Integrating Remote Cloud and Local HPC Resources

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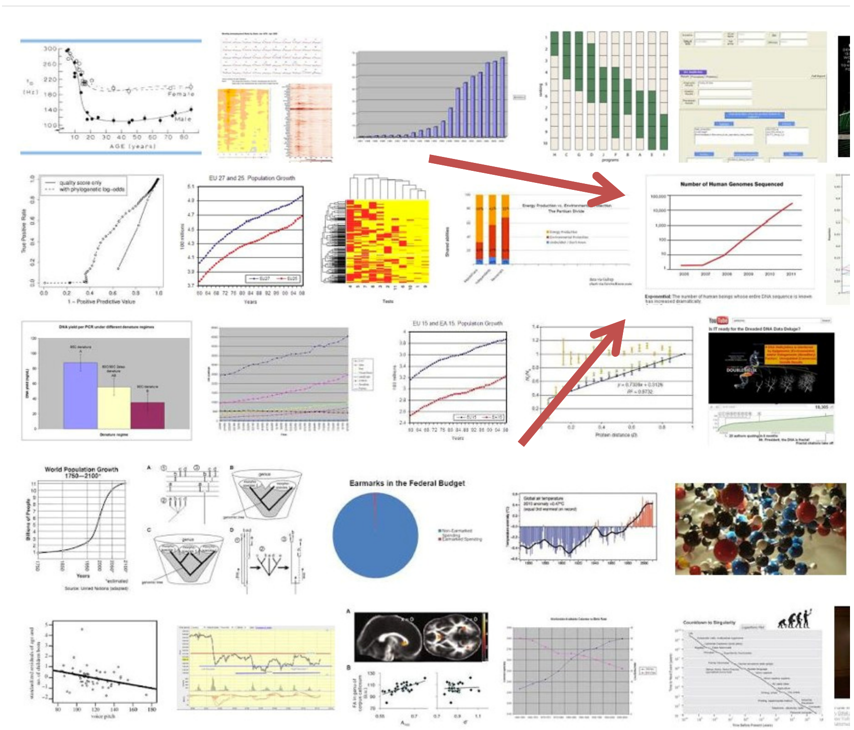
The Problem



- Not enough compute
- No where to put computational infrastructure
- Attracting IT talent easier said than done
- No academic institution does this as well as mega-corps

Cloud to the rescue!

- "Magical land of endless compute!"™
- Amazon Web Services
  - UPENN strategic partnership
- Initial usage caps are easily lifted on request
  - Went from 40 to 300 in 2 days
- Then how to integrate?

Integration to Local Resources

- I have no immediate and easy answer for you

- My 2¢:
  - Start with separate resources
  - Provide a robust transport mechanism
  - Stabilize both resources
  - Closely monitor usage patterns of both
  - THEN AND ONLY THEN start thinking about tight integration

The Cloudy Choices Before Us

- Pay someone to provide a solution
- Managed multi-tenant environments
  - Hosted provider agreements
    - E.g. POD or other non-root accessible resources
  - Set-contract VPS & managed hosting
    - Assumes administrative rights on resources
    - Can be "bear metal" dedicated servers (RackSpace)
  - IaaS providers
    - AWS, RackSpace Cloud, etc.
- [Un]managed single-tenant environments
  - IaaS where "users" request and administer resources

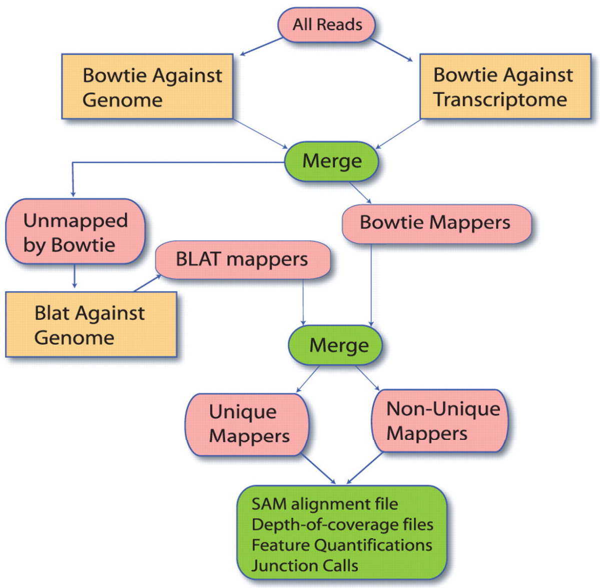
Managed Multi-tenant Environments

- Recreating current HPC environments on AWS EC2
- Known management and execution tools
- EC2 is “just different enough” to make your life a huge pain
- Costs are no longer fixed and amortized
  - chargebacks are going to be different (and variable)

