

HPC Solutions

**Best Practices and Common Sense for getting
help and keeping data and research secure**

Thursday, February 15, 2024

<https://bit.ly/COMPLECS>

About COMPLECS

COMPLECS (COMPrehensive Learning for end-users to Effectively utilize CyberinfraStructure) is a SDSC training program that covers the most important non-programming concepts and skills needed to effectively use supercomputers. Topics include parallel computing concepts, Linux tools and shell scripting, code migration, data management and batch and interactive computing.

*COMPLECS is supported by
NSF award 2320934.*



Agenda

- Motivation
- HPC Ecosystem
 - Implications on Resources Availability and Security
- Help Desk & Other Available Help Resources
- Common Issues, Solutions, Security & Best Practices
 - System Access, File Systems, Allocations, Schedulers, Applications, Performance

Motivation

- Based on experience with help desk
- Facilitate Research
 - Reduce time to solution(stress)
 - Promoting good citizenship
 - Keeping resources and research secure
 - Promote effective and efficient use resources

HPC Ecosystem

- You are not alone (HPC is a shared resource)
 - Compute resources
 - Support resources
- What all is shared
 - Login Nodes
 - File systems
 - Compute nodes
 - Licenses
 - System Administration, Security, Networking, User support
- System policies set in place to help manage



Security is a Shared Responsibility

- Resource provider is responsible to:
 - Provide Authorized Users Access to Computational Resources
 - Protect user accounts/data from unauthorized users
 - Enforce the user set permissions on data
- End user will: (review ACCESS AUP)
 - Protect personal account credentials
 - Protect personal data with appropriate permission controls
 - Use resources only for the purpose for which it has been authorized to use

What are the available Help options?

- What are the available resources
 - You
 - Project/Colleagues
 - Web (Resource providers, hardware vendors and software developers)
 - User Guide
 - Community Forums
 - Git Repositories
 - Blogs
 - Helpdesk



Help Desk: Useful Information

- Clear description of is issue
- Resource, UserID/Username, Account/Project/Allocation
- JobId
 - List of Node(s) that job ran on, Project, Start time, End time, Resources requested
 - Working directory (submit script name)
 - Location of .err and .out files
- Create new ticket for new issues
- Always be nice to the support desk! 😊



Common Issues

- Access/Logging in
 - Login issues: ssh keys, MFA, passwords
 - System unavailable: OOD portal, direct login
- File Systems
 - Sharing- chmod, chown, chgrp
 - Quotas - Usage eval - du,lfs
- Allocations/Job charging
 - Charging
- Jobs/Policies/Schedulers
 - Failed Submissions
 - Failed Jobs
- Applications/software
 - Missing software: modules, containers, compiling
- Performance and debugging
 - System tools, debuggers, profilers

Resource Access/Logging in: Common Issues

- Login Failing
 - Problem: Incorrect credentials, incomplete setup
 - Solution: review login information, userguide
 - Passwords
 - Indicator message: Enter verification code
 - Solution: check username <https://allocations.access-ci.org/profile> (if username is not available for the resource then the account has not been created yet) Generally it can take 1 business day for accounts to be fully functional.
 - ssh keys
 - Indicator message: Enter password
 - Solution: resend ssh pub key, or use `-i` option to point to location of private key
 - MFA(2FA)
 - Indicator message: not prompted for TOTP (Not set up, new device)
 - Solution: Use SDSC Passive website (<https://passive.sdsc.edu/client/>) to enroll, remove and add new device

Resource Access/Logging in Common Issues

- Unable to access system
 - Problem: System Maintenance
 - Solution: Patience, stay informed
 - Pay attention to MOTD
 - User News (Stay Subscribed to be notified)
 - Check on User Portal -- <https://support.access-ci.org/announcements>
- Hanging on login
 - Problem: Users overstimulating the file system
 - Solution: Contact Support staff
 - User Data mover nodes to move data
 - Don't run compute intensive jobs on the login nodes
 - Problem: Activating Conda in your .bashrc
 - Solution: Do not initialize conda in .bashrc, but only when needed in run scripts

Resource Access/Logging in: Tips

- Different resources can have different access protocols/mechanisms, different security policies, and different usernames
 - Access Mechanism:
 - Site local passwords
 - federated login(CI-logon)
 - MFA
 - ssh keys
 - Access Protocols:
 - Portal
 - Direct Access(ssh)
- Overarching goal is to simplify ease of access and to protect research/credentials/systems

Resource Provider Site Usernames

Below are the usernames that you have previously used to access resource provider websites.

