Outline

• Overview
• MVAPICH2 and MVAPICH2-GDR on Expanse
  • System architecture
  • Applications
  • Benchmark results
• MVAPICH2 on Voyager
  • System architecture
  • Kubernetes based usage of MVAPICH2
• INAM on Comet
  • System architecture
  • Network and Job Level Views
  • Notifications
• Summary
Overview

• SDSC operates and manages software for several HPC and AI systems with a large userbase spanning many scientific domains.
• MVAPICH2 and MVAPICH2-GDR have been an integral part of many SDSC HPC systems over the past decade including Trestles, Gordon, Comet, and Expanse.
• MVAPICH2 is being tested on machines with innovative architectures as well. This includes the Voyager heterogenous system, designed for AI workloads, which is currently in its 3-year testbed phase.
• INAM is in use on Comet to monitor network health and to identify sources of congestion.
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**EXPANSE**

**COMPUTING WITHOUT BOUNDARIES**

**5 PETAFLOP/S HPC and DATA RESOURCE**

**HPC RESOURCE**
- 13 Scalable Compute Units
- 728 Standard Compute Nodes
- 52 GPU Nodes: 208 GPUs
- 4 Large Memory Nodes

**DATA CENTRIC ARCHITECTURE**
- 12PB Perf. Storage: 140GB/s, 200k IOPS
- Fast I/O Node-Local NVMe Storage
- 7PB Ceph Object Storage
- High-Performance R&E Networking

**REMOTE CI INTEGRATION**

**LONG-TAIL SCIENCE**
- Multi-Messenger Astronomy
- Genomics
- Earth Science
- Social Science

**INNOVATIVE OPERATIONS**
- Composable Systems
- High-Throughput Computing
- Science Gateways
- Interactive Computing
- Containerized Computing
- Cloud Bursting

**NSF Award # 1928224**

**PIs: Mike Norman (PI), Ilkay Altintas, Amit Majumdar, Mahidhar Tatineni, Shawn Strande**
Expanse is a heterogeneous architecture designed for high performance, reliability, flexibility, and productivity.

**System Summary**
- 14 SDSC Scalable Compute Units (SSCU)
- 784 x 2s Standard Compute Nodes
- 100,352 Compute Cores
- 200 TB DDR4 Memory
- 56x 4-way GPU Nodes w/NVLINK
- 224 V100s
- 4x 2TB Large Memory Nodes
- HDR 100 non-blocking Fabric
- 12 PB Lustre High Performance Storage
- 7 PB Ceph Object Storage
- 1.2 PB on-node NVMe
- Dell EMC PowerEdge
- Direct Liquid Cooled
The SSCU is Designed for the Long Tail Job Mix, Maximum Performance, Efficient Systems Support, and Efficient Power and Cooling

**Standard Compute Nodes**
- 2x AMD EPYC 7742 @2.25 GHz
- 128 Zen2 CPU cores
- PCIe Gen4
- 256 GB DDR4
- 1 TB NVME

**GPU Nodes**
- 4x NVIDIA V100/follow-on
- 10,240 Tensor Cores
- 32 GB GDDR
- 1.6 TB NVMe
- Intel CPUs

**SSCU Components**
- 56x CPU nodes
- 7,168 Compute Cores
- 4x GPU nodes
- 1x HDR Switch
- 1x 10GbE Switch
- HDR 100 non-blocking fabric
- Wide rack for serviceability
- Direct Liquid Cooling to CPU nodes

**Non-blocking Interconnect**
- 1 HDR Switch/SSCU
- 10x (200 Gbps)
- 56x Compute Nodes
- 4x GPU Nodes
- 26x (200 Gbps)
- Performance Storage
- Cloud Storage
- 5 Level 2 switches
- 3x
- 2x

**SSCU – Front View**

---

SDSC - SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego
Expanse GPU Node Architecture

- 4 V100 32GB SMX2 GPUs
- 384 GB RAM, 1.6 TB PCIe NVMe
- 2 Intel Xeon 6248 CPUs
- Topology:

<table>
<thead>
<tr>
<th>GPU0</th>
<th>GPU1</th>
<th>GPU2</th>
<th>GPU3</th>
<th>m1x5_0</th>
<th>CPU Affinity</th>
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<tbody>
<tr>
<td>X</td>
<td>NV2</td>
<td>NV2</td>
<td>NV2</td>
<td>SYS</td>
<td>0-0,4-4,8-8,12-12,16-16,20-20,24-24,28-28,32-32,36-36</td>
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<tr>
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<td>X</td>
<td>NV2</td>
<td>NV2</td>
<td>SYS</td>
<td>0-0,4-4,8-8,12-12,16-16,20-20,24-24,28-28,32-32,36-36</td>
</tr>
<tr>
<td>NV2</td>
<td>NV2</td>
<td>X</td>
<td>NV2</td>
<td>SYS</td>
<td>1-1,5-5,9-9,13-13,17-17,21-21,25-25,29-29,33-33,37-37</td>
</tr>
<tr>
<td>NV2</td>
<td>NV2</td>
<td>NV2</td>
<td>X</td>
<td>SYS</td>
<td>1-1,5-5,9-9,13-13,17-17,21-21,25-25,29-29,33-33,37-37</td>
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<tr>
<td>SYS</td>
<td>SYS</td>
<td>SYS</td>
<td>SYS</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>

Legend:
- X = Self
- SYS = Connection traversing PCIe as well as the SMP interconnect between NUMA nodes (e.g., QPIUPI)
- NODE = Connection traversing PCIe as well as the interconnect between PCIe Host Bridges within a NUMA node
- PHB = Connection traversing PCIe as well as a PCIe Host Bridge (typically the CPU)
- PXB = Connection traversing multiple PCIe bridges (without traversing the PCIe Host Bridge)
- PIX = Connection traversing at most a single PCIe bridge
- NV# = Connection traversing a bonded set of # NVLinks
OSU Bandwidth Benchmark (osu_bw): Inter-node test

MVAPICH2 version 2.3.7
OSU Latency and Bandwidth (osu_latency, osu_bw) Benchmark
Intra-node, V100 nodes on Expanse

- Expanse - V100 nodes
- Latency between GPU 0, GPU 1: 1.51 µs
- Latency between GPU 1, GPU 2: 1.53 µs
- MVAPICH2 GDR 2.3.6, GCC 8.3.1
OSU Allreduce benchmark (osu_allreduce): 4096 cores

MVAPICH2 version 2.3.7, OpenMPI 4.1.3
OSU Alltoallv benchmark (osu_alltoallv): 2048 cores

MVAPICH2 version 2.3.4 through 2.3.7
## MVAPICH2 based Application Installs on Expanse

<table>
<thead>
<tr>
<th>Application</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RAxML</td>
<td>Code for sequential and parallel Maximum Likelihood based inference of large phylogenetic trees</td>
</tr>
<tr>
<td>Q-Chem</td>
<td>Commercial package for comprehensive ab initio quantum chemistry software for accurate predictions of molecular structures</td>
</tr>
<tr>
<td>AMBER</td>
<td>Suite of biomolecular simulation programs</td>
</tr>
<tr>
<td>LAMMPS</td>
<td>Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) Classical molecular dynamics code with a focus on materials modeling</td>
</tr>
<tr>
<td>NAMD</td>
<td>Parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems</td>
</tr>
<tr>
<td>ABINIT</td>
<td>Open-source software suite to calculate the optical, mechanical, vibrational, and other observable properties of materials</td>
</tr>
<tr>
<td>NEURON</td>
<td>Simulation environment for modeling individual and networks of neurons</td>
</tr>
<tr>
<td>TensorFlow w/ Horovod</td>
<td>Open-source platform for machine learning</td>
</tr>
<tr>
<td>PyTorch w/ Horovod</td>
<td>Open-source machine learning framework</td>
</tr>
</tbody>
</table>