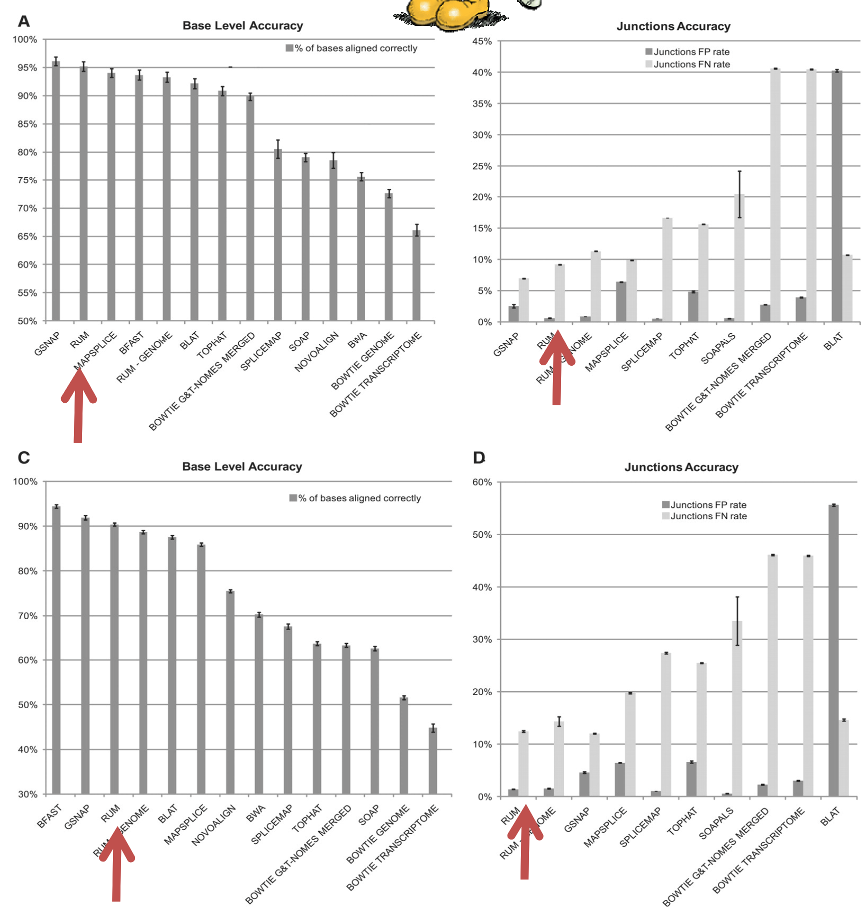
Single-tenant Managed Environments

- Bootstrapped Single Purpose Clusters (SPC™)
- Automation is **critical**
  - Permanent resources have a different management style, allow certain tradeoffs that are less palatable with cloud resources
- Able to tune SPC's for each business process
  - Instance type, how many, execution engine, storage strategy, etc.
- Let's look at an example: RNA-Seq analysis

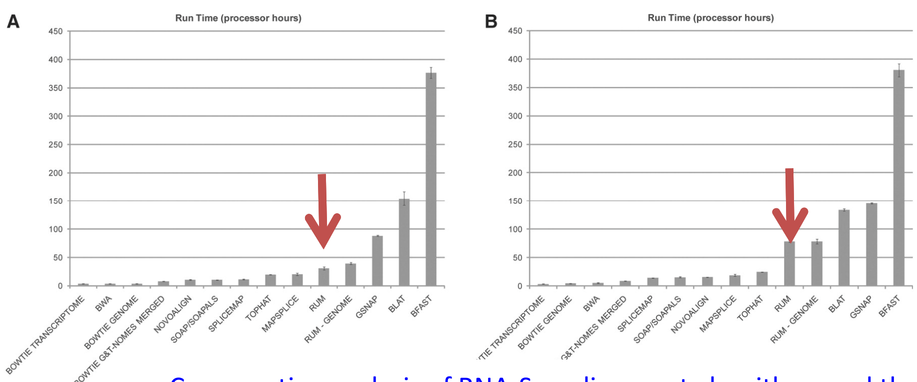
Algorithm: RNA-Seq Unified Mapper (RUM)



