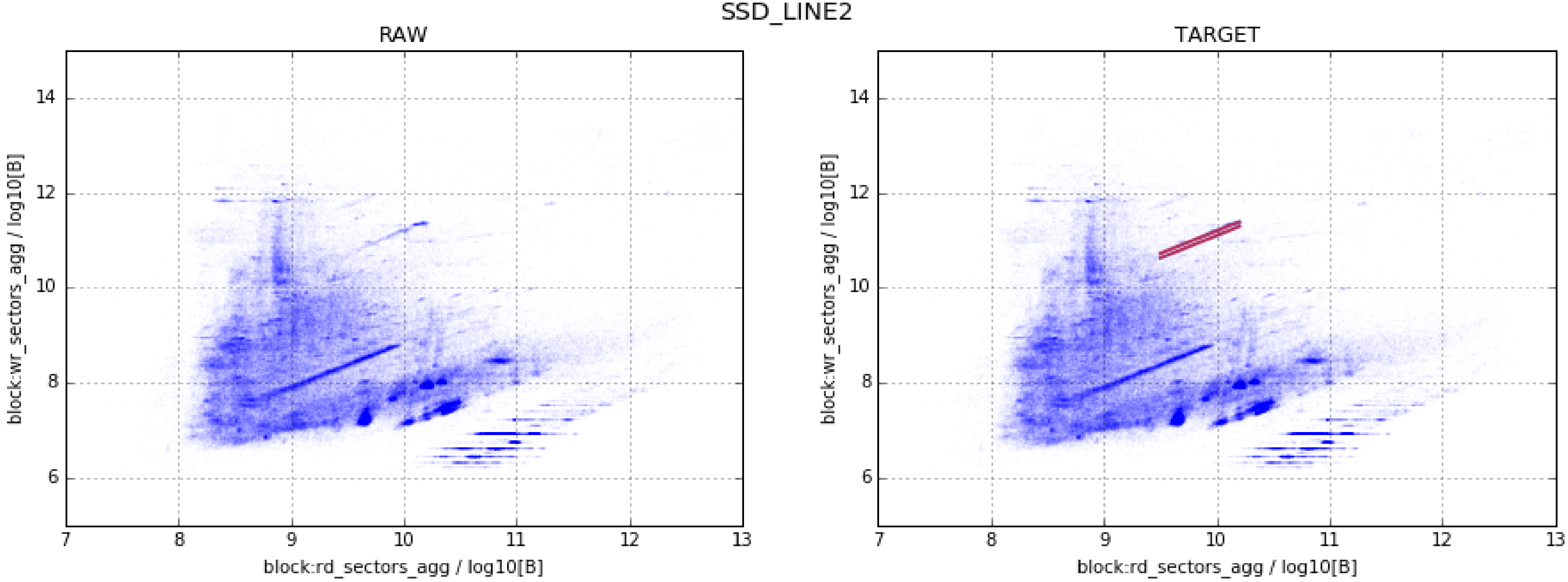
Block read versus block write pattern



- Linear patterns formed when analyzing aggregate write I/O and aggregate read I/O on the SSD
- Pertaining to all the jobs that are part of this pattern, we have seen that 1,877 (76%) jobs are Phylogentics Gateway (CIPRES running RXML code) and Neuroscience Gateway (was mostly running spiking neuronal simulation) jobs
- We know that these jobs only produce I/O to NFS
- However they used OpenMPI for their MPI communication.
- This leads to runtime I/O activity (for example memory map information) in /tmp which is located on the SSDs

Linear Pattern

Block read versus block write pattern



- *Another linear pattern formed when analyzing aggregate write I/O and aggregate read I/O on*
- *the SSD*
- *Pertaining to all the jobs that are part of this pattern, we have seen that 208 (82%) jobs have the same job name and from a particular project group*
- *Further investigation and discussion with the user showed that these I/O patterns were produced by Hadoop jobs*
- *On Comet, Hadoop is configured to use local SSD as the basis for its HDFS file system*
- *Hence, as expected, there is a significant amount of I/O to SSDs from these jobs*

