Overview of the Computer Resource Team (CRT)

Tim Fahey (Lawrence Livermore National Lab)
Ben Santos (Los Alamos National Lab)
Heidi Uphoff (Sandia National Labs)

PSAAP III Kickoff Meeting
Wednesday August 19, 2020  (Via WebEx)
Overview

- What is the CRT?
- What the CRT can do for you
- HPC customer support and problem tracking
- Training
- Documentation
- Communications
- Dedicated Runs
- Site visits
- Allocations
- LLNL compute resources
- LANL compute resources
- Sandia compute resources
- Getting accounts - SARAPE
The Computer Resource Team (CRT) is the component of the PSAAP III program that connects center researchers with the High Performance Computing (HPC) resources required to perform their work.

The CRT is comprised of representatives from each NNSA Lab who are familiar with their Lab's computing resources, personnel and policies. The following individuals serve on the CRT:

- Tim Fahey, LLNL  fahey2@llnl.gov
- Ben Santos, LANL  bsantos@lanl.gov
- Heidi Uphoff SNL  hauphof@sandia.gov

Our primary purpose is to provide assistance and guidance in all aspects related to the use of HPC resources located at LANL, LLNL, and Sandia.
What the CRT Can Do For You?

- Assist with the establishment and use of computer accounts
- Assist with accessing compute resources
- Provide essential HPC user documentation
- Provide technical support and referral to in-depth consulting
- Conduct periodic telecons to keep PSAAP users up-to-date with account, access, policy, scheduling and technical issues, and to address issues with HPC platform usage
- Interface with other individuals and groups within the Labs, such as management, networking, system administration, storage, customer support, etc., to facilitate the effective support of PSAAP users
- Track and facilitate the resolution of problems reported to each Labs' customer support “hotline”
- Provide training opportunities
What the CRT Can Do For You? (cont)

- Collect and distribute monthly machine usage statistics
- Schedule and support special/dedicated runs
- Maintain a balance of machine usage between the PSAAP centers (if needed)
- Visit PSAAP centers to discuss HPC resources, user issues and to offer technical consultation and/or training
- Showcase PSAAP research in the NNSA/ASC or DOE research exhibit booth at the annual SC conference
HPC Customer Support and Problem Tracking

- All three labs offer HPC customer support via phone and email:
  - LLNL: Livermore Computing Hotline
  - LANL: ICN Consulting Office
  - Sandia: HPC OneStop Service Desk
- Includes support for user accounting issues and for technical assistance.
- Problems and questions are tracked via a customer support database application (varies with each Lab).
- Most problems/questions are handled directly by the customer support staff on duty.
- More in-depth issues are typically referred to local subject experts.
- The labs also coordinate with hardware and software vendors for issues that require outside support.
- CRT reps coordinate routinely with each other on Tri-lab user issues.
HPC Training

Training is important – especially for new users

- Online tutorials are available
- Workshops conducted at the Labs are open to PSAAP center users
- The CRT can deliver workshops/training at your center or virtually
- The CRT can also assist with topic specific, customized workshops if that is of interest

Topics include:

- Getting started information
- Compilers
- Performance tools
- Debuggers
- Parallel programming (MPI, OpenMP, Pthreads…)
- Batch schedulers
- Machine architectures
- Visualization tools
- …
The first Getting Started training session has been scheduled for 9/2/20, 1:00PM EDT/10:00AM PDT.
Training will be held via WebEx.
All PSAAP3 users can attend regardless of account status.
This initial training will be lecture based.

