subMIT Overview

Josh Bendavid Basic Computing Services (subMIT) Review July 18, 2023

Introduction

- subMIT system provides an interactive login pool + scale-out to batch resources
 - Home directories
 - Convenient software environment (CentOS7 native, docker/singularity images, conda)
 - SSH or Jupyterhub access
 - Local batch system with O(1000) cores, >50 GPU's
 - Additional storage for software installation/development, large datasets
 - Convenient access to larger external resources (OSG, CMS Tier-2 and Tier-3, LQCD Cluster, EAPS)
- User support is a key feature of the system
 - Beyond basic troubleshooting
 - Help users make optimal use of the available resources
 - Expert advice on designing/improving workflows
 - Customize and evolve system configuration to accommodate user needs as appropriate

Introduction

- Storage and networking
 - Local storage (1TB/user), 10's of TB for larger group datasets
 - 30TB of ultra-fast NVME storage with room for future expansion
 - Fast networking: 100 Gbps ethernet
 - RoCE (RDMA over Converged Ethernet) has been partially tested/commissioned, should be possible for MPI applications
- Additional resources recently or currently being integrated
 - More disk storage (100TB contributed from ABRACADABRA)
 - Integration of existing computing resources from research groups
 - Purchase of several large core count/high memory machines by research groups for additional computing resources and to support specialized workflows and/or R&D where large single node scaling is useful
 - Current "high density" template, Dual AMD EPYC 192 core/384 thread with 0.75-1.5TB of memory

Physical Location and Infrastructure Support:

- Physical location: Machines at both Bates and Building 24 up to now
 - 100 Gbps uplink in both locations
 - Split physical location doesn't make sense for a facility of this size
 - Single location also strongly preferred for RoCE (RDMA) support
 - B24 preferred for local maintenance and support reasons
 - Network and power have been recently upgraded, current infrastructure is sufficient for a system of this size + reasonable expansion
 - Power reliability in Bates was also a concern up to this point
 - Remaining services and hardware at Bates in process of being migrated to B24
 - Expected completion in August
- Infrastructure support
 - From the fall onwards infrastructure support for subMIT is needed in B24 but not at Bates
 - LNS computing support for subMIT in B24 provided through Paul Acosta and Dave Newman
 - Infrastructure: Racks, Power, Networking
 - Network: hostnames, IP addresses, user authentication, interface with IS&T
 - Redmine server for ticketing system (also used beyond subMIT project)

Introduction: subMIT Website



Overview News People Contact About Users Guide JupyterHub

Overview

The subMIT login pool is designed to let users login safely, prepare and test their research, and submit their jobs to the large computing resource of their choice. There are for now a limited number of resources connected but we are working on quickly expanding them.



- Website (with User's Guide/Instructions): <u>https://submit.mit.edu/</u>
 - Overview and general information
 - Direct JupyterHub access
 - User's Guide:

https://submit.mit.edu/submit-users-guide/



Introduction: Project Organization

- Formally the project is organized as *Basic Computing Services* in the Physics Department
 - **Project Team:** Implementation/Operations/Maintenance of the system
 - **Users Group:** Contact point between the user community and the project team, forum for user feedback, requests, information flow to and from users
 - **Steering Committee:** Faculty oversight, funding, etc
 - See https://submit.mit.edu/?page_id=6

Users Group In Practice

- Monthly meetings
 - Advertised and open to the broader community
 - Topical presentations from project team, Users Group representatives, or other users or community members
 - Forum for feedback and information flow between the user community and the project team
 - Regular timeslot: Tuesday 10:00-11:00 EST
 - Next meeting: Tuesday July 25: <u>https://indico.mit.edu/event/802/</u>
- Users Group representatives
 - Identified representatives from research groups across the department
 - Attend the monthly meetings
 - Provide feedback from your groups/community
 - Distribute information/news from the project team

Users Group Representatives

- Users group has been formed (JB as coordinator)
- Current Users Group representative (associated faculty/group)
 - Yin Lin (Phiala Shanahan)
 - Siddharth Mishra-Sharma (Jesse Thaler)
 - Prajwal Mohan Murthy (Bob Redwine)
 - Kaliroë Pappas (LNS Neutrino/Dark Matter)
 - Sunghan Ro (Julien Tailleur)
 - Yitian Sun (Tracy Slatyer)
 - Molly Taylor (LNS Heavy Ion Group)

