

UC San Diego Research Computing Triton Shared Computing Cluster

*Ron Hawkins
October 15, 2019*



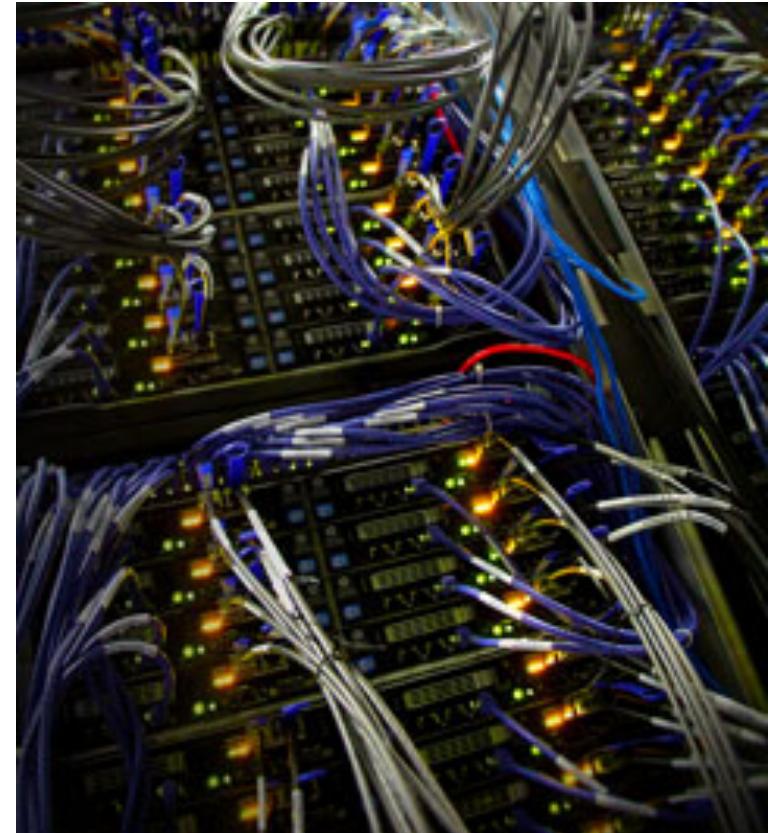
TSCC-101 Companion Material

<https://github.com/sdsc-hpc-training/tscctutorials/tree/master/tscct-101-Oct19>

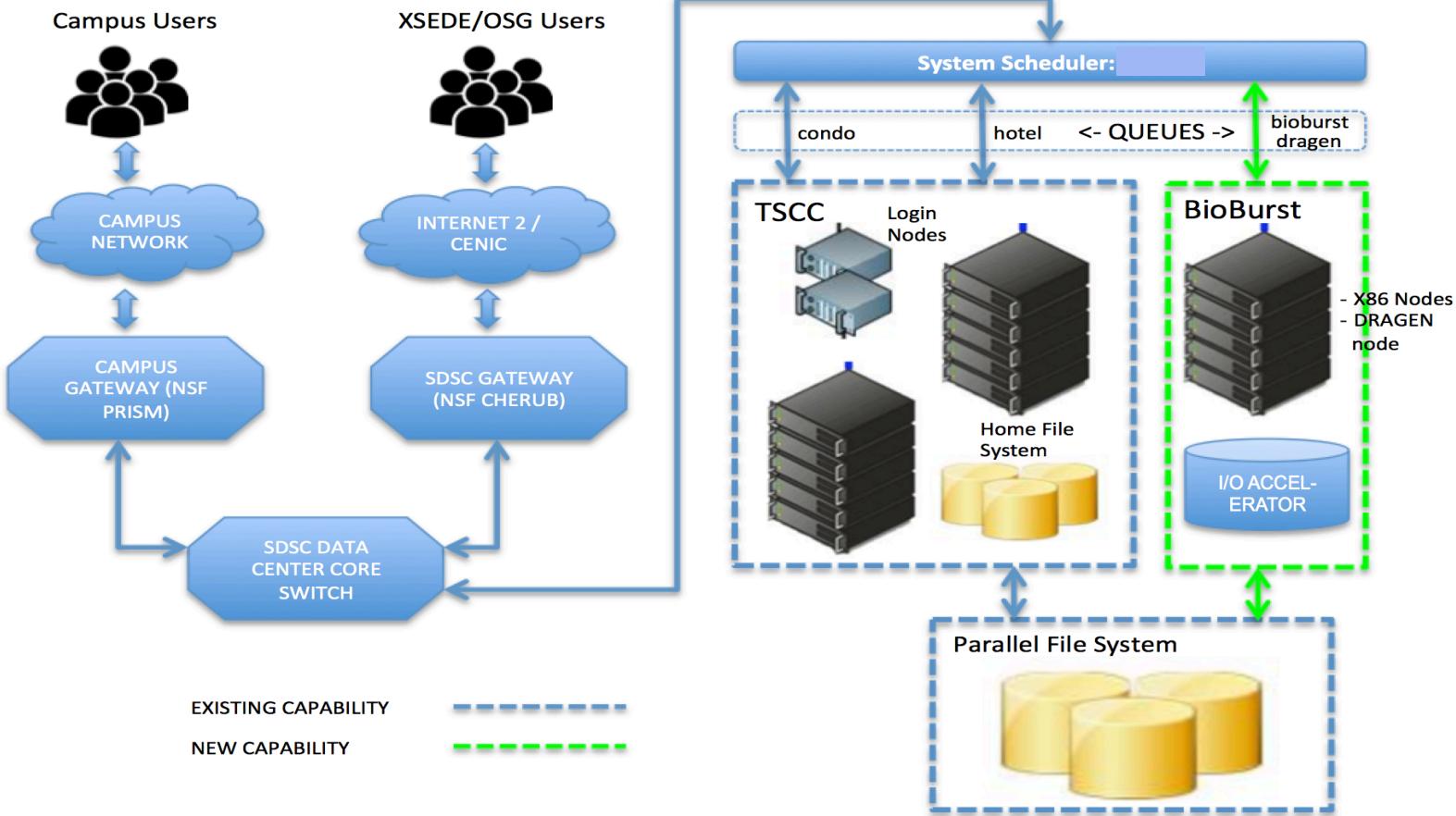
Triton Shared Computing Cluster (TSCC)