<table>
<thead>
<tr>
<th>Time (EDT)</th>
<th>Topic</th>
<th>Speaker</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:00</td>
<td>Introductions</td>
<td>Jane Herriman, LLNL</td>
</tr>
<tr>
<td>1:05</td>
<td>SARAPE account request process</td>
<td>Heidi Uphoff, SNL</td>
</tr>
<tr>
<td>1:15-2:00</td>
<td>LLNL Resources and Environment</td>
<td>Don Frederick, LLNL</td>
</tr>
<tr>
<td>2:00-2:45</td>
<td>LANL Resources and Environment</td>
<td>Giovanni Cone, LANL</td>
</tr>
<tr>
<td>2:45-3:00</td>
<td>Break</td>
<td></td>
</tr>
<tr>
<td>3:00-3:45</td>
<td>SNL Resources and Environment</td>
<td>Heidi Uphoff, SNL</td>
</tr>
<tr>
<td>3:45</td>
<td>Q &amp; A</td>
<td></td>
</tr>
</tbody>
</table>
Most of what users need to know is available online via web pages hosted by each of the Labs. Recommended starting points:

- **LLNL**
  - [https://hpc.llnl.gov/user-portal](https://hpc.llnl.gov/user-portal)
  - [https://hpc.llnl.gov/training/tutorials](https://hpc.llnl.gov/training/tutorials)

- **LANL**
  - [https://hpc.lanl.gov](https://hpc.lanl.gov) (LANL Cryptocard)
  - [https://hpcinfo.lanl.gov](https://hpcinfo.lanl.gov) (Dashboards)

- **Sandia**
  - [https://computing.sandia.gov](https://computing.sandia.gov)

- **Note:** Most LLNL web pages are open – no authentication required. Most Sandia / LANL pages require authentication.

- **Quick Start Guide for new PSAAP users:**
  - [https://asc.llnl.gov/content/assets/docs/Alliance.Quickguide.pdf](https://asc.llnl.gov/content/assets/docs/Alliance.Quickguide.pdf)
Communications

- Monthly telecons
  - Forum for discussion/questions on user topics such as accounts, access, technical issues, machine schedules, etc.
  - Open to all PSAAP center users
  - Highly recommended to have a Point-of-Contact (POC) person with some technical/computing experience from each Center attend. We'll be in touch with each Center's PI to find out who this might be.
  - Third Thursday of the month, 2:00PM EDT/11:00AM PDT
    - First call 9/17/2020; webex information on recurring meeting forthcoming

- Email list - psaap-crt-llnl@llnl.gov
  - Telecon minutes and machine usage statistics are distributed via this list to all PSAAP Center PIs & POCs, ASC HQ and various staff & managers within the Labs
  - Let us know if you want anyone else at your Center added to our list - initially it includes only your PI and POC
Communications

- Usage stats
  - Collected by each Lab's computing center and distributed with the telecon minutes
  - Present both aggregate and detailed usage (down to the user level)

- Email & phone
  - The CRT can be contacted directly by you and any of your Center's users:
    - Tim Fahey (LLNL) fahey2@llnl.gov 925-422-4228
    - Ben Santos (LANL) bsantos@lanl.gov 505-665-6153
    - Heidi Uphoff (Sandia) hauphof@sandia.gov 505-844-6119
Dedicated Runs (DATs)

- Normally, users submit their jobs to a batch system using a standard Tri-lab SLURM or LSF batch scheduler interface:
  - Jobs are then queued to wait their turn for execution.
  - There are limits on the number of nodes and number of hours that a job can use.

- Dedicated application time - DAT: can be requested by any PSAAP user:
  - Overrides normal node limits - up to the full machine
  - Overrides normal time limits
  - Typically conducted on weekends at LLNL, LANL date flexible but prefer 2-week lead time

- How to request a DAT:
  - LLNL: https://hpc.llnl.gov/accounts/forms/asc-dat
  - LANL: https://hpc.lanl.gov/dat_request
Site Visits

- Historically the CRT has been available to visit PSAAP centers:
  - Visits (2-4 hrs) by the CRT and other Lab staff
  - Focus is on the center’s *users* of HPC computing resources
  - Updates on architectures, policies, future plans at the Labs
  - Forum for discussing user issues, problems, questions
  - Not to be confused with TST visits or reviews