Accuracy

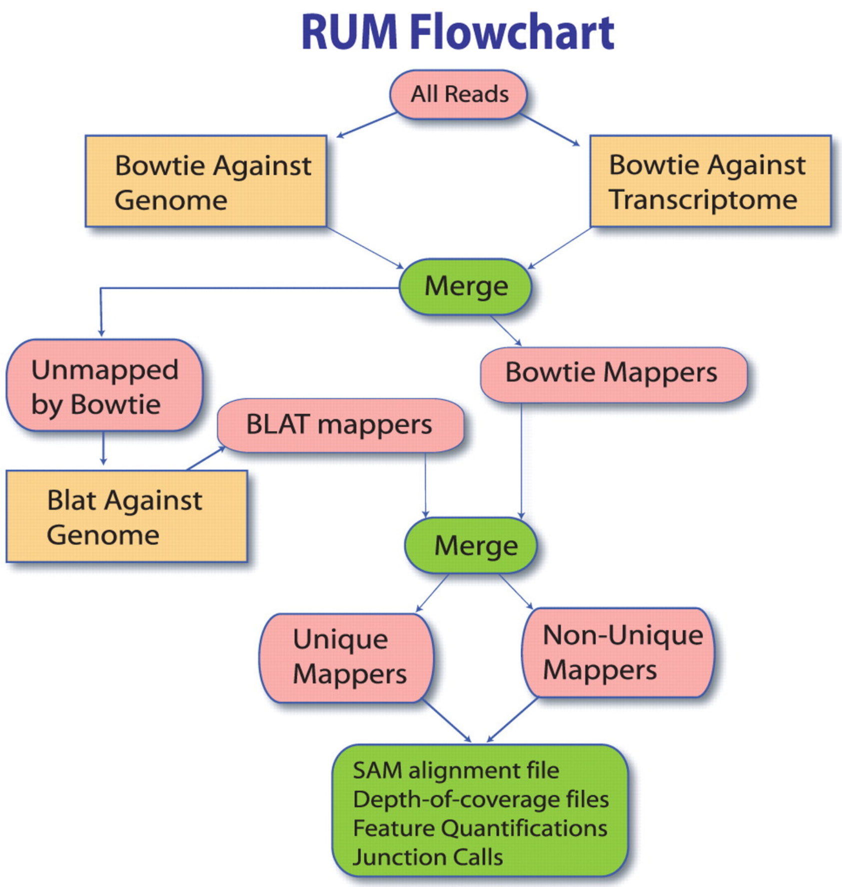


Runtime



[Comparative analysis of RNA-Seq alignment algorithms and the RNA-Seq unified mapper (RUM).]() Grant GR, Farkas MH, Pizarro AD, Lahens NF, Schug J, Brunk BP, Stoeckert CJ, Hogenesch JB, Pierce EA. Bioinformatics. 2011 Sep 15;27(18):2518-28. Epub 2011 Jul 19. PMID: 21775302

