Slurm Basics

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Setup On Kestrel..

ssh kestrel.nrel.gov

```
cd /scratch/$USER
mkdir slurm25
cd slurm25
tar -xzf /scratch/tkaiser2/shared/slurm25/slurm25.tgz

export SLURM_ACCOUNT=YOUR_ACCOUNT
export SALLOC_ACCOUNT=$SLURM_ACCOUNT
export SBATCH_ACCOUNT=$SLURM_ACCOUNT
```

. ./doall

To get the results without running...

```
tar -xzf /scratch/tkaiser2/shared/slurm25/run25.tgz
```

Introduction to Running on High Performance Computing Platforms
slurm

Slurm is the software used to manage user interactions on NREL's HPC platforms. Slurm allows users access to resources (compute nodes) for some duration of time so they can perform work.

This talk will cover the basics of slurm. After this session users should be comfortable running compute jobs on HPC platforms, including NREL's Kestrel and Swift machines.

We will give an overview of slurm. We'll discuss commands for submitting jobs, getting status, deleting jobs, getting node and job information and job history. We'll show some tools to simplify interactions with slurm. We'll discuss priority and partitions. A number of sample run scripts will be given. We'll discuss running interactively. New this year, we'll discuss array jobs and running in shared partitions.

To cover...

- Slurm, what is it, does it do?
- Basic commands for:
  - Submitting
  - Getting status
  - Killing jobs
  - Node information
  - History of jobs
  - Seeing priority
  - Partitions
- Simple run scripts
- Shared partition
- My "shortcuts"
- Array jobs
- Running interactively
- Some important options
- Links
- More scripts as time allows

Also: Start to develop some good habits

Unfortunately there are some chicken and egg issues here

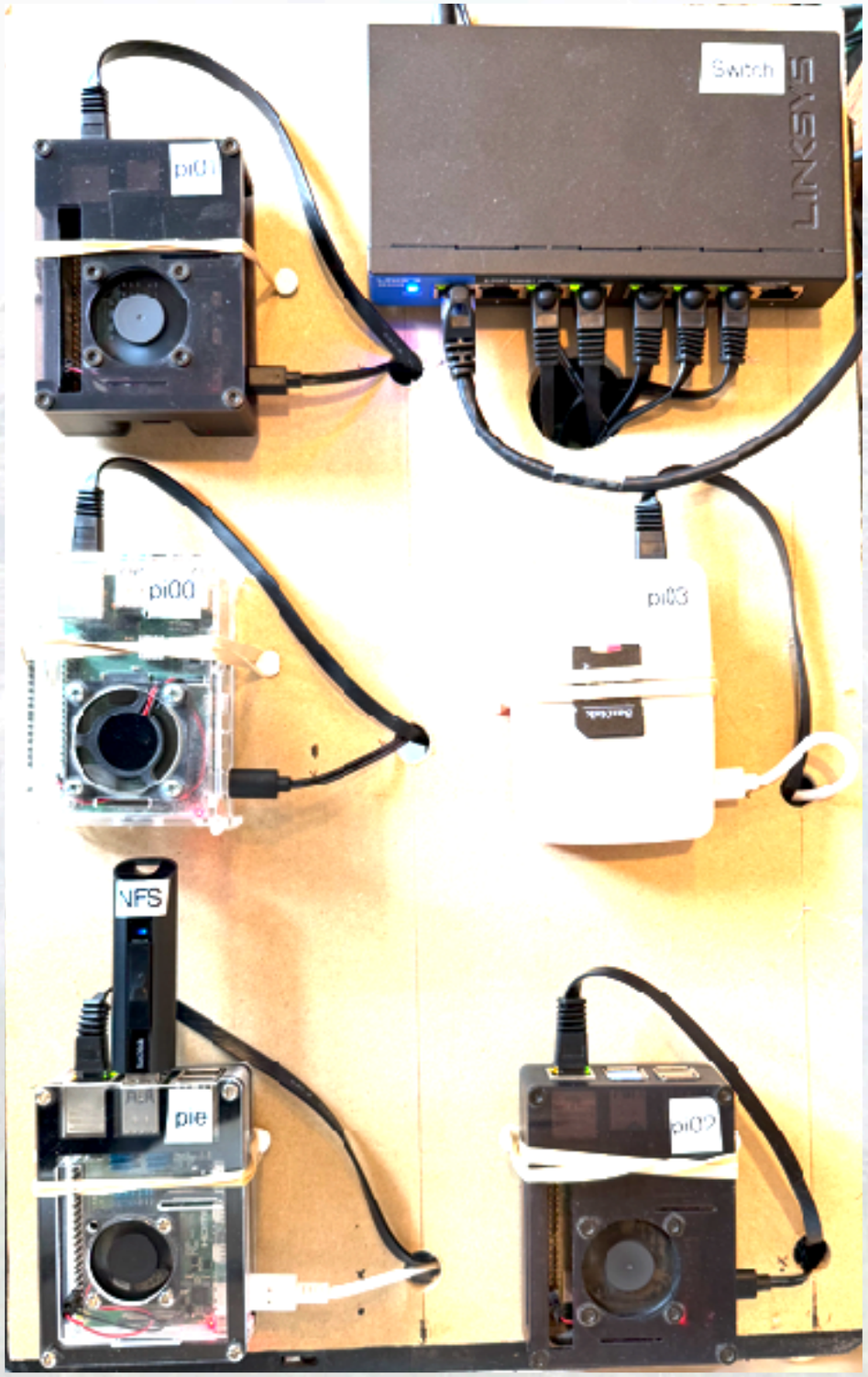
How are HPC platforms laid out?