*Additionally, libraries installed: e.g. hypre, fftw, hdf5, netcdf, netcdf, ncview*
NEURON Benchmark:
Large-scale model of olfactory bulb: 10,500 cells, 40K timesteps
ResNet50 Benchmark:
MVAPICH2-GDR 2.3.7, Horovod, V100 GPUs on Expanse

![Graph showing performance images per second (Imgs/s) vs GPUs]
AWP-ODC Performance on Expanse

<table>
<thead>
<tr>
<th>Expanse (640x320x2048)</th>
<th>Teraflop/s</th>
<th>Time (sec/step)</th>
</tr>
</thead>
<tbody>
<tr>
<td>gcc+mvapich2/2.3.7-gdr (2 nodes, 8 GPUs, A100) (non-cuda aware)</td>
<td>3.65</td>
<td>0.0361</td>
</tr>
<tr>
<td>gcc+mvapich2/2.3.7-gdr (2 nodes, 8 GPUs, A100)</td>
<td>4.03</td>
<td>0.0326</td>
</tr>
<tr>
<td>gcc+mvapich2/2.3.7-gdr (2 nodes, 8 GPUs, V100) (non-cuda aware)</td>
<td>2.40</td>
<td>0.0548</td>
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<tr>
<td>gcc+mvapich2/2.3.7-gdr (2 nodes, 8 GPUs, V100)</td>
<td>3.83</td>
<td>0.0342</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Expanse (640x640x2048)</th>
<th>Teraflop/s</th>
<th>Time (sec/step)</th>
</tr>
</thead>
<tbody>
<tr>
<td>gcc+mvapich2/2.3.7-gdr (4 nodes, 16 GPUs, V100) (non-cuda aware)</td>
<td>4.42</td>
<td>0.0599</td>
</tr>
<tr>
<td>gcc+mvapich2/2.3.7-gdr (4 nodes, 16 GPUs, V100)</td>
<td>6.09</td>
<td>0.0433</td>
</tr>
</tbody>
</table>

Credit: Dr. Yifeng Cui, Qinghua Zhou
Full results on MUG 2023 talk by Yifeng
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Category II System, NSF Award # 2005369

PI: Amit Majumdar (SDSC); Co PIs: Rommie Amaro (UCSD), Javier Duarte (UCSD), Mai Nguyen (SDSC), Robert Sinkovits (UCSD)
**Voyager** is a heterogeneous system designed to support complex AI workflows

- 42x Intel Habana Gaudi training nodes, each with 8 training processors (336 in total); all-to-all network between processors on a node
- Gaudi processors feature specialized hardware units for AI, HBM2, and on-chip high-speed Ethernet
- 2x Goya inference nodes, each with 8 Goya processors (16 in total)
- 36x Intel x86 processors compute nodes for general purpose computing and data processing
- 400 GbE interconnect using RDMA over Converged Ethernet
- 3 PB Storage system connected via 25GbE. Deployed as Ceph, but open to others
- 324 TB HFS; connectivity to compute via 25GbE

