Intro to Monsoon and Slurm

ENABLE ZOOM! (1 remote)

2/12/2019
Slides:
https://rcdata.nau.edu/hpcpub/workshops/intro.pdf

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Get logged in!

- From a Windows pc:
  - Open the putty application
    - May need to search in start menu for it
  - In the hostname field:
    - your_louie_id@monsoon.hpc.nau.edu
  - Click open button
  - And accept the security key by typing ”y”

- From a Mac:
  - Open the terminal application
  - ssh your_id@monsoon.hpc.nau.edu

Introductions

- Introduce yourself
  - Name
  - Department / Group
  - What project(s) do you plan to use monsoon for?
  - Linux or Unix experience
  - Previous cluster experience?

List of Topics

- Cluster education
  - What is a cluster, exactly?
  - Queues, scheduling and resource management
- Cluster Orientation
  - Monsoon cluster specifics
  - How do I use this cluster?
  - Group resource limits
  - Exercises
  - Question and answer

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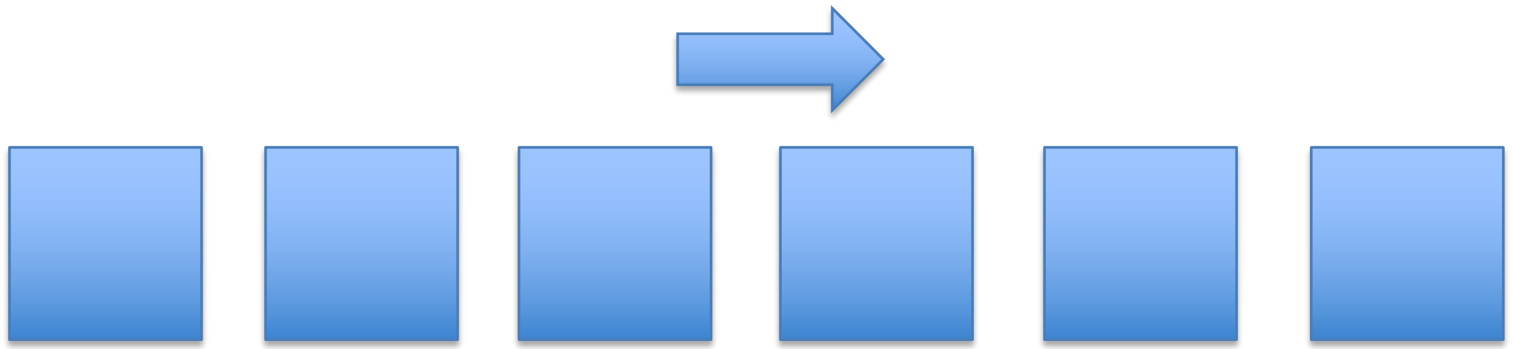
What is a queue?

- Normally thought of as a line, FIFO (Line at Starbucks)
- Queues on a cluster can be as basic as a FIFO, or far more advanced with dynamic priorities taking into consideration many factors



What is scheduling?

- *"A plan or procedure with a goal of completing some objective within some time frame"*
- Scheduling for a cluster at the basic level is much the same. Assigning work to computers to complete objectives within some time availability
- Not exactly that easy though. Many factors come into play scheduling work on a cluster.

Scheduling

- A scheduler needs to know what resources are available on the cluster in order to make accurate scheduling decisions
- Resource availability changes by the minute
- Assignment of work on a cluster is carried out most efficiently with the scheduler and resource manager working together