Linear pattern

SSD read vs Lustre write; SSD read vs Lustre read

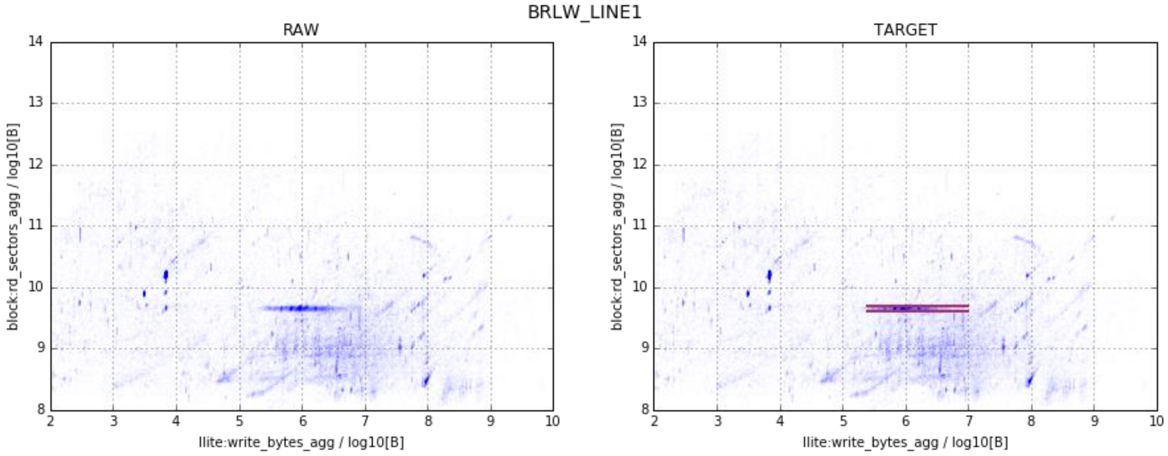


Fig. 6. Block read versus lustre write pattern (BRLW_LINE1).