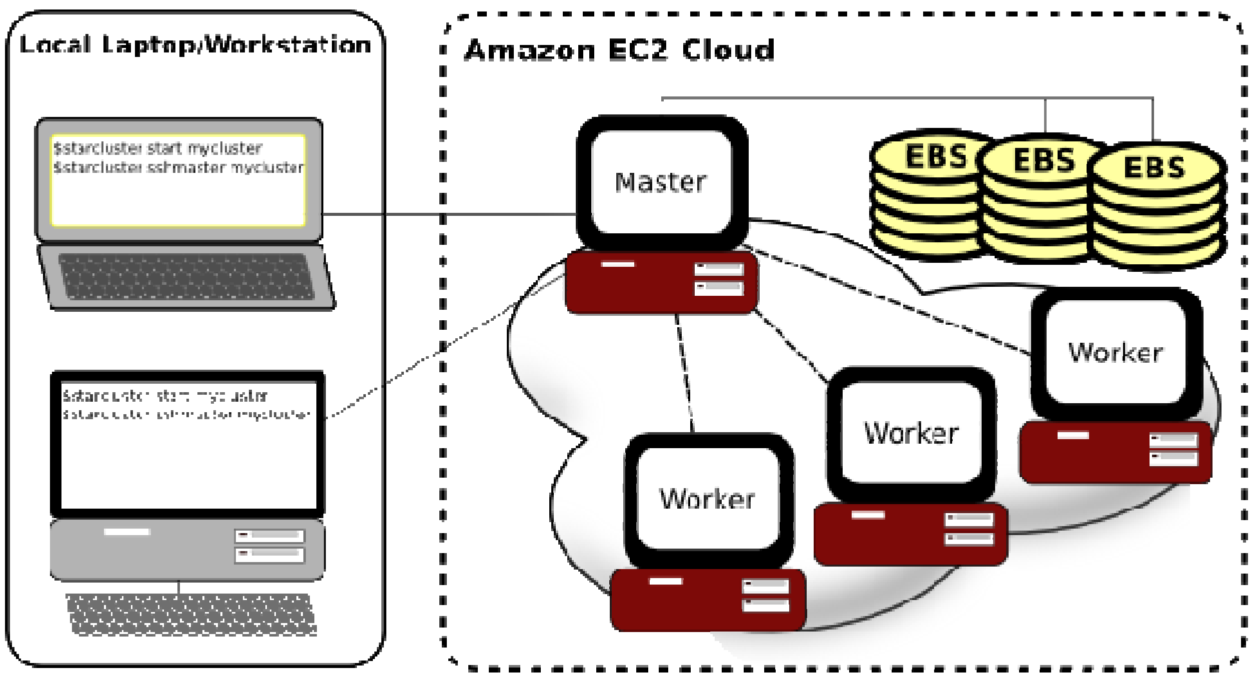
Closer look at RUM workflow



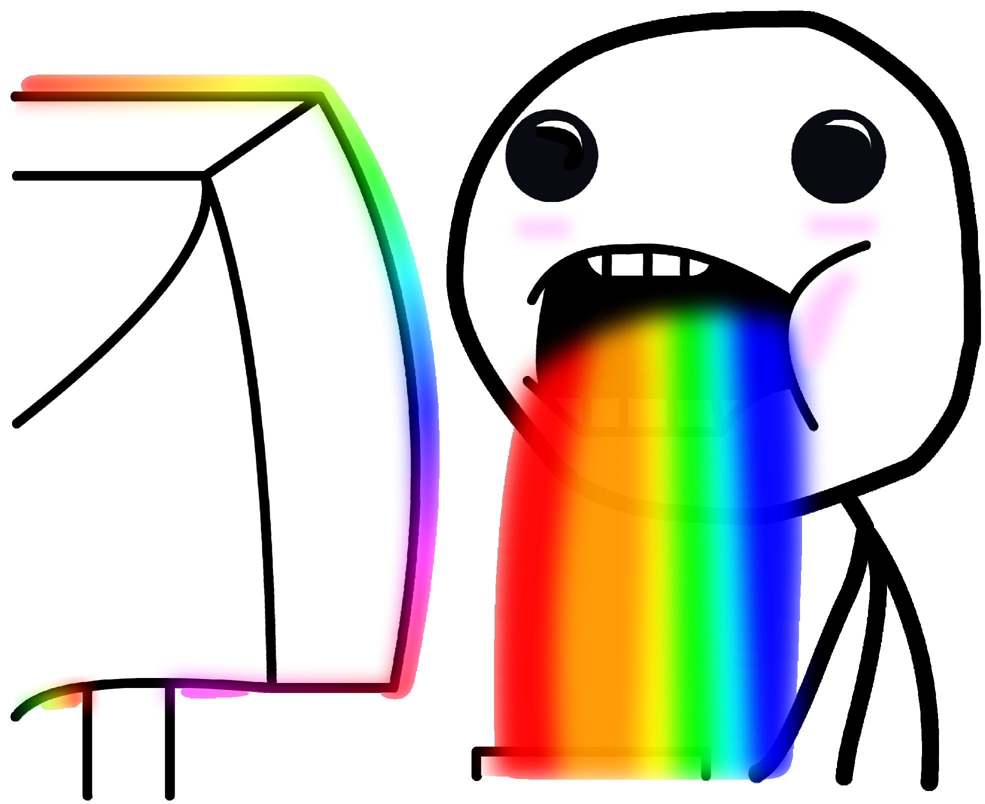
- 10MM 100bp paired end simulated data
- Lots of IO
  - 75% writes
- Essentially a map-reduce workflow
- 30 "chunks"