Resource Manager

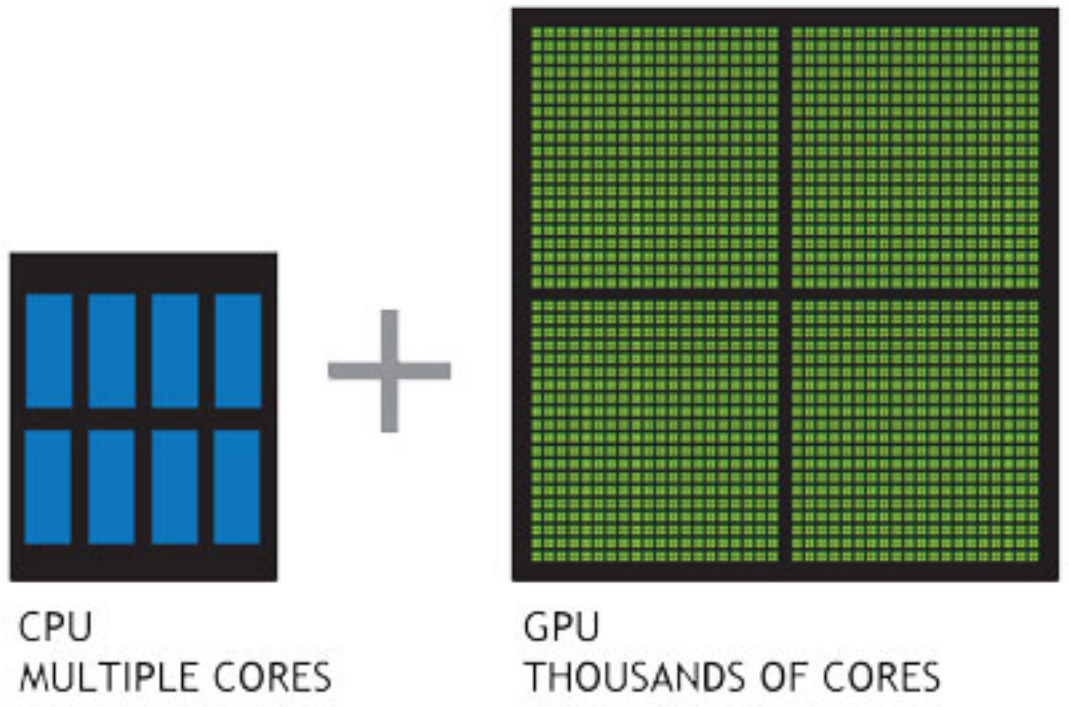
- Monitoring resource availability and health
- Allocation of resources
- Execution of resources
- Accounting of resources

Our Scheduling Goals

- Optimize quantity of work
- Optimize usage of resources
- Service all users and projects justly
- Make scheduling decisions transparent

Cluster Resources

- Node
- Memory
- CPU’s
- GPU’s
- Licenses



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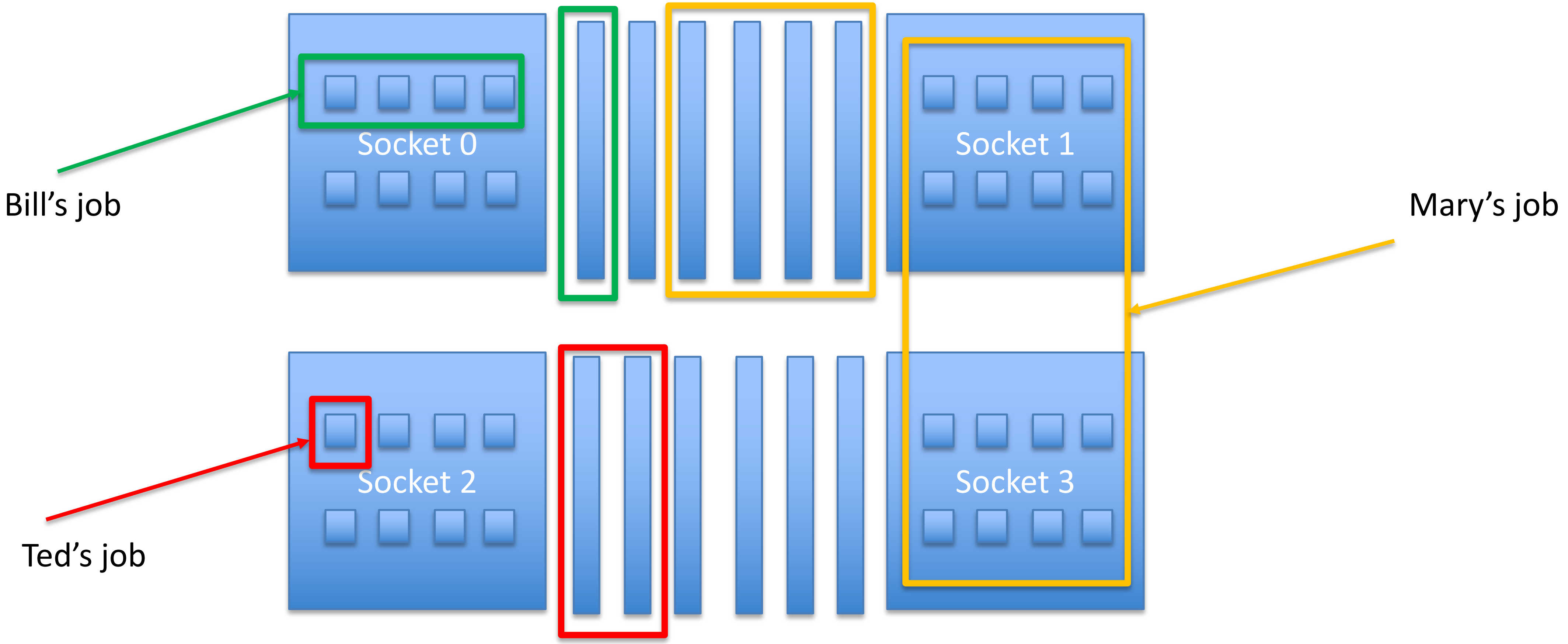
Many scheduling methods