Site	Username
ACCESS	wolter
Indiana University	wolter
OSG Consortium	wolter
Pittsburgh Supercomputing Center	wolter
San Diego Supercomputer Center	nickel
University of Kentucky	wolter
University of Texas at Austin	uxwolter

Access/Logging In: Tips (Passwords/passphrases)

- Passwords
 - Don't reuse passwords
 - Longer is better
 - Don't keep digital plaintext copies of passwords
 - Don't Hard code password in files
 - Don't share passwords
- Use password-manager program
- Use SSH keys, ssh-agent
- Multi-factor Authentication(MFA)

Access/Logging In: Tips (Passwords/passphrases)

- SDSC does not use local passwords. For direct access to SDSC systems you will need to login with your SDSC local username and
 - (for ACCESS) either ssh key(& agent forwarding) or your ACCESS-CI portal password (&MFA)
 - (For non-ACCESS) either ssh key(&agent forwarding) or UCSD AD password. (&MFA)
- For the portals SDSC uses federated login(globus)
 - (for ACCESS) user ACCESS-CI portal credential
 - (for non-ACCESS) need to get UCSD AD account and invitation

File Systems: Common Issues

- Problem: File sharing
 - Solution: Use Unix commands `chmod`, `chown`, `chgrp` to manage file permissions
 - Review file/directory ownership and permissions(`ls`)
 - Find common groups for sharing (`id`,`groups`)
- Problem: System unresponsive/slow
 - Solution: Contact user support
 - Review you usage of the files system to make sure you are not the problem
- Problem: Missing, corrupted files
 - Solution: Contact User support team
 - Review file/directory ownership



File systems: Tips

- Common File systems and their utilization
 - Home – Usually limited in space
 - Scratch - Large space, limited persistence, no backup
 - Node local scratch(SSD)- good performance, only available during job
 - Persistent storage – good performance, limited persistence
 - Archival- Slow, backup
- Types of file systems
 - Lustre
 - nsf
 - gpfs
 - ceph

File systems: Tips

- Review file permissions `ls -l`
- Review user group
 - `Groups username, id username`
- Controls: Permissions granularity levels
 - (Attribute), User, Group, Other
 - Read(4), Write(2), Execute(1)
 - Default 755 (User(read, write, execute):Group(read, execute): Other(read, execute))
- Use `chmod`, `chown` commands to modify ownership and permissions

File systems: tips

- Have a backup Plan
 - Backups should be done at regular intervals that make sense with your project
 - Frequency
 - Ensure backups are made on “good” versions
 - Use Checksum on data transfers to ensure no corruption
 - User Version Control
 - Don't back up Everything
 - Clean up unnecessary files
 - Only back up files not easily reproduced or replaces
 - Source codes, scripts config files and large output files
 - Backups should be done to a different independent resource
 - Ensure credentials would not allow hackers to get onto the external resource
 - ACCESS to HPC system and file retention is usually limited. Transferring data takes time
 - Data on the system is the users responsibility
 - Plan ahead for data transfers
 - Convert many small files into a single archive file before transfer
 - Test the backup plan with the restore process

Running jobs, Allocations, Job Charging: Common Issues

- Problem: Unable to submit jobs
 - Common errors
 - sbatch: error: Project balance is not enough to run the job
 - sbatch: error: QOSMaxNodePerJobLimit
 - Sbatch: error: Invalid account or account/partition combination specified
 - Sbatch: error: Job violates accounting/QOS policy (job submit limit, user's size and/or time limits)
 - Solution: User tools to evaluate allocations and scheduler policies
 - Solution: Request more time
- Problem: Understanding Charging
 - Charging