High Performance Computing for UC Researchers

- Medium-scale campus research cluster
- Launched 2013
- Hybrid business model: “condo” (buy in) and “hotel” (pay-as-you-go) options
- Mixed architecture:
 - ~375nodes (>7,000 cores, not incl. GPU cores) + 50 GPU nodes (~300 GPUs with mix of NVIDIA 980/1080/TitanX GPUs)
 - 250-300TF not incl. GPUs
 - 850TB parallel file system, home file system, add'l storage services
 - Ethernet + optional InfiniBand
 - High bandwidth external networks
- Provide full Linux software stack (also container support)
- 33 participating labs/groups

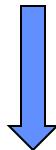
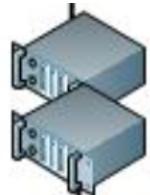


Overall Architecture

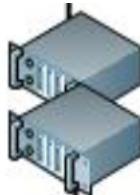


Condo Model Mechanics

**Group 1's
Purchased Nodes**



**Group 2's
Purchased Nodes**



Nodes are purchased directly and are property of the lab/group or funding agency

- Once purchased nodes are in place, group may run on purchased nodes or entire cluster according to usage rules
- Labs/groups are assessed an annual per-node operations fee



Condo Cluster

Common equipment is purchased via assessment of a one-time, per-node "infrastructure fee"



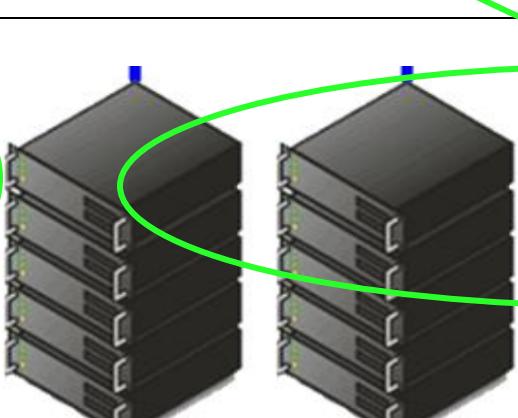
***TSCC Group Purchases
Common Infrastructure***

TSCC Operations

Condo Users



- Purchase Nodes
- Pay annual operations fee (\$495 per node – subsidized rate)
- Can run on purchased nodes or entire cluster (surge capacity for times of high computing need)
- “Glean” queue allows free use of spare capacity for short-running or re-startable jobs