<table>
<thead>
<tr>
<th>System Component</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>INTEL GAUDI TRAINING NODES</strong></td>
<td></td>
</tr>
<tr>
<td>Node count</td>
<td>42</td>
</tr>
<tr>
<td>Training processors/node</td>
<td>8</td>
</tr>
<tr>
<td>Host x86 processors/node</td>
<td>2</td>
</tr>
<tr>
<td>Memory/node</td>
<td>512 GB DDR4</td>
</tr>
<tr>
<td>Memory/training processor</td>
<td>32 GB HBM2</td>
</tr>
<tr>
<td>Local NVMe</td>
<td>6.4 TB</td>
</tr>
<tr>
<td><strong>INTEL GOYA INFEERENCE NODES</strong></td>
<td></td>
</tr>
<tr>
<td>Node count</td>
<td>2</td>
</tr>
<tr>
<td>Inference processors/node</td>
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</tr>
<tr>
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<td>2</td>
</tr>
<tr>
<td>Memory/node</td>
<td>512 GB DDR4</td>
</tr>
<tr>
<td>Memory/inference processor</td>
<td>16 GB DDR4</td>
</tr>
<tr>
<td>Local NVMe</td>
<td>3.2 TB</td>
</tr>
<tr>
<td><strong>STANDARD COMPUTE NODES</strong></td>
<td></td>
</tr>
<tr>
<td>Node count</td>
<td>36</td>
</tr>
<tr>
<td>x86 processors/node</td>
<td>2</td>
</tr>
<tr>
<td>Memory capacity</td>
<td>384 GB</td>
</tr>
<tr>
<td>Local NVMe</td>
<td>3.2 TB</td>
</tr>
<tr>
<td><strong>STORAGE SYSTEM</strong></td>
<td></td>
</tr>
<tr>
<td>High performance storage: HDD:NVMe</td>
<td>3 PB:140 TB</td>
</tr>
<tr>
<td>High performance filesystems</td>
<td>Ceph, Lustre</td>
</tr>
<tr>
<td>Home filesystem storage: HDD:NVMe</td>
<td>324 TB: 12.4 TB</td>
</tr>
<tr>
<td>File system</td>
<td>NFS</td>
</tr>
</tbody>
</table>
Gaudi: Architected for performance and efficiency

- Fully programmable Tensor Processing Cores (TPC) with tools & libraries
- Configurable Matrix Math Engine (GEMM)
- Multi-stage memory hierarchy with 32GB HBM2 memory
- Integrated 10 x 100 Gigabit Ethernet for multi-chip scale-out training
Voyager’s three distinct networks support application performance, data movement, and systems management

- 400 GbE for scale-out training
  - Six connections from each Gaudi node to a single 230 Tbps Arista 7808 non-blocking switch

- 25 GbE Bonded Control and data network
  - Every node has a bonded 50GbE (2 X 25GbE) connection.

- 1 GbE out-of-band management network for IPMI and other traffic.
Gaudi servers supports all-to-all connectivity

- 8 Gaudi OCP OAM cards
- 24 x 100GbE RDMA RoCE for scale-out
- Non-blocking, all-2-all internal interconnect across Gaudi AI processors
- Separate PCIe ports for external Host CPU traffic

Example of Integrated Server with eight Gaudi AI processors, two Xeon CPU and multiple Ethernet Interfaces
Gaudi design enables highly efficient scaling

- Natively integrated RoCE on Gaudi processor
- 6x Quad-100 GbE per node (8x Gaudi)
- 7808 Arista 400 GbE switch
6x400 connections from each Gaudi node to Arista 400GbE non-blocking switch

200 Tb/s of bandwidth (42x6x400)
Software Stack Overview: Synapse AI

- Train deep learning models on Gaudi with minimal code changes
- Natively integrated with TensorFlow & PyTorch
- Popular computer vision and NLP models
- Habana Developer Site & GitHub
- Support with reference models, kernel
- Libraries, docs & “how-to” guides
- Advanced users can write their own custom software kernels

Containerized Software Stack

https://vault.habana.ai

Experience using MVAPICH2 on Voyager

• Dr. Panda’s group provided the MVAPICH2 complied install binaries and libraries. The install is done to host path location mounted within a Kubernetes pod making it easily usable by others.

• MPI jobs on Voyager are run using the Kubeflow MPI operator. The MVAPICH2 install can be bind mounted into the right location in the pods:

```
volumeMounts:
- name: home
  mountPath: /home/mahidhar
- name: mv2install
  mountPath: /usr/local/apps/mvapich2gdr
```

• With this mount addition, the install is usable by all users with host access to the install location.
MVAPICH2 on Voyager