Users Group Meetings

- E.g. presentation from April Users Group meeting on Visualization of Geant Simulations on subMIT
- <u>https://indico.mit.edu/event/752/</u>



Users Group Meeting Tuesday Apr 25, 2023, 10:00 AM → 11:00 AM America/New_York Kolker Room (26-414) (MIT) Description https://mit.zoom.us/i/96743699673?pwd=b3h2O3c3cVOwYW12blhMUG5SWXZCZz09 10:00 AM → 10:10 AM News/Introduction Speakers: Joshua Bendavid (Massachusetts Institute of Technology), Matthew Heine (staff@mit.edu) UserGroup_04_25_2... 10:10 AM → 10:30 AM Visualization of Geant Simulations Speaker: Richard Foster (Massachusetts Institute of Technology) Foster_SubMIT_Par...
Foster_SubMIT_Par... 10:30 AM → 10:45 AM Roundtable Speakers: Kaliroe Pappas (MIT laboratory for nuclear science), Molly Taylor (Massachusetts Institute of Technology), Prajwal Mohan Murthy (MIT LNS), Siddharth Mishra-Sharma (MIT), Sunghan Ro (MIT), Yin Lin (Massachusetts Institute of Technology), Yitian Sun (Massachusetts Institute of 10:45 AM → 11:00 AM Discussion ⊙15m Q-

Storage breakdown

- Several different storage areas are available covering different use cases
 - /home/submit/<username>
 - Home directories (nfs server), redundant disk array with backups
 - 5GB quota
 - Use for software development and (small) critical data
 - /work/submit/<username>
 - Work directory (nfs server), no backups (but redundant disk array)
 - 50GB quota
 - Use for software installation (conda or docker/singularity images)
 - /data/submit/<username>
 - Large distributed disk system, no backups, but redundancy against disk failure ("erasure coding")
 - 1TB user quota, larger quotas available in dedicated group directories
 - Store large datasets here
 - /scratch/submit/<username>
 - Fast NVMe SSD array
 - Commissioned by several groups for high performance data analysis
 - o /cvmfs/
 - Read-only distributed storage for distributing software, singularity images, etc
 - Several CERN-related repositories are available
 - Local repository /cvmfs/cvmfs.cmsaf.mit.edu where additional software or data can be added if needed
- Flexible tiered storage system, can accommodate a wide range of user needs
- Larger datasets encouraged to use shared group space, but quotas can be increased when needed

Interactive Use: Terminal or JupyterHub



Select a job profile:

Slurm - Submit - 1 CPU, 500 MB

Quick introduction: Spawn server menu · Slurm - Submit - 1 CPU, 500 MB: spawns a server on submit slurm partition Slurm - Submit - 2 CPUs, 1000MB; similiar as above, with more resources allocated. · Slurm - SubmitGPU - 1 GPU: spawns a server on submit-gpu slurm partition, requesting 1 GPU. · Slurm - SubmitGPU1080 - 1 GPU: spawns a server on submit-gpu1080 slurm partition, requesting 1 GPU. Local server - Submit01 - 1 CPU. 500 MB. /home/submit/(username)/: spawns on submit01. in your /home/submit/(username)/ directory. Local server - Submit01 - 1 CPU, 500 MB, /work/submit/{username}/: spawns on submit01, in your /work/submit/{username}/ directory · GPUs: you can use GPU resources in your notebooks or Jupyterhub's terminal if you spawn a server on submit-opu or submit-opu 1080 supported through Slrum. · Conda: your conda environments should be automatically loaded as kernels by Jupyterhub, and can be used in notebooks. See User Guide for more info · Singularity: you can manually set up a kernel based on a singularity environment's python. See User Guide for more info For more information about Submit, conda, GPUs, Jupyterhub, etc., see



For any questions, comments, or feedback, please send an email to submit-jupyter.