- FIFO
  - Simply first in first out
- Backfill
  - Runs smaller jobs with lower resource requirements while larger jobs wait for higher resource requirements to be available
- Fairshare
  - Prioritizes jobs based on a users recent resource consumption

Inside a Node



Monsoon Today

- The Monsoon cluster is a resource available to the NAU research enterprise
- 103 systems (nodes) – cn[3-105]
- 2860 Intel Xeon cores
- 16 GPUs, NVIDIA Tesla K80, and P100
- Red Hat Enterprise Linux 6.9
- 24TB memory - 128GB/node min, 1.5TB max
- 500TB high-speed scratch storage (Lustre)
- 615TB long-term storage (ZFS)
- High speed interconnect: FDR Infiniband

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Slurm … yummm

- Slurm (Simple Linux Utility for Resource Management)
- Excellent resource manager and scheduler
- Precise control over resource requests
- Developed at LLNL, continued by SchedMD
- Used everywhere from small clusters to the largest clusters:
  - Summit (#1), 2.4M cores, NVIDIA Volta GPUs, 200 PF, 9.7k kW - USA
  - Sierra (#2), 1.5M cores, 125 PF, 7.4k kW - USA

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Small Cluster!

Dual core?

Largest Cluster!

2.4M cores

Monsoon scheduling

- Combination of scheduling methods
- Currently configured to utilize backfill along with a multifactor priority system to prioritize jobs

Factors attributing to priority

- Fairshare (predominant factor)
  - Priority points determined on users recent resource usage
  - Decay half life over 12 hours
- QOS (Quality of Service)
  - Some QOS have higher priority than others, for instance: debug
- Age – how long has the job sat pending
- Job size - the number of nodes/cpus a job is requesting

Storage

- /home – 10GB quota
  - Keep your scripts and executables here
  - Snapshotted twice a day: /home/.snapshot
  - Please do not write job output (logs, results) here!!
  - Run the command “quota” now
- /scratch – 500TB, 30 day retention
  - Very fast storage, capable of 11GB/sec
  - Quota: 20TB, 1M files
  - Checkpoints, logs
  - Keep all temp/intermediate data here
  - Should be your default location to perform input/output

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Storage

- /projects – 615TB
  - Long-term storage project shares
  - 10TB is assigned to faculty member for group to share
  - $24/TB/year above 10TB
  - Snapshots available
  - Backups available - $.10/GB/month
- /common
  - Cluster support share
  - Contrib: place to put software/libs/confs/db's for others use

Data Flow

1. Keep scripts and executables in /home
2. Write logs/temp/intermediate data to /scratch
3. Copy data to /projects/<group_project>, for group storage and reference in other projects
4. Cleanup /scratch

