OAK RIDGE National Laboratory

Deploying Summit

Presented to
PEARC 2020 HPCSYSPROS Symposium

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HPC Systems Task Lead

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U.S. DEPARTMENT OF ENERGY

Summit IBM AC922

Specifications and Features

- Processor: IBM Power9™ (2/node)
- GPUs: 27,756 NVIDIA Volta V100s (6/node)
- Nodes: 4,626
- Node Performance: 42TF
- Memory/node: 512GB DDR4 + 96GB HBM2
- NV Memory/node: 1.6TB
- Total System Memory: >10PB DDR4 + HBM + Non-volatile
- Interconnect Topology: Mellanox EDR 100G InfiniBand, Non-blocking Fat Tree
- Peak Power Consumption: 13MW

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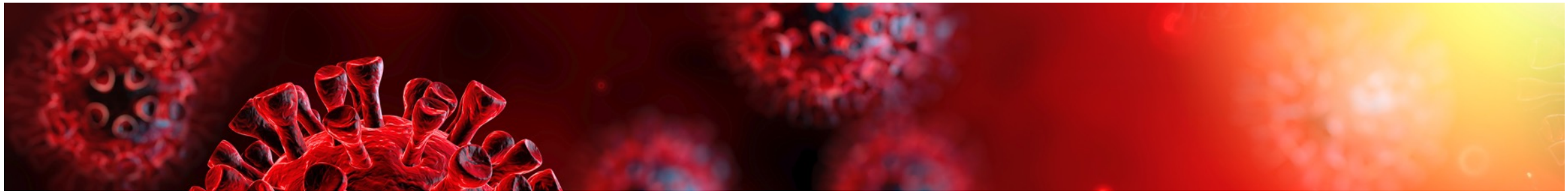
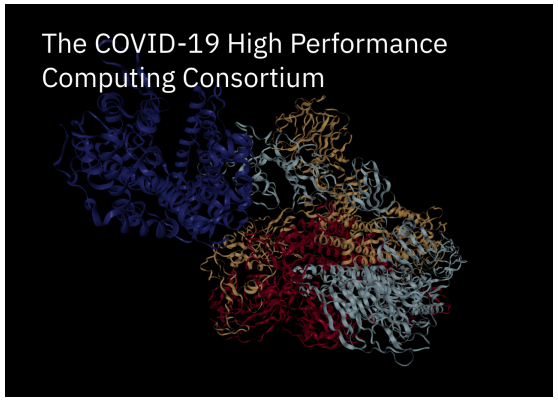
Summit COVID Hardware



3 New COVID-19 Cabinets (54 additional nodes) June 2020

Hardware improvements for COVID workloads:

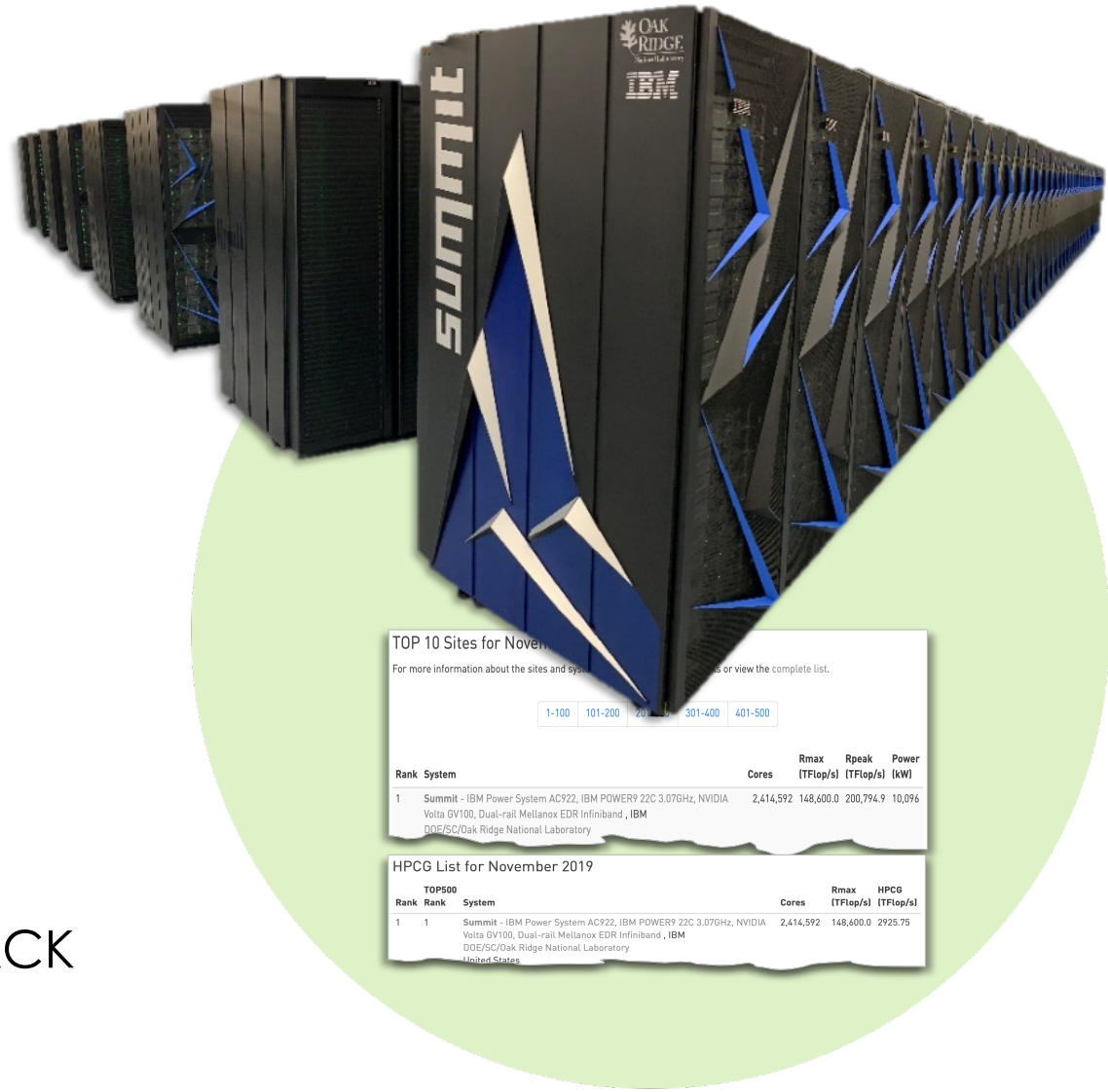
2 TB DDR4 CPU memory
32 GB HBM2 memory per GPU
6.4 TB NVMe Flash Drive



https://covid19-hpc-consortium.org

Summit Software

- Currently
  - RHEL 7.6
  - CUDA 10.1
  - MOFED 4.7
  - LSF 10.1.0.9
  - xCAT 2.15
- Summit IBM HPC Software Stack Upgrade
  - Released June 19th
  - Software Updates
    - RHEL 8.1
    - CUDA 11
    - MOFED 4.9
    - LSF 10.1.0.10
    - xCAT 2.16
    - Updates to LAPACK, LAPACKE, and LAPACK GPU support in ESSL
    - GDRCopy support in Spectrum MPI
    - JSM
      - Improved GPU Binding options
      - Support for multiple SMPI installs with a single JSM



Capability Usage (Summit) IBM AC922

Leadership usage	CY19 target	CY19 actual	CY20 target	CY20 actual[a]
INCITE	NAM	39.8%	NAM	40.2%
ALCC	NAM	52.7%	NAM	34.7%
All projects	**30%**	**47.6%**	**35%**	**38.2%**

[a] Jan-May 2020

2019 Capability Usage (47.6% average) demonstrates effective scheduling policy and application workload (large, scalable jobs)

- Leadership-class jobs must use no less than 20% of the available Summit nodes, and receive a +10 day aging boost from scheduler
- OLCF further boosts (+15d) the largest (>60%) jobs

Summit scheduling policy

Bin	Min nodes	Max nodes	Walltime hours	Aging boost (days)
1	2,765	4,608	24.0	15
2	922	2,764	24.0	10
3	92	921	12.0	0
4	46	91	6.0	0
5	1	45	2.0	0