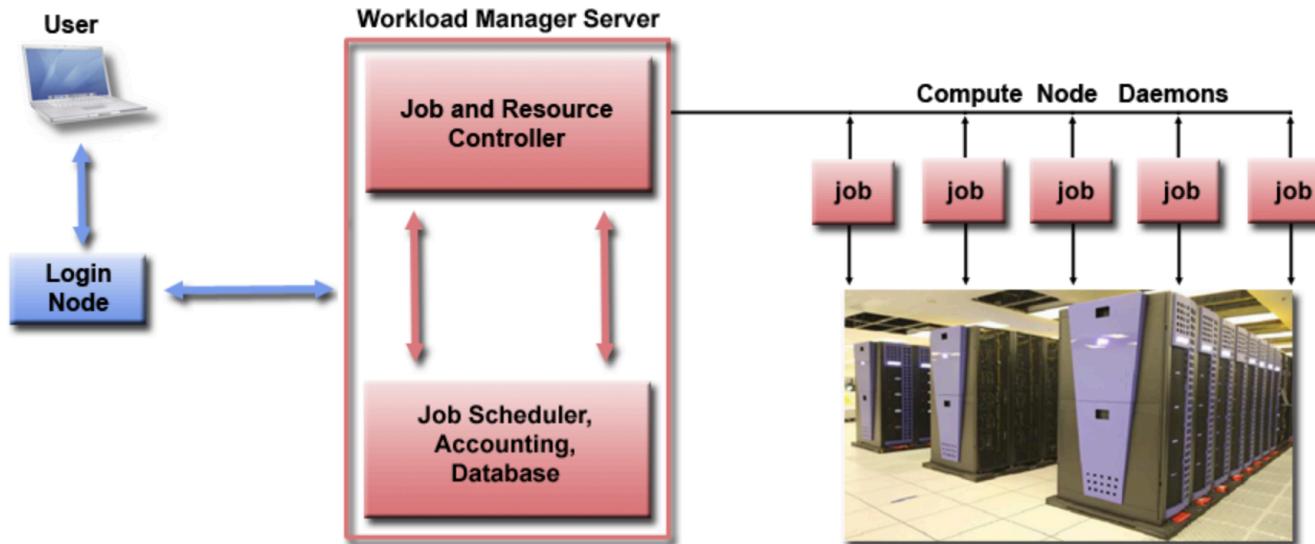
Hotel Users



- Purchase Time (2.5 c per core-hour e.g. \$250 for 10,000 core-hours)
- Run only on hotel nodes

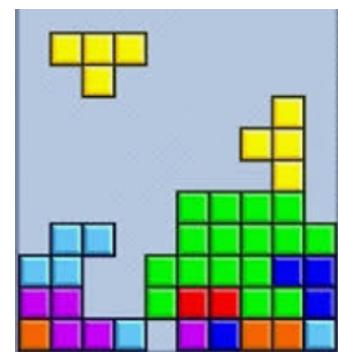


TSCC is a Batch-Scheduled Cluster



Think of the scheduler like a game of Tetris...

User	Workload Manager	Cluster
<ul style="list-style-type: none">◦ Logs into cluster◦ Creates job script and submits it to workload manager◦ Monitors and interacts with job via workload manager◦ Queries workload manager for job and cluster information	<ul style="list-style-type: none">◦ Typically runs on a separate server as multiple processes◦ Receives job submissions, commands, queries from user◦ Matches job requirements to available machine resources◦ Evaluates, prioritizes and queues jobs◦ Schedules jobs for execution on cluster◦ Tracks job and cluster information◦ Sends jobs to compute node daemons for actual execution	<ul style="list-style-type: none">◦ Workload Manager daemons run on compute nodes◦ Daemons manage compute resources and job execution◦ Daemons communicate with Workload Manager server processes



Source: <https://computing.llnl.gov/tutorials/moab/>

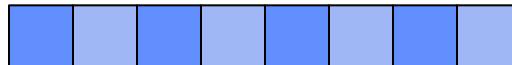
TSCC Queues

HOTEL



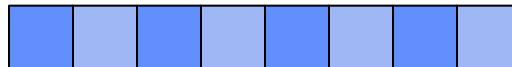
- *Run on Hotel Nodes*
- *Max Wall Clock 168 hrs*

CONDO



- *Run on Condo Nodes*
- *Max Wall Clock 8 hrs*

HOME



- *Run on Home Nodes*
- *Max Wall Clock unlimited**

GLEAN



- *Run on Condo Nodes*
- *Max Wall Clock unlimited*
- *Immediately Preemptible*

**Up to limit of annual allocation*

DRAGEN Bio-IT Platform

DRAGEN is a fully reconfigurable FPGA-based platform that can be reconfigured in seconds to host a number of different highly optimized analysis pipelines.

Ultra-Rapid Genomic Analysis Platform

- The power of the platform makes it possible to perform an extremely fast and accurate secondary analysis, which results in significant cost savings.
- Pipelines currently available include Whole Genome, Exome, RNASeq, Methylome, Microbiome, Joint Genotyping, Population Calling, Cancer and more.
- DRAGEN accepts FASTQ/BCL, and BAM/CRAM files as input and provides output in standard BAM/VCF/gVCF file formats.
- DRAGEN offers supreme flexibility of data analysis with both the ability to stream BCL data directly from sequencer storage.
- DRAGEN also offers the ability to convert BCL to FASTQ or BAM/CRAM. DRAGEN can read and output compressed or uncompressed files.