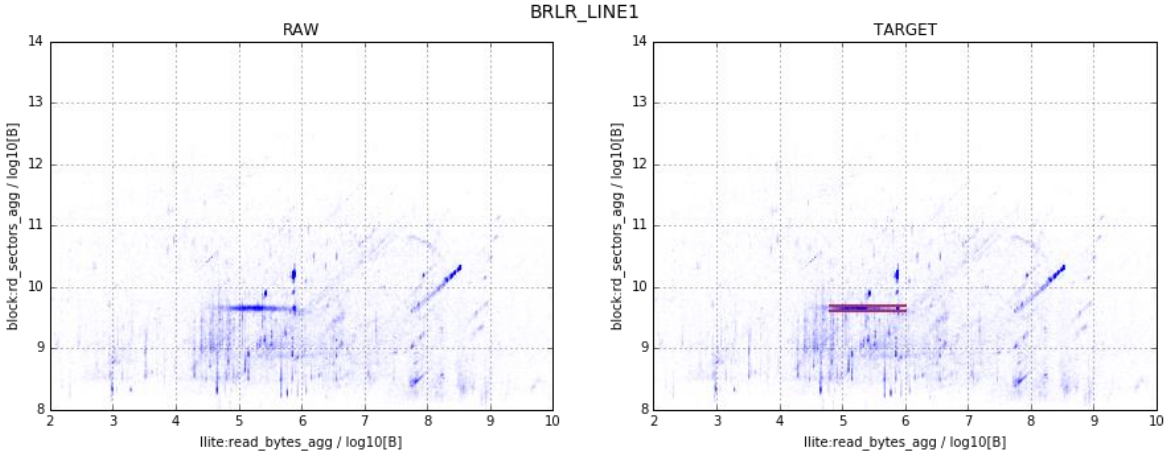


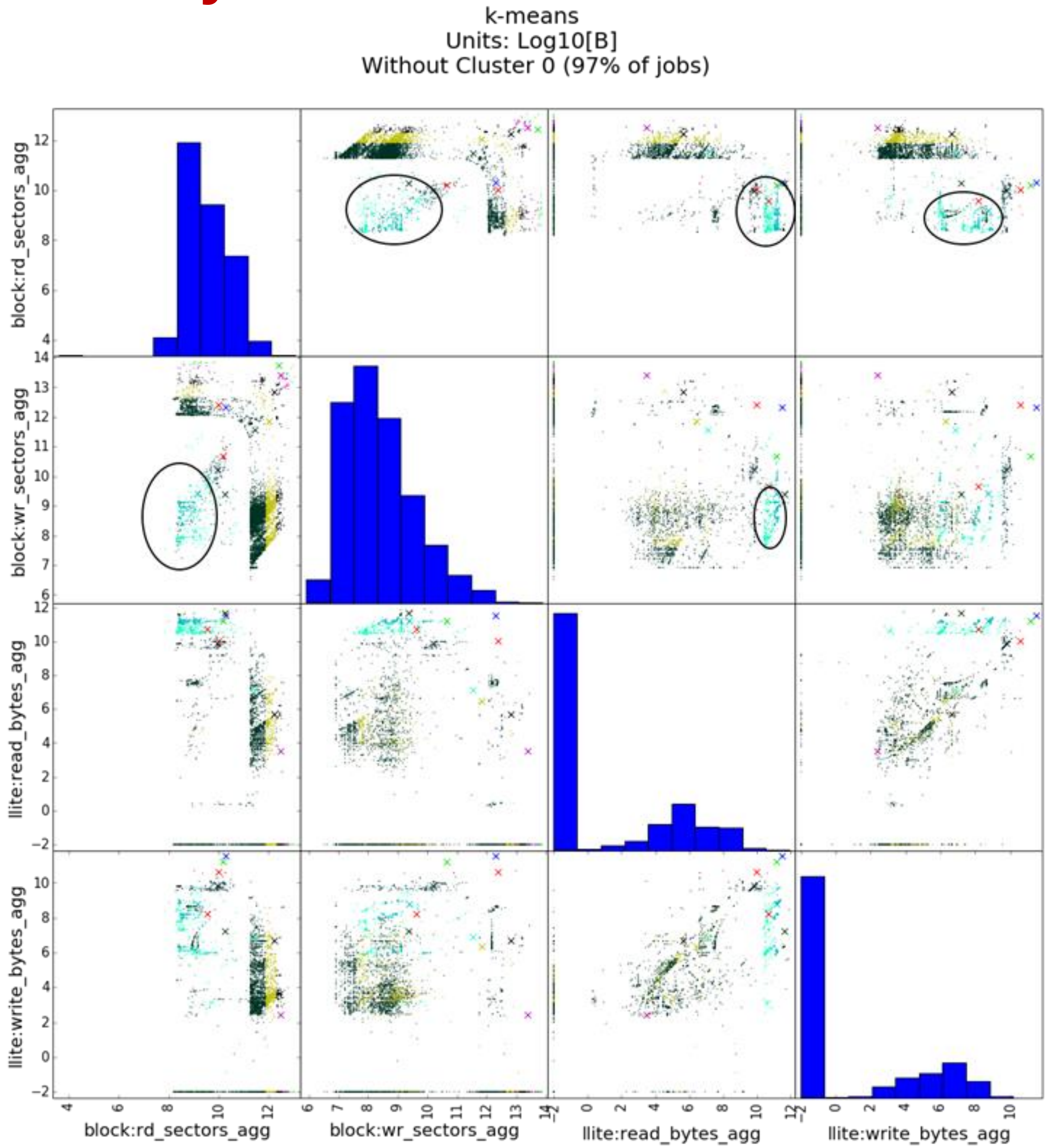
Fig. 7. Block read versus lustre read pattern (BRLR_LINE1) – horizontal line.

Linear pattern

SSD read vs Lustre write; SSD read vs Lustre read

- Horizontal linear patterns on SSD read I/O against Lustre Write I/O and Lustre Read I/O respectively
- Both show similar patterns.
- This indicates that they were both created by similar applications
- BRLW_LINE1 contains 232 (28%) VASP and CP2K jobs and 134 (16%) NAMD jobs
- We can say these applications require ~4 GB of read from the local SSD (this includes both scratch and system directories) and between 100 kB and 10 MB Lustre I/O (both read and write) to run the job

K-means analysis cluster center marks 'X' and cluster 10 encircled



K-means cluster analysis

- The teal colored cluster as shown in Figure, is characterized by low SSD read and SSD write (100 MB - 1 GB)
- However, this cluster shows very high Lustre read (>10 GB) and variable Lustre write (100 kB - 1 GB)
- At least 324 (89%) of these jobs had projects that indicate that these are astrophysics jobs

Summary

- **We did some other analysis such as using DBSCAN, longer (than 10 mins) time window for data etc.**
  - No distinct patterns
- **Presented work show we were able to analyze distinct patterns in the dataset caused by different applications**
- **We only looked at aggregate data**
  - In the future examine time series data - beginning, middle end of job
- **We can also analyze jobs separately based on parameters like run time of the job**

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