Orchestration via StarCluster

- Python command line tool to configure and launch single-tenant clusters on AWS



```
>>> Configuring cluster took 5.672 mins
>>> Starting cluster took 6.576 mins
```



Our StarCluster Plugins

- Extend StarCluster’s bootstrapping procedure
- GrideEngine Tweaks
  - Alter the number of slots on the master
  - Enable h_vmem on execution hosts
  - Enable exclusive reservation of hosts
- RAID0 Ephemeral storage
  - Formats all ephemeral disks into a single BTRFS volume
- GlusterFS on ephemeral storage
  - Parallel shared file system
  - Uses above to get massive single-namespace parallel filesystem
- PVFS2 on ephemeral storage
  - Alternate parallel shared file system
  - Built for high I/O workflows

https://github.com/PGFI/StarClusterPlugins

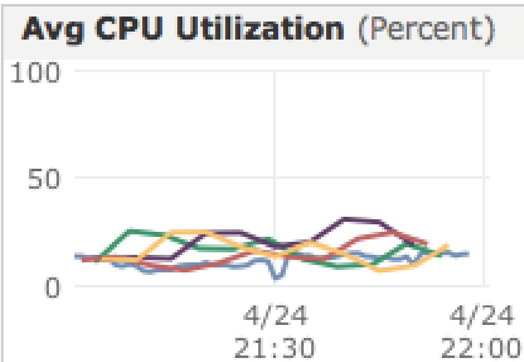
Experiment: Effect of a Shared File System on Run Time

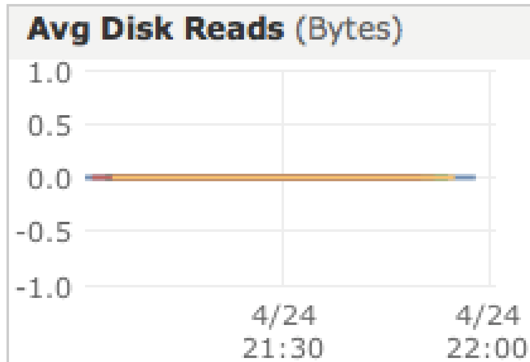
- NFS from the master host
  - Native to StarCluster default strategy, on EBS
- GlusterFS
  - FUSE-based, slower than kernel modules
  - All nodes on cluster join their ephemeral storage as one distributed GlusterFS volume
- PVFS2
  - Kernel module shunts requests via a pvfs2-client daemon
  - Distributed striped volumes across ephemeral storage

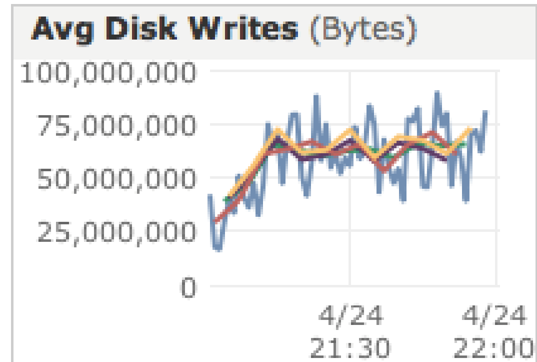
PVFS2 Results

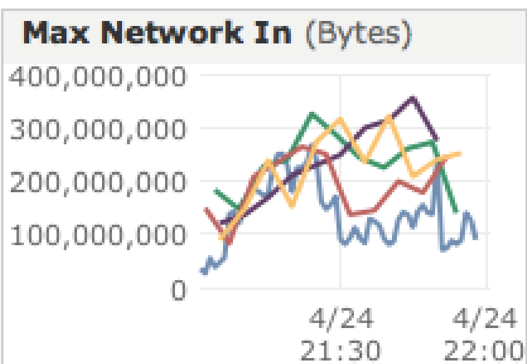
- Killed PVFS2 after 232 minutes
  - Master process looked for files and aggressively cleaned up after itself
  - Restarted each “chunk” analysis
  - Your algorithm may work better
  - There are tuning parameters that allow more file system consistency
  - Can tune the data server and metadata server layout configuration