Issues

- LSF
  - Scheduling requirements needed fairly significant development effort
    - Job size ranges as a priority factor
    - User group priority
    - Limits on the number of jobs that can be dispatched in one scheduling cycle
    - Job steps
    - Job "plans" to avoid large job starvation
  - New features meant new bugs that destabilized the product for a period of time
- Mellanox Ethernet Switches
  - LDAP packets being dropped
  - Buffers weren't sufficient, so flow-control was required reducing bandwidth
  - IBM replaced all switches to fix the issue
- Mellanox IB Fabric
  - Adaptive Routing
  - Reroutes take up to 30 seconds
- Spectrum MPI/jsrun
  - Two new development efforts which, as above, took some time to stabilize
  - Still see layout issues with jsrun
- Burst Buffer
  - Solution required 25% of resources on each ESS (GPFS) server for a VM
  - Several security issues found with the code
  - Integration with LSF required running jobs as root
  - Custom API for applications not portable

Jobstat

ORNL contact – Matt Ezell

- Python-based LSF job viewer
- Uses LSF API
- Modeled after MOAB showq output
  - Jobs categorized into Running / Eligible to Run / Blocked
  - Within each category, highest priority to lowest
  - usage: jobstat [-h] [-u USER] [-q QUEUE] [-r] [-e] [-b] [-c] [-a]
    [--format {cols,text,yaml,xml}] [--raw] [--version]
    [jobid] [field]

---------- Running Jobs: 77 (batch: 4622/4622=100.00% + batch-hm: 28/53=52.83%) ----------

JobID	User	Queue	Project	Nodes	Remain	StartTime	JobName
227382.1	sindhu	batch	MED111	2	5:50:50	07/16 13:58:53	equil-5-[1-25]
227382.2	sindhu	batch	MED111	2	14:24:14	07/16 22:32:17	equil-5-[1-25]
224740	hyuan	batch	NFI114	400	3:28:16	07/16 23:36:19	nekRS
228134	sehr	batch	CHM169	4	15:28:16	07/16 23:36:19	covid19-rem
224478	mlupopa	batch	MAT020	1700	11:41:28	07/16 23:51:57	LSMS-FeSi

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---------- Eligible Jobs: 92 ----------

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---------- Blocked Jobs: 429 ----------

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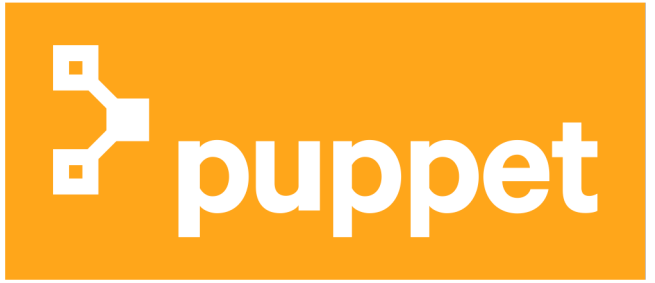
Configuration Management for Summit

ORNL contact – Chris Muzyn

- Combination of xCAT and Puppet.

- **Puppet** (NCCS Center-wide)
  - Backed by git
  - Templated configuration files



- **xCAT**
  - Combination of files and databases that are not versioned
  - Because of the databases, not easily manageable by our Puppet instance.

TTTAx- The Thing That Assembles xCAT

ORNL contact – Chris Muzyn

- Written in Ruby
- Manages xCAT's flat files **and** databases
  - ERB templating for flat files
  - YAML for databases/definitions
- Git repo for agile development
- Runs on RHEL and Ubuntu

Cgroupsysd

ORNL contact – Don Maxwell

- Solution for shared resource exhaustion on Summit login nodes
- Python script with a yaml configuration file
  - Utilizes systemd cgroups-v1
  - Default cgroup values with all resources configurable on a per-user basis
  - Calls via pam sshd and cron job
- Other solutions exist but none included a feature to first reduce and then kill processes with configurable limits
- Per-User Default Login Node Resource Limits
  - Cgroup
    - 16 hardware threads / 16 GB memory / 1 GPU
  - Reduce
    - Process reaches 4 hours of CPU time
      - .5 hardware thread
  - Kill
    - Process reaches 8 hours of CPU time
      - Kill process
- Login node limits are set per user and not per individual login session. All user processes on a node are contained within a single cgroup and will share the cgroup's limits.