- Login node
- Compute nodes
- Service nodes
  - File system
  - Monitoring
  - Management
- All connected together via a network
- Kestrel: https://www.nrel.gov/hpc/kestrel-system-configuration.html

Kestrel

- Login nodes:
  - kestrel.hpc.nrel.gov (CPU)
    - kl1.hpc.nrel.gov (CPU)
    - kl2.hpc.nrel.gov (CPU)
    - kl3.hpc.nrel.gov (CPU)
  - kestrel-gpu.hpc.nrel.gov
    - kl5.hpc.nrel.gov (GPU)
    - kl6.hpc.nrel.gov (GPU)
- Compute nodes:
  - 2,314 with 104 Intel CPUs
  - 134 nodes with AMD processors and 4 H100 GPUs

On small systems...



- Login nodes might also be the file system and management node
- My home machine (Runs slurm, MPI, OpenMP, Julia, Fortran, C, Spack, Web Server...)
  - pie
    - Login
    - Service (slurm)
    - File Server (nfs)
  - 4 Compute nodes
    - pi00-pi03
    - 4 cores / 4 - 8GB
  - Switch

Slurm, what is it, does it do?

- Simple Linux Utility for Resource Management
- It manages compute resources
- It allows for fair sharing of resources
- It is the software that allows you, and others to run jobs on compute nodes

https://slurm.schedmd.com/quickstart.html

Some definitions

- Node:
  - What is normally thought of as a computer that you could, in theory, login. Slurm manages the compute nodes and assigns jobs to them.
- Partition:
  - A collection of compute nodes often that have similar characteristics (memory, disk, core, gpus) or just grouped for management purposes.
  - Every compute node is part of one or more partitions.

Slurm, what is it, does it do?

- Typical usage:
  - You create a "batch" script that says:
    - What you want to run
    - Resources required
    - How long
    - Will most often have a "srun" command to launch multiple instances of the same program in parallel
  - You tell slurm to "run" your script
  - Slurm will run your job on compute nodes (after some waiting for resource to become available)

Running Batch Scripts

- A batch script is submitted to **slurm**
  - Command to submit scripts
    - **sbatch myscript**
  - Options you add to the batch line overrule what you have in the script
    - **sbatch --nodes=1 myscript**
  - Scripts can use variables defined in your environment.
- The scheduler decides where and when to run your job
  - Each job is given a number
  - Jobs are also given a name so that you can track them in the system
  - Each job has a priority that goes up over time
  - Wait for nodes to become available
  - Start the job and let it run until it finishes or runs out of time