Accounting/Charging: Tips

- Different resources use different home grown tools to help users evaluate their usage.
 - `expanse-client` tool (SDSC)
 - `TSCC_client` tool (TSCC)
 - `projects` (PSC)
 - `taccinfo` (TACC)
- Expanse uses `expanse-client` tool
 - Per User
 - Per Project
 - Per Resource
- ACCESS Portal accounting updated at various intervals
- Slurm tools : `sacct`

```
login01 ~]$ expanse-client user train112 -p
```

```
Resource expanse
```

```
NAME    STATE PROJECT TG PROJECT  USED  
AVAILABLE USED BY PROJECT
```

```
-----  
-----  
train112 allow gue998 TG-CIE960001S 337  
200000      114621
```

Jobs/Policies/Schedulers: tips (charging)

- All systems charge differently
 - Each resource has a unique definition of an SU
 - Some are in core hours, some are in node hours, etc
 - Some charge for other components such as memory
- Visit the user guide for specifics
 - Check for opportunities to save
- Allocations are shared
- Charging is generally based on what is requested, not how resources are used
- Do test jobs to evaluate
 - Slurm commands to collect information
 - `sacct -u $USER`
 - `sacct -j $JOBID`

Jobs/Policies/Schedulers: Common Issues

- Problem: Unable to submit jobs
 - Solution: Review errors
 - Common Sbatch errors:
 - Invalid account or account/partition
 - Job violates accounting/QOS policy (job submit limit, user's size and/or time limits)
 - Project balance is not enough
 - QOS Max NodePerJobLimit
- Problem: Jobs not running
 - Solution: Use `squeue` to identify “reasons” for pending jobs
 - Solution: Check user notifications for pending or active System Maintenance
 - <https://support.access-ci.org/outages>

Running Jobs: Tips Jobs/Policies/Schedulers(Slurm)

- Slurm tools to help monitor and manage jobs
 - squeue: view running or queued job and job step information
 - sacctmgr: view or modify Slurm account information
 - scontrol: view or modify Slurm configuration including jobs, job steps, nodes, partitions, reservations, and overall system configuration.
 - sacct: displays job accounting data
 - sinfo: view partition and node information
 - User Guide

Jobs/Policies/Schedulers : tools

(**queue: Job Status**)

- `queue [OPTIONS...]` (PBS,MAUI: `qstat,showq`)
 - View information about queued or running jobs

```
[nickel@login01 ~]$ queue | more
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST (REASON)
13574113	compute	80dgree_	yweng3	PD	0:00	2	(MaxMemPerLimit)
12668967	compute	0-xtensi	kavousi	PD	0:00	1	(MaxMemPerLimit)
14756880	compute	job001_p	amysai	PD	0:00	10	(Reservation)
14800161	compute	namd-com	sasadian	PD	0:00	6	(QOSMaxCpuPerUserLimit)
14800218	compute	namd-com	sasadian	PD	0:00	6	(QOSMaxCpuPerUserLimit)
14789098	compute	bl_8JHNp	uscms	PD	0:00	1	(MaxJobsPerAccount)

- Running jobs

14813206	compute	post0110	lpegolot	R	16:30:28	1	exp-9-35
14800090	compute	namd-com	sasadian	R	16:13:01	6	exp-2-29,exp-3-23,exp-4-33,exp-7-20,exp-9-[03,26]
14764467	compute	V1WTRERU	aminkvh	R	16:08:56	1	exp-2-54
14773832	compute	V4R1639Q	aminkvh	R	15:55:58	1	exp-8-14
14800092	compute	namd-com	sasadian	R	15:29:28	6	exp-4-29,exp-7-[07,39-40],exp-9-[28,41]
14812166	compute	scratch	mlaskow2	R	15:53:59	1	exp-10-20
14812167	compute	scratch	mlaskow2	R	15:39:34	1	exp-8-48
14800158	compute	namd-com	sasadian	R	15:17:18	6	exp-2-[26,50],exp-4-[52-53],exp-7-[42-43]
14812168	compute	scratch	mlaskow2	R	15:20:01	1	exp-10-37

Jobs/Policies/Schedulers : tools

(**queue: Job Status**)

- Queue states
 - PD –PENDING, R – RUNNING, S – SUSPENDED, CA – Canceled, CG – COMPLETING, CD – COMPLETED
- **queue** – Common “reasons” for pending jobs
 - MaxMemPerLimit
 - QOSMaxNodePerUserLimit
 - Priority
 - ReqNodeNotAvail, Unavailable nodes: exp-x-xx
 - ReqNodeNotAvail, Reserved for maintenance
 - Licenses
 - Dependency (file system, license, another job)
 - Priority
- **System Maintenance**
 - <https://support.access-ci.org/outages>

Jobs/Policies/Schedulers: tools (scontrol)

- scontrol [OPTIONS...]
[COMMAND...]
 - scontrol show job <<local_jobid>>
 - view or modify Slurm configurations and state on currently queued or running jobs