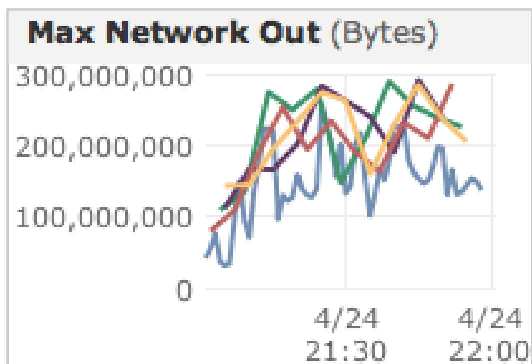
PVFS2 Profile Data
(something is not right)







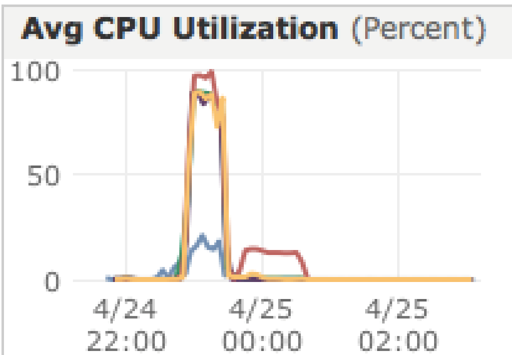


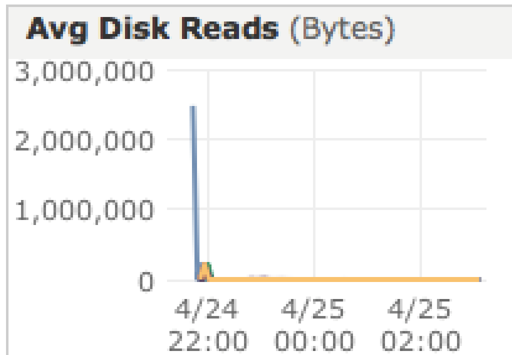


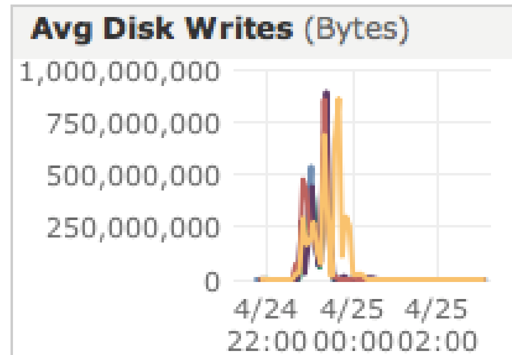
GlusterFS Results

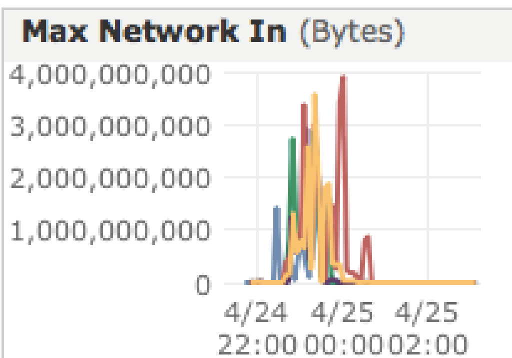
- Completed in 112 minutes
  - 10MM paired end RNASeq data ~ $7.50 to align
  - VERY CLEAN SIMULATED DATA
- We've tried using 2 dedicated GlusterFS file servers to service the cluster, and that failed badly.
  - NFS time outs, lots of EBS => $$$
- Much better performance to use it as scratch space on ephemeral drives
  - Also cheap, since it utilizes ephemeral drives