A Simple Slurm Script hostname

```
#!/bin/bash

#SBATCH --job-name="atest"
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=8
#SBATCH --time=00:02:00
#SBATCH -o stdout
#SBATCH -e stderr
#SBATCH --export=ALL
##SBATCH --account=hpcapps
##SBATCH --partition=debug
##SBATCH --mail-type=ALL
##SBATCH --mail-user=joeuser@nrel.gov

#----------------------
cd /scratch/$USER
srun hostname > hostlist
```

Scripts contain comments designated with a # that are interpreted by SLURM.

and normal shell commands

Lines with ## are ignored by slurm

Go to your scratch directory

srun - run a command in parallel

slurm0

A Simple Slurm Script for a “parallel” job

#!/bin/bash	This is a bash script
#SBATCH --job-name="atest"	Give our job a name in the scheduler
#SBATCH --nodes=2	We want 2 nodes
#SBATCH --ntasks-per-node=8	We expect to run 8 tasks/node
#SBATCH --time=00:02:00	We want the node for 2 minutes
#SBATCH --output=stdout	Output will go to a file “stdout”
#SBATCH --error=stderr	Errors will go to a file “stderr”
#SBATCH --export=ALL	Pass current environment to nodes
##SBATCH --mail-type=ALL	Send email on abort,begin,end
##SBATCH --mail-user=auser@nrel.gov	Address for email
#SBATCH --account=hpcapps	Your account (not hpcapps)
#SBATCH –partition=debug	The scheduler partition
#----------	Just a normal “comment”
cd /scratch/$USER	Go to this directory first
srun hostname	Run hostname on 8 cores / node (2 nodes)

Submitting and Output

```
[tkaiser2@kl1 system]$ sbatch slurm0
...
...
```

```
[tkaiser2@kl1 slurm25]$cat hostlist
x1005c2s4b0n1
x1005c2s4b0n1
x1005c2s4b0n1
x1005c2s4b0n1
x1005c2s4b0n1
x1005c2s4b0n1
x1005c2s4b0n1
x1005c2s4b0n1
x1005c2s4b1n0
x1005c2s4b1n0
x1005c2s4b1n0
x1005c2s4b1n0
x1005c2s4b1n0
x1005c2s4b1n0
x1005c2s4b1n0
x1005c2s4b1n0
[tkaiser2@kl1 slurm25]$
```

Color added for clarity

Time format

```
#SBATCH --time=dd-hh:mm:ss

          Days (followed by -)
         Hours (followed by :)
       Minutes (followed by :)
                       Seconds
All are optional except Seconds

These are "legal"
--time=48:00:00
--time=120:00
--time=47:59:59
--time=2-00:00:00
--time=10:00
```

- Time is required for sbatch and salloc
- Can be useful for srun

Mail

--mail-type=
- NONE
- BEGIN
- END
- FAIL
- ALL
- TIME_LIMIT_90

--mail-user=**A_VALID_EMAIL_ ADDRESS_PLEASE**

Standard Output/Error

- If you don't specify
  - #SBATCH -o stdout
  - #SBATCH -e stderr
- Output goes to:
  - slurm-xxx.out/err where xxx is the job number.
- You can create unique files for each job by including the following in your "file name":

```
%j      jobid of the running job.
%u      User name.
%x      Job name.
```

```
#SBATCH -o X_%j_%u_%x.out  gives us  X_9366638_tkaiser2_atest.out
```