```
login01]$ scontrol show job 32658556
JobId=32658556 JobName=NGBW-JOB-BEAST2_XSEDE-43842C4A2D8C4B5085E71285ADC4D5DB
  UserId=testuser(505687)  GroupId=use300(6099)  MCS_label=N/A
  Priority=4509 Nice=0  Account=sds121  QOS=shared
  JobState=RUNNING Reason=None Dependency=(null)
  Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
  RunTime=00:46:22 TimeLimit=03:00:00 TimeMin=N/A
  SubmitTime=2024-07-30T12:22:15 EligibleTime=2024-07-30T12:22:15
  AccrueTime=2024-07-30T12:22:15
  StartTime=2024-07-30T12:22:16 EndTime=2024-07-30T15:22:16 Deadline=N/A
  SuspendTime=None SecsPreSuspend=0 LastSchedEval=2024-07-30T12:22:16
Scheduler=Main
  Partition=shared AllocNode:Sid=login01:2295441
  ReqNodeList=(null) ExcNodeList=(null)
  NodeList=exp-16-53
  BatchHost=exp-16-53
  NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
  ReqTRES=cpu=1,mem=1G,node=1,billing=3600
  AllocTRES=cpu=1,mem=1G,node=1,billing=3600
  Socks/Node=* NtasksPerN:B:S:C=1:0:*:* CoreSpec=*
  MinCPUsNode=1 MinMemoryNode=1G MinTmpDiskNode=0
  Features=(null) DelayBoot=00:00:00
  Reservation=cipres-shortjobs
  OverSubscribe=OK Contiguous=0 Licenses=cipres:1 Network=(null)
  Command=._batch_command.run
  WorkDir=/exppanse/projects//NGBW-JOB-BEAST2_XSEDE-
43842C4A2D8C4B5085E71285ADC4D5DB
  StdErr=/exppanse/projects//NGBW-JOB-BEAST2_XSEDE-
43842C4A2D8C4B5085E71285ADC4D5DB/_scheduler_stderr.txt
  StdIn=/dev/null
  StdOut=/exppanse/projects//NGBW-JOB-BEAST2_XSEDE-
43842C4A2D8C4B5085E71285ADC4D5DB/_scheduler_stdout.txt
  Power=
  MailUser=user@sdsc.edu
MailType=INVALID_DEPEND,BEGIN,END,FAIL,REQUEUE,STAGE_OUT
```

Jobs/Policies/Schedulers: tools (sacct)

- `sacct [OPTIONS...]`
 - View accounting data for completed jobs and job steps

```
l@login01 user_support]$ sacct -j 32659299 -l
```

JobID	JobIDRaw	JobName	Partition	MaxVMSize	MaxVMSizeNode	MaxVMSizeTask	AveVMSize	MaxRSS	MaxRSSNode	MaxRSSTask	Ave		
RSS	MaxPages	MaxPagesNode	MaxPagesTask	AvePages	MinCPU	MinCPUNode	MinCPUTask	AveCPU	NTasks	AllocCPUS	Elapsed	State	Ex
itCode	AveCPUFreq	ReqCPUFreqMin	ReqCPUFreqMax	ReqCPUFreqGov	ReqMem	ConsumedEnergy	MaxDiskRead	MaxDiskReadNode	MaxDiskReadTask	AveDis			
kRead	MaxDiskWrite	MaxDiskWriteNode	MaxDiskWriteTask	AveDiskWrite	ReqTRES	AllocTRES	TRESUsageInAve	TRESUsageInMax	TRESUsageInMaxNode	T			
RESUsageInMaxTask	TRESUsageInMin	TRESUsageInMinNode	TRESUsageInMinTask	TRESUsageInTot	TRESUsageOutMax	TRESUsageOutMaxNode	TRESUsageOutMaxTas	k	TRESUsageOutAve	TRESUsageOutTot			

- For formatted output