- Technical "training" sessions were offered if desired

- In our current environment is is highly likely these will be virtual. The CRT will work with each center to schedule these sessions.
Allocations - Production Machines

PSAAP centers have allocations on eight ASC funded, Tri-lab production machines:

- PSAAP allocations vary by machine; shared at the group level
- Able to use more than allocation if there are available cycles

<table>
<thead>
<tr>
<th>Machine</th>
<th>Lab</th>
<th>Total available core-hr/mo</th>
<th>PSAAP allocation</th>
<th>PSAAP total core-hr/mo</th>
</tr>
</thead>
<tbody>
<tr>
<td>QUARTZ</td>
<td>LLNL</td>
<td>78,209,280</td>
<td>31.25%</td>
<td>24,440,400</td>
</tr>
<tr>
<td>LASSEN*</td>
<td>LLNL</td>
<td>25,310,560</td>
<td>10.0%</td>
<td>2,531,056</td>
</tr>
<tr>
<td>SOLO</td>
<td>Sandia</td>
<td>9,828,720</td>
<td>1.0%</td>
<td>98,287</td>
</tr>
<tr>
<td>ECLIPSE</td>
<td>Sandia</td>
<td>39,104,640</td>
<td>1.0%</td>
<td>391,046</td>
</tr>
<tr>
<td>ATTAWAY</td>
<td>Sandia</td>
<td>39,104,640</td>
<td>1.0%</td>
<td>391,046</td>
</tr>
<tr>
<td>GRIZZLY</td>
<td>LANL</td>
<td>39,157,200</td>
<td>1.0%</td>
<td>391,572</td>
</tr>
<tr>
<td>SNOW</td>
<td>LANL</td>
<td>9,671,040</td>
<td>1.0%</td>
<td>96,710</td>
</tr>
<tr>
<td>CAPULIN</td>
<td>LANL</td>
<td>7,154,000</td>
<td>1.0%</td>
<td>71,540</td>
</tr>
</tbody>
</table>

* Lassen allocation is subject to change
**Quartz**

- Intel Xeon E5-2695v4 (Broadwell) architecture; 2.1 GHz
- 3018 nodes with 36 cores each
- 108,648 total cores
- 128 GB memory per node; 344,064 TB total memory
- Omni-Path interconnect; ~100 Gb/sec pt2pt MPI
- 3.23 petaflops peak
- Details at [https://hpc.llnl.gov/hardware/platforms/Quartz](https://hpc.llnl.gov/hardware/platforms/Quartz)
LLNL PSAAP Compute Resources

- **Lassen**
  - IBM Power 9 architecture at 3.5 GHz
  - 792 compute nodes with 44 cores each; 34,848 total cores
  - 4 NVIDIA V100 GPU’s per node; 3168 total GPU’s
  - 256 GB CPU-memory and 64 GB GPU-memory per node
  - Infiniband EDR interconnect
  - 23 petaflops peak
  - Details at [https://hpc.llnl.gov/hardware/platforms/lassen](https://hpc.llnl.gov/hardware/platforms/lassen)
**LLNL PSAAP Compute Resources**

- **HPSS Archival Storage**
  - Mounted from all unclassified production clusters
  - Users automatically get an HPSS account with their machine accounts
  - 300TB quota for FY2020
  - 154 PB total archive storage
  - 6 PB disk cache

- **Visualization Cluster – Pascal**
  - Intel Xeon E5-2695 v4 (Broadwell)
  - 164 nodes, 36 cores/node
  - 2 NVIDIA Tesla P100 GPUs/node
  - 256GB memory/node
  - 16GB GPU global memory/node
  - Available upon request
LANL PSAAP Compute Resources