- You can specify an absolute path for your output

Slurm defines Variables:

```
SLURM_MPI_TYPE=pmi2
SLURM_STEP_ID=0
SLURM_NODEID=0
SLURM_TASK_PID=29272
SLURM_PRIO_PROCESS=0
SLURM_CPU_BIND_VERBOSE=quiet
SLURM_SUBMIT_DIR=/scratch/tkaiser2
SLURM_CPUS_PER_TASK=4
SLURM_STEPID=0
SLURM_SRUN_COMM_HOST=192.168.1.1
SLURM_PROCID=0
SLURM_JOB_GID=131364
SLURM_CPU_BIND=....
SLURM_ACCOUNT=hpcapps
SLURMD_NODENAME=c1-28
SLURM_TASKS_PER_NODE=32
SLURM_NNODES=1
SLURM_LAUNCH_NODE_IPADDR=192.168.1.1
SLURM_STEP_TASKS_PER_NODE=32
SLURM_JOB_NODELIST=c1-28
SLURM_CLUSTER_NAME=swift
SLURM_NODELIST=c1-28
SLURM_NTASKS=32
SLURM_UMASK=0002
SLURM_JOB_CPUS_PER_NODE=128
SLURM_TOPOLOGY_ADDR=c1-28
```

```
SLURM_WORKING_CLUSTER=swift:192.168.1.4:6817:9472:101
SLURM_STEP_NODELIST=c1-28
SLURM_JOB_NAME=atest
SLURM_SRUN_COMM_PORT=34097
SLURM_JOBID=143033
SLURM_CONF=/etc/slurm.conf
SLURM_JOB_QOS=normal
SLURM_TOPOLOGY_ADDR_PATTERN=node
SLURM_CPUS_ON_NODE=128
SLURM_JOB_NUM_NODES=1
SLURM_JOB_UID=131364
SLURM_JOB_PARTITION=debug
SLURM_PTY_WIN_ROW=60
SLURM_CPU_BIND_LIST=....
SLURM_JOB_USER=tkaiser2
SLURM_PTY_WIN_COL=146
SLURM_NPROCS=32
SLURM_SUBMIT_HOST=swift-login-1.swift.hpc.nrel.gov
SLURM_JOB_ACCOUNT=hpcapps
SLURM_STEP_LAUNCHER_PORT=34097
SLURM_PTY_PORT=37177
SLURM_JOB_ID=143033
SLURM_CPU_BIND_TYPE=mask_cpu:
SLURM_STEP_NUM_TASKS=32
SLURM_STEP_NUM_NODES=1
SLURM_LOCALID=0
```

```
mkdir -p $SLURM_JOB_NAME/$SLURM_JOB_ID
cd       $SLURM_JOB_NAME/$SLURM_JOB_ID
cat $0 > script.$SLURM_JOB_ID
```

Using variables defined in your environment

Script with variables

```
[tkaiser2@kl1 slurm0]$cat docommand
#!/bin/bash
#SBATCH --job-name="atest"
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=8
#SBATCH --time=00:01:00

srun $COMMAND > $OUTFILE
```

Set variables ; submit script

```
[tkaiser2@kl1 slurm0]$export COMMAND='date +%s.%N'
[tkaiser2@kl1 slurm0]$export OUTFILE=spread


[tkaiser2@kl1 slurm0]$sbatch --partition=debug docommand
Submitted batch job 7773917
[tkaiser2@kl1 slurm0]$
```

Results

```
[tkaiser2@kl1 slurm0]$sort spread
1743690724.618852371
1743690724.618885719
1743690724.619073134
1743690724.619128815
1743690724.619943391
1743690724.620182445
1743690724.620212055
1743690724.620769746
1743690724.635477415
1743690724.635745630
1743690724.635746714
1743690724.635955550
1743690724.635969448
1743690724.636509942
1743690724.636712457
1743690724.636839603
[tkaiser2@kl1 slurm0]$
```

Allows you to submit a bunch of different jobs with different data sets without editing your script.