- MVAPICH2 Install location on host
- Container image with Synapse AI software
- MVAPICH2 mount location in Kubernetes worker pods
MVAPICH2 on Voyager

```bash
~/shared/MPI# /usr/local/apps/mvapich2gdr/bin/mpirun_rsh -np 8 -hostfile /home/mahidhar/hosts MVZ_ENABLE_GPU=1 MVZ_IS_PT2PT=0 LD_PRELOAD=/usr/local/apps/mvapich2gdr/lib/libmpi.so /usr/local/apps/mvapich2gdr/libexec/osu-micro-benchmarks/mpi/collective/osu_allreduce -d synp
  * Starting OpenBSD Secure Shell server sshd
    ...done.

# OSU MPI-SYNP Allreduce Latency Test v7.0
# Size    Avg Latency(us)
  4        79.67
  8        75.30
  16       74.61
  32       75.79
  64       76.80
  128      75.29
  256      77.00
  512      74.93
  1024     72.27
  2048     71.40
  4096     72.53
  8192     72.66
 16384     77.78
 32768     73.96
 65536     74.68
 131072    75.96
 262144    75.52
 524288    72.74
1048576    73.39
```

Credit: Chen-Chun, OSU; Full details in Chen-Chun’s MUG 2023 talk
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Center For Western Weather and Water Extremes (CW3E) has made exclusive use of Comet starting July 2021 after it was retired from NSF XSEDE/ACCESS service

Comet is being used for West-WRF ensemble runs during wet-seasons for near real-time forecasts. In addition, it used by CW3E researchers for several research projects.

Managed by the San Diego Supercomputer Center (SDSC)

Represents over 1 billion core hours (SUs) of computing over the period of 2.5 years from July 2021 through December 2023

Highlights: ~440 M CPU hours / year, ~1.2 M GPU hours / year, >12 PB of storage
Comet Network Architecture

InfiniBand compute, Ethernet Storage

- **Node-Local Storage**
  - 320 GB
  - 72 HSWL
  - 36 GPU
  - 4 Large Memory

- **FDR 36p**
  - 18 switches
  - 27 racks

- **Core InfiniBand**
  - (2 x 108-port)

- **18-Ethernet Bridges**
  - (4 x 18-port each)

- **Arista 40GbE**
  - (2x)

- **CW3E Lustre Storage**
  - 12 PB, 2MDS, 18 OSS

- **Research and Education Network Access Data Movers**
  - Internet 2
  - Juniper 100 Gbps
  - Arista 40GbE (2x)
  - Data Mover Nodes

- **Additional Support Components**
  - (not shown for clarity)
  - Ethernet Mgt Network (10 GbE)
  - NFS Servers for Home Directories
  - Virtual Image Repository
  - Gateway/Portal Hosting Nodes
  - Login Nodes
  - Rocks Management Nodes

- **72 HSWL**
  - 7x 36-port FDR in each rack wired as full fat-tree, 4:1 over subscription between racks.
Motivation for INAM on Comet

- CW3E workloads can involve both IO intensive and communication intensive workloads. Sometimes this leads to performance issues. The goal is to use both historical and live data to troubleshoot such issues.
- Monitoring of network fabric health, utilization with notification thresholds set for errors and utilization.
- Enable Lustre traffic monitoring to get a handle on the IO aspect of workloads
- Use MPI information from jobs in combination with Lustre info to evaluate impact on network
INAM Experience on Comet

• OSU INAM group helped build a custom INAM RPM for Comet OS and OFED stack.

• There was an issue parsing the switch map file. Worked ok after we removed all of the blank lines in our map file. Suggestion to fix as the map file can be parsed as is by other tools.

• At present the install is setup for internal use. Will need user/auth setup additions to enable end user access.

• PhantomJS took some time to build up cached info initially, but web service has been good since.