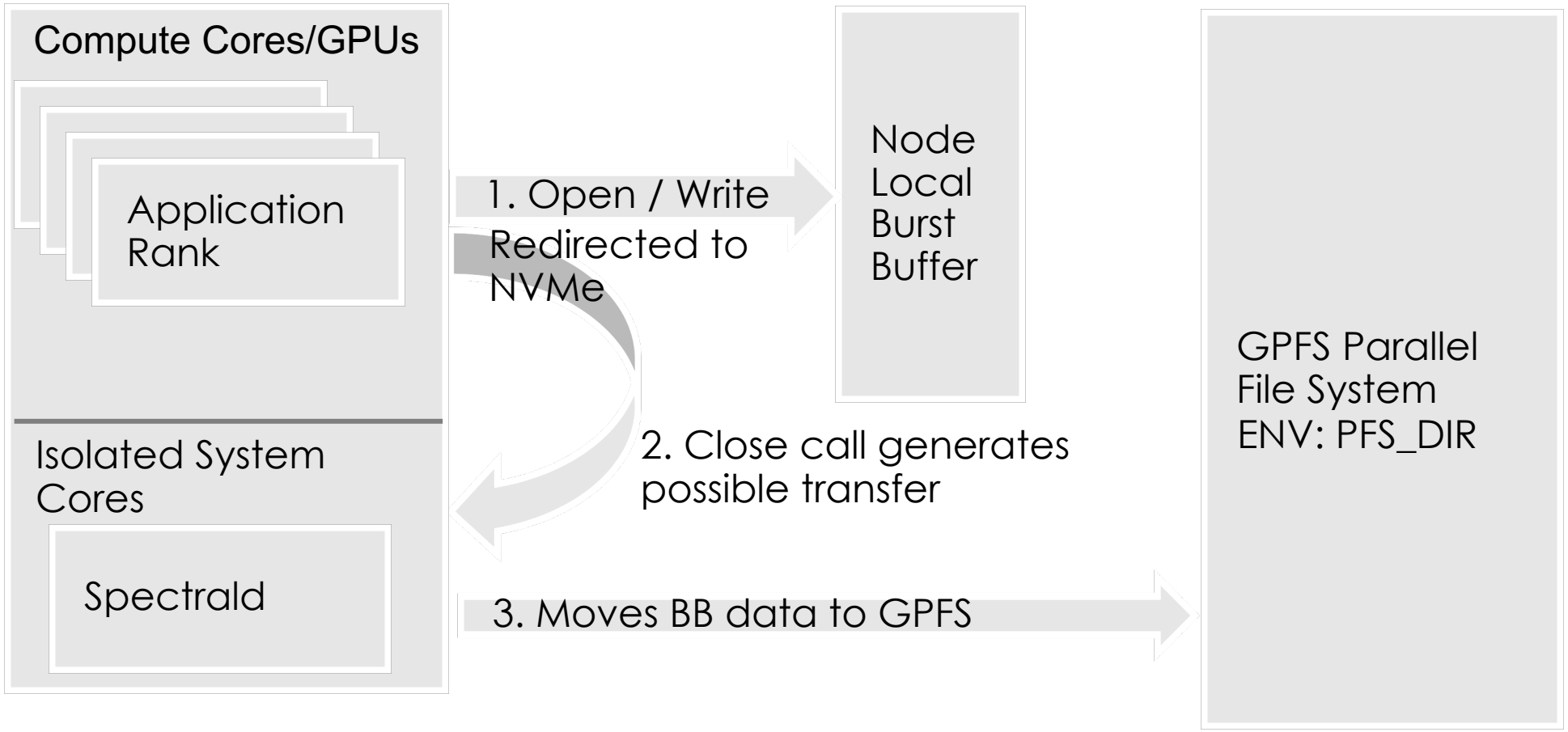
Spectral

ORNL contact – Chris Zimmer

- On node copy agent
  - Runs on isolated cores as system agent
- Application Interface Transparent
  - No code modifications (LD_PRELOAD)
    - Changes limited to job scripts
  - Application only has knowledge of a single namespace
- Preserves portability with single namespace
- Now supports shared files