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Interactive Jupyter session available directly from website with touchstone authentication (subMIT account still required)

- SLURM is used to efficiently share resources between interactive and batch use
- Primary usage is research, but education applications also possible
 - Limited trial has been conducted for 802 exercises

Communication Channels

- User support mailing list: submit-help@mit.edu
- Experimental large language model application under development for interactive user support and to augment support ticket handling
 - Joint project with College of Computing, with dedicated funding
 - More discussion later + dedicated talk at LLM workshop on Friday https://indico.mit.edu/event/759/
- Slack workspace: https://mit-submit.slack.com
 - "help-desk" channel
- Monthly Users Group Meetings
 - Open for discussion
 - Open for user contributions: full set of Users Group representatives can be contacted at submit-usersgroup@mit.edu
- Annual subMIT workshop
 - January 2023 workshop: <u>https://indico.mit.edu/event/647/</u>
- In addition to direct interaction with the subMIT project team, users are encouraged to discuss with Users Group representative from their own group or "nearby" group

subMIT and ORCD

- subMIT provides Basic Computing Services tailored to the physics department
 - Easier in terms of scale and scope than institute-wide solutions
 - subMIT system is already up and running and successfully supporting research across the department
- "Local" nature of support and physics expertise of project team:
 - Fast turnaround time
 - User guidance on workflow design and optimization
 - System design and evolution targeted towards physics research needs
- Longer term relationship of subMIT with ORCD and balance between institute-wide and department-level services to be defined in coming year(s)

Linux Distribution Upgrade

- Current CentOS 7 distribution reaches EOL for maintenance updates in June 2024
- Decision by Red Hat to reorganize CentOS project and releases has disrupted logical upgrade path from CentOS 7->8
- Decision taken to upgrade from CentOS 7 to Alma Linux 9, considering:
 - Ease of transition
 - Support lifetime
 - Functionality
 - Direction being taken at other universities and labs (CERN, Fermilab, etc)
- Discussion has included Users Group and broader community
- Ease transition for users through well-supported and documented use of containers
- Test instances for interactive and batch usage with Alma 9 are being set up for initial user feedback
- Performance-sensitive services already upgraded (NVME storage)
- New large 384-thread machines using Alma 9 from the start
- Recent change (June 21, 2023) by Red Hat to CentOS source code policy introduces further uncertainty to enterprise linux ecosystem and Alma/Rocky Linux Projects
 - Carefully monitoring developments, but continuing with Alma 9 migration
 - Current plan from Alma Linux project is to maintain ABI compatibility with RHEL but not 1:1 source code or bug compatibility

Today's Review

- Indico page with timetable and slides:
 - <u>https://indico.mit.edu/event/761/</u>
- Overview of subMIT project, resources, software environment
- Discussion of User Support
- Usage Metrics
- Kolker Room + Zoom

0-Basic Computing Services (subMIT) Review Tuesday Jul 18, 2023, 2:00 PM → 4:00 PM America/New_York • Kolker Room (26-414) (MIT) 🕲 10m 🖉 -2:00 PM → 2:10 PM Opening Remarks from the Steering Committee Speaker: Christoph Paus (staff@mit.edu) 2:10 PM → 2:25 PM Introduction / Overview 🛈 15m 🖉 -Speaker: Joshua Bendavid (Massachusetts Institute of Technology) 🛈 15m 🖉 -2:25 PM → 2:40 PM Recent & Future Upgrades Speaker: Zhanggier Wang (Massachusetts Institute of Technology) 2:40 PM → 3:05 PM System Usage & JupyterHub User Accommodation 🛈 25m 🖉 -Speakers: Matthew Heine (Massachusetts Institute of Technology), Luca Lavezzo 3:05 PM → 3:15 PM Break () 10m 3:15 PM → 3:35 PM User Support & Slurm User Accommodation 🛈 20m 🖉 -Speaker: Chad Freer (staff@mit.edu) 𝔅 15m 🖉 ▪ 3:35 PM → 3:50 PM Community Engagement Example: MKI Speaker: Joshua Borrow (Massachusetts Institute of Technology) 3:50 PM → 4:00 PM Closing Remarks & Discussion ()10m 2 -Speaker: Joshua Bendavid (Massachusetts Institute of Technology)