• We will be installing INAM for Expanse as well. Plan to evaluate use of ClickHouse DB backend.
Rack Level Network View from INAM

- 18 nodes per switch
- 4 switches at first level that feed into 3 switches in the next tier
Network Views from INAM

Single Switch with 18 nodes

Node LID, GUID, Name info
## Notifications from INAM

### Notifications & Criteria

<table>
<thead>
<tr>
<th>Notification ID</th>
<th>Criteria ID</th>
<th>Category</th>
<th>Metric</th>
<th>Condition</th>
<th>Threshold Value</th>
<th>Time</th>
<th>Additional Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1</td>
<td>Port Counters</td>
<td>Symbol errors</td>
<td>Greater than</td>
<td>50</td>
<td>22 Aug 2023 15:33:30</td>
<td><code>MFS;switch-01588ee5:0000:000:0000:000;1 - comet-34-08 HCA-1 (52480d073f03050c:39e1), MFS;...</code></td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>Port Counters</td>
<td>Link utilization (percentage)</td>
<td>Greater than</td>
<td>95</td>
<td>22 Aug 2023 09:25:57</td>
<td><code>comet-01-LO1 (b0146214038008e4330);7 - cv2a-00a-1-9 HCA-1 (b0b8428103009000)</code></td>
</tr>
</tbody>
</table>

Showing 1 to 2 of 2 rows

### Notification Criteria

<table>
<thead>
<tr>
<th>Criteria ID</th>
<th>Category</th>
<th>Metric</th>
<th>Comparison</th>
<th>Threshold Value</th>
<th>Is Recurring</th>
<th>Action</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>Port Counters</td>
<td>Symbol errors</td>
<td>Greater than</td>
<td>50</td>
<td>✔</td>
<td>✔</td>
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<tr>
<td>2</td>
<td>Port Counters</td>
<td>Link downed</td>
<td>Greater than</td>
<td>1</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>3</td>
<td>Port Counters</td>
<td>Link utilization (percentage)</td>
<td>Greater than</td>
<td>95</td>
<td>✗</td>
<td>✔</td>
</tr>
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</table>

Showing 1 to 3 of 3 rows
Notifications from INAM

### Notifications & Criteria

<table>
<thead>
<tr>
<th>Notification ID</th>
<th>Criteria ID</th>
<th>Category</th>
<th>Metric</th>
<th>Additional Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1</td>
<td>Port Counters</td>
<td>Symbol errors</td>
<td>MFO:switch-928eee:5X6036/U1 (0x248a070300f25580):11 - comet-34-08 HCA-1 (0x248a0703005c39e1)</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>Port Counters</td>
<td>Link utilization (percentage)</td>
<td>MFO:switch-928eee:5X6036/U1 (0x248a070300f25580):12 - comet-34-07 HCA-1 (0x248a0703005c39f1)</td>
</tr>
</tbody>
</table>

Showing 1 to 2 of 2 rows
Job level view from INAM
Summary

- MVAPICH2 and MVAPICH2-GDR used as the performant option for several application on Expanse.
- Voyager - Heterogenous system designed for AI workloads. Currently in 3-year testbed phase. MVAPICH2 development and testing ongoing.
- INAM installed and in use on Comet. Will be used for network health/performance monitoring and to identify sources of congestion. An install is planned on Expanse as well.
- Upcoming work includes use of MVAPICH2 on the Prototype National Research Platform (PNRP) which is a nationally distributed, open system that features CPUs, FP32- and FP64- optimized GPUs, and FPGAs.
Thank you to our collaborators, partners, users, and the SDSC team!
Voyager would not be possible without a dedicated team of professionals and experts

Rommie Amaro
Haisong Cai*
Trevor Cooper
Chris Cox*
Javier Duarte
Tom Hutton*
Christopher Irving*
Marty Kandes
Amit Majumdar
Tim McNew*
Dmitry Mishin
Mai Nguyen
Susan Rathbun
Paul Rodriguez
Scott Sakai
Manu Shantharam
Robert Sinkovits
Fernando Silva*
Shawn Strande
Tom Tate*
Mahidhar Tatineni
Mary Thomas
Cindy Wong
Nicole Wolter

Supermicro Team
Habana Team
Arista

* A special thanks to the HPC Systems Group and the Data Center staff who performed onsite work under COVID restrictions to get the system ready for production.