** Remember, /scratch is a scratch filesystem, used for high-speed temporary, and intermediate data

Remote storage access

- scp
  - scp files nauid@monsoon.hpc.nau.edu:/scratch/nauid
  - WinSCP (windows)
  - Cyberduck (mac)
- samba / cifs
  - \\nau.froot.nau.edu\cirrus (windows)
  - smb://nau.froot.nau.edu/cirrus (mac)
- Globus
  - https://nau.edu/high-performance-computing/globus/

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Groups

- NAU has a resource called Enterprise groups
- They are available to you on the cluster if you'd like to manage access to data
- https://my.nau.edu
  - "Go to Enterprise Groups"
  - Take a look at our FAQ :: nau.edu/hpc/faq
- If they are not working for you, contact ITS help desk
- What groups are you in? Run the command "groups", or "I"

Software

- ENVI / IDL
- Matlab
- Mathematica
- Intel Compilers, and MKL
- SAS
- R
- Qiime2
- Anaconda Python
- WRF
- Amber
- Tensorflow
- Lots of bioinformatics programs

- Full list here: “module avail”
- Request additional software to be installed!

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Modules

- Software environment management handled by the *modules* package management system

- module avail – what modules are available
- module list – modules currently loaded
- module load <module name> - load a package module
- module display <module name> - detailed information including environment variables effected

MPI

- Quick note on MPI
- Message Passing Interface for parallel computing
- Open MPI set as default MPI
- Mpich, and Mvapich2 also available
  - module unload openmpi
  - module load mvapich2
- Example MPI job script:
  - /common/contrib/examples/job_scripts/mpijob.sh

Interacting with Slurm

- What resources are needed?
  - 2 cpus, 12GB memory, for 2 hours?
- What steps are required?
  - Run prog1, then prog2 … etc
  - Are the steps dependent on one another?
- Can your work, or project be broken up into smaller pieces? Smaller pieces can make the workload more agile.
- How long should your job run for?
- Is your software multithreaded, uses OpenMP or MPI?

Example Job script

- #!/bin/bash
- #SBATCH --job-name=test
- #SBATCH --output=/scratch/nauid/output.txt   # the stdout from your program goes here
- #SBATCH --time=20:00   # shorter time = sooner start
- #SBATCH --workdir=/scratch/nauid   # default location slurm searches

- # replace this module with software required in your workload
- module load anaconda/latest   # loads our supported conda distribution (v2)

- # example job commands
- # each srun command is a job step, so this job will have 2 steps
- srun sleep 300
- srun python -V

Job Parameters

You want	Switches needed
More than one cpu for the job	--cpus-per-task=2, or -c 2
To specify an ordering of your jobs	--dependency=afterok:job_id, or -d job_id
Split up the output, and errors	--output=result.txt --error=error.txt
To run your job at a particular time/day	--begin=16:00 --begin=now+1hour --begin=2010-01-20T12:34:00
Add MPI tasks/ranks to your job	--ntasks=2, or -n 2
To control job failure options	--norequeue –requeue
To receive status email	--mail-type=ALL

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Contraints and Resources

You want	Switches needed
To choose a specific node feature (e.g. avx2)	--constraint=avx2
To use a generic resources (e.g. a gpu)	--gres=gpu:tesla:1
To reserve a whole node for yourself	--exclusive
To chose a partition	--partition

Submit the script

```
[user1@wind ~ ]$ sbatch jobscript.sh
Submitted batch job $\boxed{85223}$
```

- slurm returns a job id for your job that you can use to monitor or modify constraints

Login node vs Compute node

- When you log into “monsoon” you are placed on a login node
- The login node is a shared system used solely for:
  - Developing scripts
  - Transferring data
  - Submitting work to the scheduler
  - Analyzing results
  - Debug work less than 30 minutes in length
- The compute nodes are what make the supercomputer “super”.