```
@login01 user_support]$ sacct -j 28582088 --format=JobID%20,Partition,CPUTime,MaxRSS,MaxDiskRead,MaxDiskWrite,NCPUS,ReqNodes,NNodes,ReqMem
```

JobID	Partition	CPUTime	MaxRSS	MaxDiskRead	MaxDiskWrite	NCPUS	ReqNodes	NNodes	ReqMem
28582088	shared	16-00:27:44				64	1	1	112.50G
28582088.batch		16-00:27:44	12143272K	232.05M	120.89M	64	1	1	
28582088.extern		16-00:27:44	1856K	0.01M	0.00M	64	1	1	

Jobs/Policies/Schedulers: Tools (acctmrg, sinfo)

- Tools for reviewing system partition activity and setup
 - sacctmrg – used to view and modify slurm account information
 - sinfo –used to view information about nodes and partitions
- User Guide

```
[nickel@login01 ~]$ sinfo
PARTITION   AVAIL  TIMELIMIT  NODES  STATE NODELIST
compute     up  2-00:00:00    3  drain$ exp-14-30,exp-16-[53-54]
compute     up  2-00:00:00    1  maint  exp-9-23
compute     up  2-00:00:00    2  down*  exp-12-12,exp-14-53
compute     up  2-00:00:00    3  comp  exp-8-29,exp-9-25,exp-13-19
compute     up  2-00:00:00    1  drng   exp-8-26
compute     up  2-00:00:00    2  drain  exp-9-30,exp-14-50
compute     up  2-00:00:00    8  resv   exp-13-[55-56],exp-16-[55-56],exp-17-[53-
30,39-40,42,44,46-47],exp-13-[01-07,12,16,20,22,27,42,46,48,50,52,54],exp-14-[01-02,04,
compute     up  2-00:00:00   375  alloc  exp-1-[01-21,23-24,27-47,50,56],exp-2-[03
-[21-28,34,38-54],exp-12-[01-11,13-16,29,31-38,41,43,45,48-56],exp-13-[08-11,13-15,17-1
compute     up  2-00:00:00   154  idle   exp-4-[15-56],exp-5-[01-56],exp-6-[01-56]
```