Script to build/run a Parallel (MPI/OpenMP) Job

```
#!/bin/bash
##SBATCH --job-name="atest"
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=8
#SBATCH --time=00:02:00
#SBATCH -o /scratch/%u/%j.out
#SBATCH -e /scratch/%u/%j.err
##SBATCH --partition=debug
##SBATCH --account=hpcapps
##SBATCH --mail-type=ALL
##SBATCH --mail-user=joeuser@nrel.gov

# Setup
export BASE=$SLURM_SUBMIT_DIR
mkdir -p $BASE/$SLURM_JOB_ID
cd $BASE/$SLURM_JOB_ID

# Save info
cat $0   > $SLURM_JOB_ID.script
printenv > $SLURM_JOB_ID.env

# Get and build glorified "Hello World"
module load intel-oneapi-mpi
curl -s https://raw.githubusercontent.com/timkphd/examples/master/hybrid/pstream.c -o pstream.c
mpicc -fopenmp pstream.c -o  pstream

echo "First run"
export OMP_NUM_THREADS=1
srun ./pstream -F -D -t 5
echo "Second run:"
export OMP_NUM_THREADS=18
srun --nodes=1 --ntasks=4 --ntasks-per-node=4 ./pstream -F -D -t 5 > pstream.out

mv $SLURM_SUBMIT_DIR/$SLURM_JOB_ID.out .
```

Scripts contain "comments" designated with a # that are interpreted by SLURM and normal shell commands

##SBATCH are also comments

srun is the "normal" command to run something in parallel

Slurm1

Output

```
[tkaiser2@kl1 7577744]$ls -lt
total 96
-rw-rw---- 1 tkaiser2 tkaiser2  5042 Mar 21 10:02 pstream.out
-rw-rw---- 1 tkaiser2 tkaiser2    40 Mar 21 10:02 7577744.err
-rw-rw---- 1 tkaiser2 tkaiser2  1278 Mar 21 10:02 7577744.out
-rw-rw---- 1 tkaiser2 tkaiser2 22692 Mar 21 10:02 7577744.env
-rw-rw---- 1 tkaiser2 tkaiser2   951 Mar 21 10:02 7577744.script
-rwxrwx--- 1 tkaiser2 tkaiser2 36544 Mar 21 10:02 pstream
-rw-rw---- 1 tkaiser2 tkaiser2 14420 Mar 21 10:02 pstream.c
[tkaiser2@kl1 7577744]$cat *err
srun: Step created for StepId=7577744.1
[tkaiser2@kl1 7577744]$head pstream.out
MPI VERSION Intel(R) MPI Library 2021.12 for Linux* OS

task    thread             node name  first task    # on node  core
0001      0016        x3101c0s13b0n0        0000         0001  0002
0001      0005        x3101c0s13b0n0        0000         0001  0006
0001      0004        x3101c0s13b0n0        0000         0001  0005
0001      0001        x3101c0s13b0n0        0000         0001  0003
0001      0010        x3101c0s13b0n0        0000         0001  0008
0001      0017        x3101c0s13b0n0        0000         0001  0009
0001      0012        x3101c0s13b0n0        0000         0001  0004
[tkaiser2@kl1 7577744]$
[tkaiser2@kl1 7577744]$
[tkaiser2@kl1 7577744]$head 7577744.out
First run
MPI VERSION Intel(R) MPI Library 2021.12 for Linux* OS

task    thread             node name  first task    # on node  core
0007      0000        x3101c0s13b0n0        0000         0007  0009
0006      0000        x3101c0s13b0n0        0000         0006  0008
0015      0000         x3104c0s5b0n0        0008         0007  0008
0001      0000        x3101c0s13b0n0        0000         0001  0003
0000      0000        x3101c0s13b0n0        0000         0000  0002
0004      0000        x3101c0s13b0n0        0000         0004  0006
[tkaiser2@kl1 7577744]$
```

Output

```
[tkaiser2@kl1 7577744]$cat 7577744.out | egrep "task|^00" | sort -r
task    thread             node name  first task    # on node  core
0015      0000         x3104c0s5b0n0        0008         0007  0008
0014      0000         x3104c0s5b0n0        0008         0006  0007
0013      0000         x3104c0s5b0n0        0008         0005  0006
0012      0000         x3104c0s5b0n0        0008         0004  0005
0011      0000         x3104c0s5b0n0        0008         0003  0004
0010      0000         x3104c0s5b0n0        0008         0002  0003
0009      0000         x3104c0s5b0n0        0008         0001  0002
0008      0000         x3104c0s5b0n0        0008         0000  0001
0007      0000        x3101c0s13b0n0        0000         0007  0009
0006      0000        x3101c0s13b0n0        0000         0006  0008
0005      0000        x3101c0s13b0n0        0000         0005  0007
0004      0000        x3101c0s13b0n0        0000         0004  0006
0003      0000        x3101c0s13b0n0        0000         0003  0005
0002      0000        x3101c0s13b0n0        0000         0002  0004
0001      0000        x3101c0s13b0n0        0000         0001  0003
0000      0000        x3101c0s13b0n0        0000         0000  0002
[tkaiser2@kl1 7577744]$
```