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Interactive / Debug Work

- Run your compiles and testing on the cluster nodes by:
  - srun –p all gcc hello.c –o a.out
  - srun –qos=debug -c12 make -j12
  - srun Rscript analysis.r
  - srun python analysis.py

  - Try this now:
    - srun hostname
    - hostname

Long Interactive work

- salloc
  - Obtain a SLURM job allocation that you can work with for an extended amount of time interactively. This is useful for testing/debugging for an extended amount of time.

```
 [user1@wind ~ ]$ salloc -c 8 --time=2-00:00:00
 salloc: Granted job allocation 33442
[user1@wind ~ ]$ srun python analysis.py
[user1@wind ~ ]$ exit
salloc: Relinquising job allocation 33442
[user1@wind ~ ]$ salloc -N 2
salloc: Granted job allocation 33443
[user1@wind ~ ]$ srun hostname
cn3.nauhpc
cn2.nauhpc
[user1@wind ~ ]$ exit
salloc: Relinquising job allocation 33443
```

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Monitoring your job

- squeue
  - view information about jobs located in the SLURM scheduling queue.
- squeue --start
- squeue -u login
- squeue -o “%j %u … “
- squeue -p partitionname
- squeue -S sortfield
- squeue -t <state> (PD or R)

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Cluster info

- sinfo
  - view information about SLURM nodes and partitions.
- sinfo -N –l
- sinfo –R
  - List reasons for downed nodes and partitions

Monitoring your job

- sprio
  - view the factors that comprise a job’s scheduling priority
- sprio –l

  -- list priority of users jobs in pending state
- sprio -o “%j %u … “
- sprio -w

Monitoring your job

- sstat
  - Display various statistics and information of a running job
- sstat -j jobid
- sstat -o AveCPU,AveRSS

- Only works with jobs where analysis is executed with “srun”

Controlling your job

- scancel
  - Used to signal jobs or job steps that are under the control of Slurm.
- scancel -j jobid
- scancel -n jobname
- scancel -u mylogin
- scancel -t pending (only yours)

Controlling your job

- scontrol
  - Used to view and modify Slurm configuration and state.
  - Can change job constraints while it’s in pending state, once the job starts, it can no longer be modified
- scontrol show job 85224
- scontrol update jobid=6880341 timelimit=4:00:00

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Job Accounting

- sacct
  - displays accounting data for of your jobs and job steps in the SLURM job accounting log or SLURM database
- sacct -j jobid -o jobid,elapsed,maxrss
- sacct -N nodelist
- sacct -u mylogin

- Try our alias “jobstats”
  - jobstats -r
  - jobstats -j <jobid>

Job Accounting

- sshare
  - Tool for listing the shares of associations to a cluster.
- sshare -l : view and compare your groups cpu minutes usage
- sshare -a : view all users fairshare
- sshare –A –a <account> : view all members in your account (group)
- group_efficiency <account>

Account hierarchy

- Your user account belongs to a parent faculty account (group)
- Your user account shares resources that are provided for your group
- Example:
  - account1
    - user1
    - user2
- View the account structure you belong to with: “sshare -a –A <account>”
- Example:
  - sshare -a -A account1

Limits on the account (group)

- Limits are in place to prevent intentional or unintentional misuse of resources to ensure quick and fair turn around times on jobs for everyone.
- Groups are limited to a total number of cpu minutes in use at one time: 5M, and gpu minutes: 64K
- This cpu resource limit mechanism is referred to as: “TRESRunMins”.
- This limiting mechanism has nothing to do with priority!

TRESRunMins Limit

- What the heck is that!?
- A number which limits the total number of remaining cpu minutes which your ***running*** jobs can occupy.
- Enables flexible resource limiting
- Staggers jobs
- Increases cluster utilization
- Leads to more accurate resource requests

- Sumofjobs(cpus * timelimit remaining)

Examples

- 14400 = 10 jobs, 1 cpu, 1 day in length
- 144000 = 10 jobs, 10 cpu, 1 day in length
- 720000 = 10 jobs, 10 cpu, 5 days in length
- 720000 = 1000 jobs, 1 cpu, ½ day in length
- 1105920 = 1 job, 1024 cpus, 18 hrs in length

Questions?