Ben Santos
LANL PSAAP Compute Resources

- **Grizzly**
  - Intel Xeon Broadwell E5-2695 2.1 GHz
  - 1490 nodes with 36 cores each; 53640 total cores
  - 128 GB memory per node; 191 TB total memory
  - Intel OmniPath interconnect
  - 1806 teraflops peak
  - 23.5 PB Lustre (global scratch)
  - [https://hpc.lanl.gov/grizzly_home](https://hpc.lanl.gov/grizzly_home)
LANL PSAAP Compute Resources

- **Snow**
  - Intel Xeon Broadwell E5-2695 2.1 GHz
  - 368 nodes with 36 cores each; 13248 total cores
  - 128 GB memory per node; 47.1 TB total memory
  - Intel OmniPath interconnect
  - 445 teraflops peak
  - 23.5 PB Lustre (global scratch)
  - [https://hpc.lanl.gov/snow_home](https://hpc.lanl.gov/snow_home)
LANL PSAAAP Compute Resources

- **Capulin**
  - Cray XC50 Cavium ThunderX2 ARM
  - 175 nodes with two TX2 56 cores per node; 9800 total cores
  - 256 GB memory per node; 45 TB total memory
  - Cray Aries interconnect
  - 196 teraflops peak
  - 23.5 PB Lustre (global scratch)
  - [https://hpc.lanl.gov/capulin_home](https://hpc.lanl.gov/capulin_home)
LANL PSAAAP Compute Resources

- **Turquoise Archival Storage**
  - Accessible from ar-tn.lanl.gov via wtrw.lanl.gov
  - Mounts the scratch spaces, internet staging and archive
  - [http://hpc.lanl.gov/turquoise_archive](http://hpc.lanl.gov/turquoise_archive)

- **Fast File Transfer Service**
  - Data Transfer Nodes (DTN)
    - Globus supported endpoint ([https://hpc.lanl.gov/globus_intro](https://hpc.lanl.gov/globus_intro))
    - Utilize scp and parallel bbcp
  - Uses a 2-hop method (temporary internet staging storage)
  - [https://hpc.lanl.gov/dtn](https://hpc.lanl.gov/dtn)
Sandia PSAAP Compute Resources

Heidi Uphoff
Sandia PSAAP Compute Resources

- ECLIPSE

  - Intel Broadwell E5-2695 v4; 2.1 GHz
  - 1,488 nodes with 36 cores each; 53,568 total cores
  - 128 GB memory per node
  - Intel Omni-Path high speed interconnect / Mellanox ConnectX4
  - 1.800 petaflops peak
  - In SARAPE, request "SRN Capacity Clusters" (US citizenship required)
ATTAWAY

- Intel Xeon Gold 6140; 2.3 GHz
- 1488 nodes with 36 cores each; 53,568 total cores
- 192 GB memory per node
- Intel Omni-Path high speed interconnect / Mellanox ConnectX4
- 3.943 petaflops peak
- In SARAPE, request "SRN Capacity Clusters" (US citizenship required)
Sandia PSAAP Compute Resources

- **SOLO**
  - Intel Broadwell E5-2695 v4; 2.1 GHz
  - 374 nodes with 36 cores each; 13,464 total cores
  - 128 GB memory per node
  - Intel Omni-Path high speed interconnect / Mellanox ConnectX4
  - 460 teraflops peak
  - In SARAPE, request “ECN Capacity Clusters”
Sandia PSAAP Compute Resources

- **Sandia Mass Storage System (SMSS)**
  - High Performance Storage System (HPSS) provides high-end near-line storage for HPC systems
  - In SARAPE, request “Restricted Sandia Mass Storage System (RSMSS)” for the SRN network and “ECN Capacity Clusters” for the ECN and OHPC network.