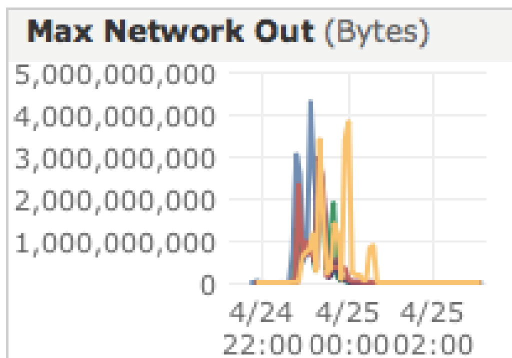
GlusterFS Profile Data









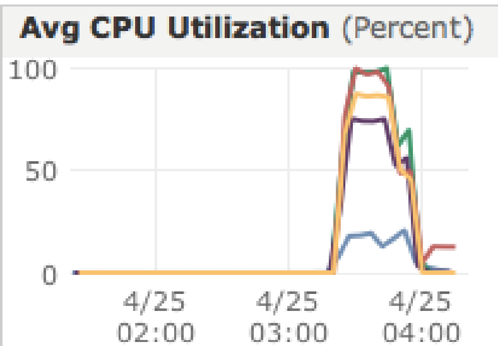


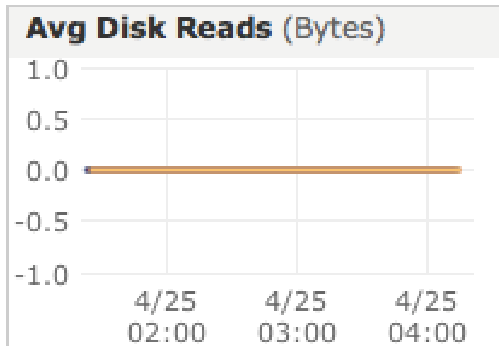
NFS from the master node

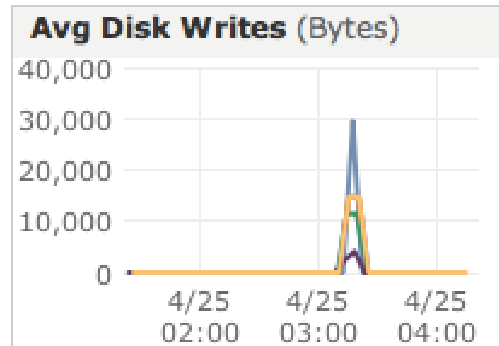
- Finished in 91 minutes
- Not much faster than GlusterFS

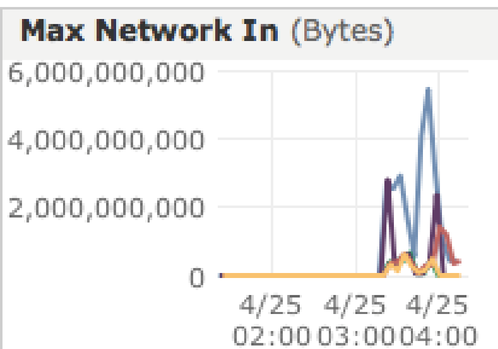
- We have seen it fail hard under heavy loads
  – 10-15 servers, 90 processes
- Unless you RAID, limited to 1TB volumes
- Probably best to use local scratch space on nodes, copy back final results to NFS space

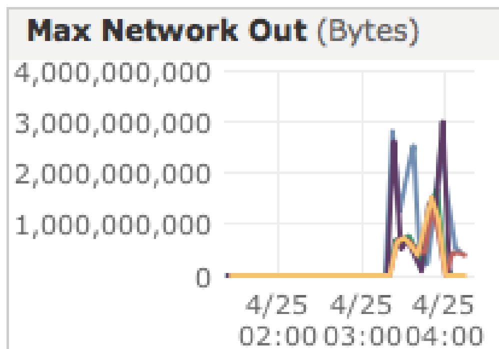
NFS Profile Data











Conclusions

- Profile your algorithms, tune Single Purpose Clusters (SPC™) for CPU and IO
- **COMPLETELY** automate the process of bootstrapping SPC's
  - Automate the process of bringing them up and bringing them down
- Once you have achieved "set it and forget it" status, treat it as a single algorithm/service that gets integrated with local resources