- Check your groups cpu min usage:
  - sshare -l

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TRES run minutes (demo)

- Say, groupA’s total cpu minute limit is: 5000
- Example, groupA submits three jobs
  - Job1:
    - 1 core
    - 1 day timelimit (1440 minutes)
    - 1 GB memory
  - Job2:
    - 2 core
    - 1 days (1440 minutes)
    - 16 GB memory
    - 2880 minutes total !
  - Job 3:
    - 1 core
    - 1 day (1440 minutes)
    - 1GB memory

TRES run minutes

– Assuming there are available monsoon resources
– How many jobs start?

– How many cpu minutes are in use?

– When is job 3 ELIGIBLE to start?

TRES run minutes

- Assuming there are available monsoon resources
- How many jobs start?
  - 2
- How many cpu minutes are in use?
  - 1440+2880 = 4320
- When is job 3 ELIGIBLE to start?
  - After ~6 hours (6*60 = 360), and 2 jobs (360*2) = 720 minutes

  - We have only 5000-4320 = 680 minutes available initially
  - After ~ 1/4 day goes by (360 minutes) * 2 (two jobs) = 720 minutes
  - 680 + 720 = 1400
  - After another 40 minutes we’ll have 1440 at which point job starts

Helpful Linux Commands

List Files	ls options -l – to show more information
Change Directory	cd <directory path> cd by itself will return you to your home directory
Show/print current working directory	pwd
Copy Files	cp <source> <destination> use a period for the destination to copy a file to your current directory
Move or rename a file	mv <source> <destination>
Delete a file	rm <filename>
Create a directory	mkdir <directory name>
View contents of a file	more <filename> less <filename> cat <filename>
Edit a file	nano <filename>
Exit your terminal session (log off)	exit

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Exercise 1

Get to know monsoon and Slurm, on your own.

1. How many nodes make up monsoon?
   – Hint: use “sinfo”
2. How many nodes are in the **all** partition?
3. How many jobs are currently in the running state ?
   – Hint: use “squeue -t R”
4. How many jobs are currently in the pending state? Why?
   – Hint: use “squeue –t PD”

Exercise 2

- Create a simple job in your home directory
- Example here: /common/contrib/examples/job_scripts/simplejob.sh (copy it if you like ☺)
- Name your job: “exercise”
- Name your jobs output: “exercise.out”
- Output should go to /scratch/<user>/exercise.out
- Load the module “workshop”
- Run the “date” command
- And additionally, the “secret” command
- Save your job
- Submit your job with sbatch, i.e. “sbatch simplejob.sh”

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Exercise 3

- Edit the jobscript file from previous exercise 2
- Make your job sleep for 5 minutes (sleep 300)
  - Sleep is a command that creates a lazy process that … sleeps and does nothing
- Monitor your job
  - squeue -u your_nauid
  - squeue -t R
  - scontrol show job jobnum
  - sacct -j jobnum
    - Inspect the steps

- Cancel your job
  - scancel jobnum

Exercise 4 (note Slurm bug)

- Copy job script and edit:
  - /common/contrib/examples/job_scripts/lazyjob.sh
- Edit the job with your user id
- Submit the job, it will take 65 sec to complete
- Use sstat and monitor the job
  - sstat -j <jobid>
- Review the resources that the job used
  - jobstats -j <jobid>
- We are looking for "MaxRSS", *MaxRSS is the max amount of memory used*
- Edit the job script, reduce the memory being requested in MB and resubmit, edit "--mem=" , e.g. --mem=600
- Review the resources that the optimized job utilized once again
  - jobstats -j <jobid>

- Ok, memory looks good, but notice that the usercpu is the same as the elapsed time

*Usercpu = num utilized cpus * elapsed time*

- This is because the application we were running only used 1 of the 4 cpus that we requested
- Edit the lazy job script, comment out first srun command, and uncomment the second srun command.
- Resubmit
- Rerun jobstats -j <jobid>, notice now usercpu is a multiple times the elapsed time, in this case (4). Because we were allocated 4 cpus, and **used** 4 cpus.
- Now address the egregious time estimate!