DRAGEN Node Performance Examples

- Running BWA, samtools, Picard tools, & GATK-3.6 haplotype caller on a single whole human genome sample at 48X coverage completed in 1.5 hours. Another run on a different sample at 49.5X coverage completed in 2 hours
- Running BWAmeth on WGBisulfite data (bisulfite treated sequence alignment) completed in under 2 hrs compared to 20-30 hours on standard nodes



NSF Campus Cyberinfrastructure PI and Cybersecurity Innovation for Cyberinfrastructure PI Workshop

September 23 – 25, 2019 | Minneapolis, MN

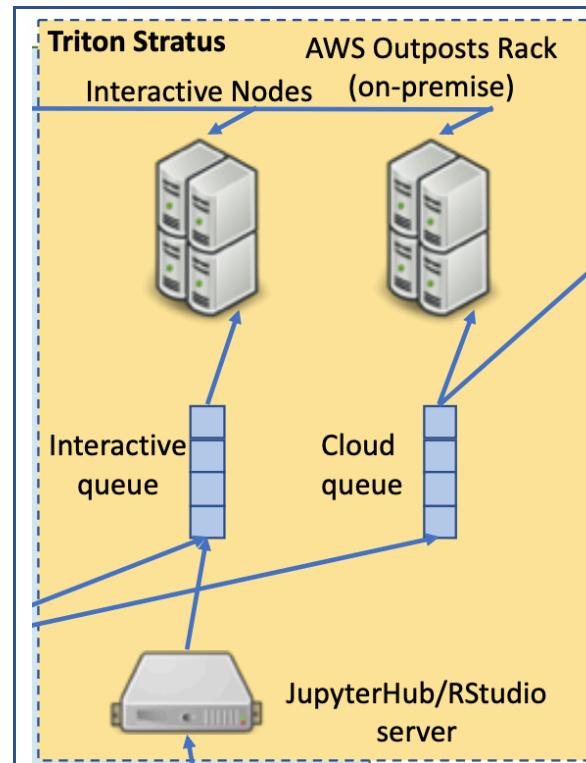
CC* Compute: Triton Stratus

Challenge Project Seeks to Address:

- Increasing use of interactive tools such as Jupyter Notebooks and RStudio
- Attracting researchers used to GUI/portal-driven interfaces
- Facilitating, simplifying use of cloud computing for campus researchers
- Integrating with and scaling to commercial cloud resources for elastic HPC

Deliverables:

- 28 new cluster nodes for interactive use
- Software for migration of scientific apps to commercial clouds
- User GUI (JupyterHub, Open OnDemand)
- Cloud integration for scaling tested notebooks/scripts
- On-premise cloud appliance (Amazon Outposts) for low-latency cloud testing and access
- OSG integration to campus cluster



Broader Impact:

- Reach new generation of researchers
- Support reproducible research
- Improve training & outreach for scientific computing
- “Living” documentation as means of communicating research broadly

Metadata tag:

- <https://www.sdsc.edu/services/hpc/hpc_systems.html#tscc>
- <Just getting started!>
- <Your input welcome!>
- <Student engagement>

Getting Started

- **Trial accounts granted upon request**
 - 250 service units good for 90 days (can accommodate larger trials on a case-by-case basis)
 - Need your name, group, contact information, UCSD AD username
- **For Hotel usage, simply need an index number to recharge**
- **User accounts include remote login and home directory with 50GB quota**
- **Condo Process**
 - Discuss your needs with us
 - We provide an initial budget estimate for review
 - Obtain firm pricing from vendor
 - Work with your fund manager to place order
 - Receive nodes, install and test
 - ~6 weeks for entire process

Future Plans

- Compute node upgrade for Hotel cluster (over time)
- OS & kernel upgrades (almost complete)
- Lustre expansion (in progress)
- Network fabric upgrade (25GbE and EDR InfiniBand)
- JupyterHub and Rstudio server support (interactive support via Triton Stratus)
- “Cloud bursting” to commercial compute clouds (e.g., Amazon Web Services)

**We need your
support &
advocacy!!**

For More Information Contact:

- **Ron Hawkins**
 - Email rhawkins@sdsc.edu or tscc-info@sdsc.edu
 - Tel (858) 534-5045
 - [http://www.sdsc.edu/services/hpc/hpc systems.html](http://www.sdsc.edu/services/hpc/hpc_systems.html)
- **Mary Thomas** (mthomas@sdsc.edu)
- **Subha Sivagnanam** (sivagnan@sdsc.edu)