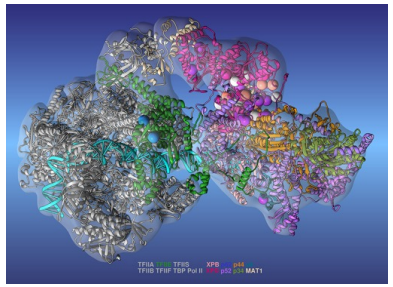
Spectral Data Flow

ORNL contact – Chris Zimmer



OLCF Systems Enable Breakthrough Science

Genetic Diseases

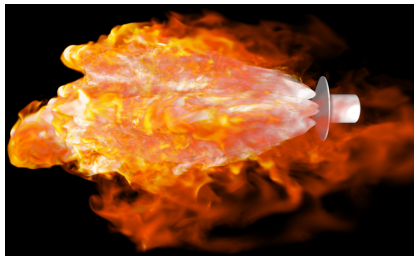


Ivaylo Ivanov
Georgia State U.

A Georgia State Univ. team used Summit to develop an integrative model of the transcription preinitiation complex (PIC), a complex of proteins vital to gene expression. This work is a foundation for more precisely pinpointing the mutations that cause genetic diseases ranging from degenerative neurological disorders to different types of cancers.

Chunli Yan, et al. 2019. *Nature Structural & Molecular Biology*. **26**.

Mars Exploration

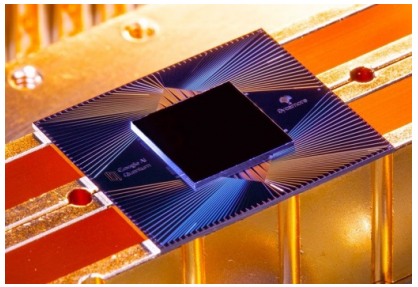


Eric Nielsen
NASA Langley

A NASA team is using Summit to simulate engine-powered deceleration (retropropulsion) — a promising engineering solution for landing humans on Mars by the mid- to late-2030s. CFD simulations on Summit are helping predict how the vehicle's engines should be designed and controlled.

A. M. Korzun, et al. 2019. *Int. Astronautical Congress*, Washington, D.C.

Quantum Supremacy

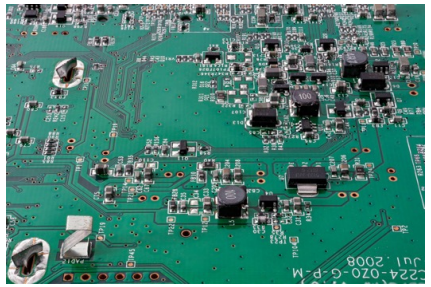


Travis Humble
ORNL

A joint research team from Google Inc., NASA Ames, and ORNL demonstrated that a quantum computer can outperform a classical computer at certain tasks, a feat known as quantum supremacy. To prove quantum supremacy, scientists used Summit to rule out that classical supercomputers could perform computational tasks at the same speed as Google's Sycamore quantum computer.

F. Arute et al., 2019. *Nature.* **574.**

Semiconductors

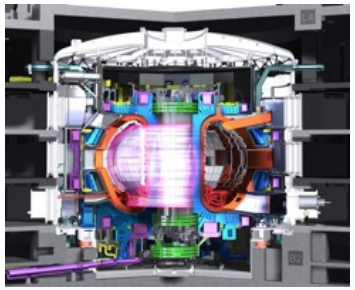


Torsten Hoefler
ETH Zürich

A Gordon Bell Prize-winning team led by ETH Zurich studied transistors by simulating quantum transport. They performed a 10,000-atom simulation of a 2D slice of a transistor on Summit and developed a map of where heat is produced in a single transistor. The results could be used to inform the production of new semiconductors with optimal heat-evacuating properties.

A. Ziogas. 2019. *Proceedings of SC19*.

Fusion Energy



Christopher Holland
UC San Diego

A team led UC San Diego is using Summit to better understand turbulence, an important characteristic of plasma behavior that affects performance in fusion devices such as ITER. Augmenting experiment with high-performance computing, the team is analyzing experimental data from the DIII-D tokamak and carrying out unprecedented simulations with their new CGYRO gyrokinetic code on Titan and Summit.

J. Candy, et al. 2019. *Computers and Fluids*. **188**.

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All from 2019 work conducted on Titan and Summit

Questions?