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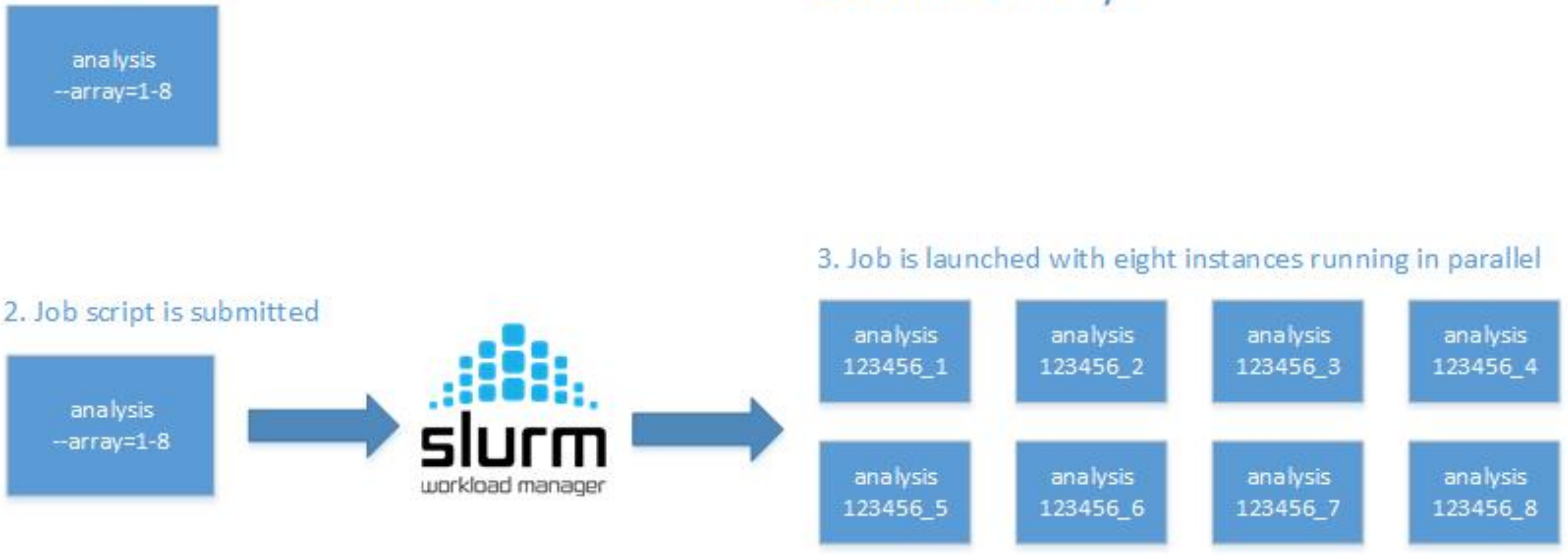
Slurm Arrays

1. Job script is created

2. Job script is submitted

3. Job is launched with eight instances running in parallel



Useful environment variables

SLURM_ARRAY_JOB_ID:	the job array's ID (parent)
SLURM_ARRAY_TASK_ID:	the id of the job array member n (child)
%A	
%a	

Slurm Arrays Exercise

- From your scratch directory: “/scratch/nauid”
- tar xvf /common/contrib/examples/bigdata_example.tar
- cd bigdata
- edit the file “job_array.sh” so that it works with your nau id replacing all NAUID with yours
- Submit the script “sbatch job_array.sh”
- Run “squeue”, notice there are 5 jobs running, how did that happen!

MPI Example

- Refer to the MPI example here:
  - /common/contrib/examples/job_scripts/mpijob.sh
- Edit it, for your work areas, then experiment:
  - Change number of tasks, nodes … etc
- Also can run the example like this:
  - srun --qos=debug –n4 /common/contrib/examples/mpi/hellompi

Keep these tips in mind

- Know the software you are running, is it multi-threaded?
- Request resources accurately
- Supply an accurate time limit for your job
- Don’t be lazy, it will effect you and your group negatively

Question and Answer

- More info here:

  http://nau.edu/hpc

- FREE – Linux command line book:
  - http://linuxcommand.org/tlcl.php
- FREE - Intro to Linux command line video:
  - https://www.lynda.com/Linux-tutorials/Welcome/435539/482226-4.html
  - Info here: https://nau.edu/HPC/Linux-External-Resources/
- And on the nauhpc listserv
  - nauhpc@lists.nau.edu

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