```
[nickel@login01 ~]$ sacctmgr show qos format=name%20,MaxWall,MaxTRESPU%20,MaxJobsPU,MaxSubmitPU,MaxTRESPA%20,MaxJobsPA,MaxSubmitPA
-----
Name           MaxWall           MaxTRESPU MaxJobsPU MaxSubmitPU           MaxTRESPA MaxJobsPA MaxSubmitPA
-----
normal         2-00:00:00        cpu=8192,node=64      32         64      cpu=16384,node=128      32         64
shared-normal  2-00:00:00        cpu=8192,node=64     4096       4096      cpu=16384,node=128     4096      4096
large-shared-normal 2-00:00:00          2          4          4          4          4
preempt-normal 7-00:00:00          128         128        cpu=4096,node=32      128
gpu-normal     2-00:00:00        cpu=160,gres/gpu=16+   4          8      gres/gpu=32,node=8      8         16
gpu-shared-normal 2-00:00:00        cpu=240,gres/gpu=24+  24         24      cpu=320,gres/gpu=32+    24         24
gpu-preempt-normal 7-00:00:00        gres/gpu=24,node=6    12         16      gres/gpu=48,node=12     16         20
```

Application Software: Common Issues

- Problem: Missing software
 - Solution: User Module commands to id if software is available
 - Solution: Compile own software in personal directory space
- Problem: Missing software version
 - Solution: Use containers
- Problem: Unable to load software
 - Solution: User module spider command to see all dependencies to load
- Problem: Need Licensed Software (Gaussian, VASP)
 - Solution: Contact help desk

Applications/software: tips

- Software is made available
 - Modules
 - Compile
 - Containers
 - Ask help desk
- Most HPC system use module to manage their software stacks
 - Check for available software with the module commands
 - `module [options] sub-command [args ...]`
- Login nodes, compute nodes are different
 - Compiling codes need to happen on the nodes on which they will run
 - Modules need to be loaded on the nodes on which applications will run
- Software managed by the resource provider has usually been tested and fine tuned for the specific resources

Software: Navigating with Modules

Command	Description
<code>module list</code>	Currently Loaded Modules
<code>module avail</code>	List of available software modules based on your current module path
<code>module spider</code>	List all available software and versions on the system
<code>module spider <application name></code>	List available application specific modules and module details, including versions and dependencies
<code>module load [module file]</code>	Load module(s) or specify unresolved dependencies
<code>module show [module file]</code>	Display information about loaded modules including changes, dependencies, versions and paths
<code>module unload [module file]</code>	Unloads a specified module form the environment
<code>module purge</code>	Unloads all the loaded modules
<code>module reset</code>	Reset modules to default settings

System Performance: Common Issues

- Login Nodes
- Compute nodes
 - GPU
 - CPU
- Filesystems
 - Lustre (project storage, scratch)
 - NSF (home)

System Performance : Monitoring Resource Utilization

- System evaluation Tools
 - top, htop, atop : display Linux processes
 - mpstat : display processors related statistic
 - sar : display system activity report
 - free: display memory statics
 - ps: display active processes
 - nvidia-smi: display gpu activity and statistic
- Job evaluation tools
 - seff(slurm efficiency) after job is complete
 - Slurm tools: sacct, sacctmgr
- Profiling tools
 - gprof
- Debuggers
 - Totalview, dbx

Best Practices: Getting help

- Understand your problem
- Engage with appropriate support tools
- Help Desk
 - While help desk staff are exceptional, they should be considered general practitioners
 - Provide relevant and adequate information for helpdesk to reduce iterations
 - Username, Account, System, Jobid, specific error message if available, etc.
 - The user with the problem should submit the help ticket
- Always be nice to the support desk! 😊

Best Practices: Risk Management

- Manage/secure your credentials
- Manage/secure your personal devices
- Manage directory and file access
 - Use least privileges
 - Use `chmod`, `chown` commands to modify ownership and permissions
- Data Resiliency
 - Clean up unnecessary files
 - Back up Data
 - Use integrity checking
 - Data transfers, bad hardware
- Have a contingency plan(Data recovery plan)
 - Off site backup

Best Practices: jobs and job charging

- Check user guide for accounting policies
- Use system tools for most up to date accounting information
 - Slurm for individual job details
 - sacctmgr
 - sacct
 - squeue
 - scontrol
 - sinfo
 - Home grown tools for accounting information
 - Expanse-client

Best Practices: Software

- Review user guide for tools available
- Use system installed applications when available
- Use containers to manage out of date software

In Conclusion

- Manage your risks by securing your accounts, research and data
- Be a good citizen
- There is help available if you know where to look

Review and helpful links

- ACCESS AUP
 - <https://identity.access-ci.org/aup.html>
- SSH Key setup
 - <https://github.com/sdsc-hpc-training-org/hpc-security>
- Comet Webinar- Indispensable Security: Tips to Use SDSC's HPC Resources Securely
 - https://www.sdsc.edu/event_items/202007_CometWebinar.html
- Expanse Webinar: Enduring Security: The Journey Continues
 - https://education.sdsc.edu/training/interactive/202204_expanse_enduring_security/index.html
- Access Allocations:
 - <https://allocations.access-ci.org/>
- Training Catalog
 - https://www.sdsc.edu/education_and_training/training_hpc.html#catalog

Questions

- [How to Reach Support](#)
 - consult@sdsc.edu
 - <https://support.access-ci.org/>