- **LYNX**
  - Sandia’s HPC file transfer agent nodes
  - Mounts the same parallel file systems available on the compute clusters
  - 10 gigabit and InfiniBand (IB) technology to optimize file transfer performance to/from Sandia SMSS
  - High performance data transfer tools HSI, HTAR, and PFTP
  - In SARAPE, request "SRN Capacity Clusters"
Testbed systems

- Request accounts through SARAPE (sarape.sandia.gov)
- Research systems from several vendors
- Some require NDAs
- Not for production computing
- Systems come and go, lifetime usually a year or less
- Users cannot expect mature hardware/software
- Support available via Sandia HPC OneStop (e.g. email to <machine-name>-help@sandia.gov)
- In-depth support typically provided by research teams
Not for production computing cycles - but can be provided to Test Pilot users
Both hardware and software are intended to be highly dynamic
Closer to prototypes and technology development drivers
Multiple nodes available but more important to explore a diverse set of architectural alternatives, than push large scale
Available for PSAAP access, via SARAPE.

<table>
<thead>
<tr>
<th></th>
<th>Mayer</th>
<th>White</th>
<th>Blake</th>
<th>Morgan</th>
<th>Stria</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>CPU</strong></td>
<td>4 Computes B0 ThunderX2 (beta) 43 computes A1 ThunderX2</td>
<td>Dual IBM Power 8, 10 cores</td>
<td>Dual-Socket Intel Xeon Platinum</td>
<td>Five dual socket Intel IvyBridge with Xeon Phi co-processor and four Intel 32-core Haswell nodes</td>
<td>2.0 GHz Arm Cavium Thunder-X</td>
</tr>
<tr>
<td><strong>Accelerator</strong></td>
<td>None</td>
<td>NVIDIA K40 2 per node</td>
<td>None</td>
<td>Intel Xeon Phi Co-processor (codenamed Knights Corner) 2 per node</td>
<td>None</td>
</tr>
<tr>
<td><strong>Nodes</strong></td>
<td>47</td>
<td>9</td>
<td>40</td>
<td>9</td>
<td>266</td>
</tr>
<tr>
<td><strong>Interconnect</strong></td>
<td>Mellanox EDR Infiniband with SocketDirect</td>
<td>Mellanox EDR Infiniband</td>
<td>Intel OmniPath</td>
<td>Mellanox Quad Data Rate Infiniband</td>
<td>Infiniband</td>
</tr>
<tr>
<td><strong>Other</strong></td>
<td>n/a</td>
<td>Technology on the path to anticipated CORAL systems</td>
<td>Each processor core has dual AVX512 vector processing units that are FMA capable.</td>
<td>Hetero testbed on restricted network</td>
<td>* On SRN network (US citizenship required)</td>
</tr>
</tbody>
</table>

http://www.sandia.gov/asc/computational_systems/HAAPS.html
Each Lab has its own policies, forms and procedures, however there is a single-entry portal (sarape.sandia.gov) for requesting an account at any of the 3 Labs.
Computer Accounts - SARAPE

- Centers need at least one account authorizer (also called a GPA). This can be a PI, POC and/or a trustworthy, knowledgeable designee.

- Account authorizers are responsible for overseeing and approving (via SARAPE) the accounts for all of their Center's users. Here's who we have as of today:
  - Colorado – Richard Regueiro
  - Illinois - Mike Anderson
  - Stanford – Corinne Beck, Vi Nguyen
  - Texas – Karl Schulz
  - Buffalo – James Chen
  - MIT – Jean Sofronas
  - Maryland – Johan Larsson
  - New Mexico – Tracy Wenzl
  - Oregon State - Kyle Niemeyer

- Having a “backup” authorizer is important if the primary authorizer is often not available.
After a SARAPE account request is approved by the Center's account authorizer, it is routed to the appropriate Lab for review, collection of additional information and approval.

- Typically takes 1-2 weeks for US citizens
- Account processing for non-US citizens requires additional time and “paperwork” - allow 30-90 days (plan ahead!).
- Lilia Martinez (Sandia: lmartin@sandia.gov 505-845-7967 ) manages the sarape.sandia.gov user accounts portal and has already contacted the PIs of each PSAAP II Center to get the account request process going.

- Questions? Contact Lilia Martinez or one of the CRT representatives.
Questions?
Backup