Setting Default Accounts and Partition

- Jobs are "charged" against an account
- The account must be specified for a job to run
- You were given an account when you got your allocation
- One way to set account is with variables
  - SLURM_ACCOUNT - used by srun
  - SALLOC_ACCOUNT - used by salloc
  - SBATCH_ACCOUNT - used by sbatch
    - Most likely, just want to set them all the same

```
export SLURM_ACCOUNT=hpcapps
export SALLOC_ACCOUNT=$SLURM_ACCOUNT
export SBATCH_ACCOUNT=$SLURM_ACCOUNT
```

export SBATCH_PARTITION=short

More about srun

- sbatch will get you a collection of nodes
- srun will actually launch your program in parallel
- In most cases you will use srun instead of mpirun/mpiexec
- How many instances:
  - Defaults to what is given in your script header

```
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=8
```

  - Can also:
    - `srun --tasks-per-node=4 --ntasks=8  myprogrm`
    - `Many options See: man srun`

Getting Status and Information

- squeue
- sinfo
- scontrol show node
- sacctmgr

squeue

- Shows what is running or waiting to run
- By default it shows everyone's jobs
- Just show yours:
  - squeue -u $USER
- squeue has many potential output fields
- The --format option allows to to select fields

squeue: default output

```
 JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
461291  debug    benchmar  slarsen PD       0:00      1 (ReqNodeNotAvail)
581892  standard  install  joetrip PD       0:00      1 (Priority)
581891  parallel  install  joetrip PD       0:00      1 (Priority)
489530  parallel  install  joetrip PD       0:00      1 (Priority)
489529  parallel  install  joetrip PD       0:00      1 (Priority)
488899  parallel  install  joetrip PD       0:00      1 (Priority)
594990  parallel  install  joetrip PD       0:00      1 (Priority)
594989  parallel  install  joetrip PD       0:00      1 (Priority)
594988  parallel  install  joetrip PD       0:00      1 (Priority)
582732      test   jaguar    toads  R    5:51:25      2 c9-[45-47]
582728      test   jaguar    toads  R    5:55:47      1 c4-49
582726      test   jaguar    toads  R    5:57:24      1 c4-49
582712      test   jaguar    toads  R    6:08:34      1 c8-8
581890      test  install  joetrip PD       0:00      1 (Resources)
```

squeue with a format

I have an alias "sq" for squeue with a format:

```
alias sq='squeue -u $USER --format='\"%10A%15l%15L%6D%20S%15P%15r%20V%N'\"'
```

```
[tkaiser2@el1 runior]$ sq
JOBID     TIME_LIMIT TIME_LEFT  NODES START_TIME          PARTITION  REASON            SUBMIT_TIME         NODELIST
9382137   1:00:00    1:00:00    2     N/A                 debug      QOSMaxJobsPerUs   2022-06-03T10:42:54
9382131   1:00:00    1:00:00    2     N/A                 debug      QOSMaxJobsPerUs   2022-06-03T10:42:37
9382129   1:00:00    59:42      2     2022-06-03T10:42:39 debug      None              2022-06-03T10:42:22 r102u[34-35]
9382130   1:00:00    59:42      2     2022-06-03T10:42:39 debug      None              2022-06-03T10:42:29 r104u33,r105u33
[tkaiser2@el1 runior]$
```

squeue -i 10 -u $USER

Run squeue every 10 seconds

squeue --start -u $USER

“Estimate”of when your jobs will start

sprio

List priorities of all jobs

```
[tkaiser2@kl6 pstream]$sq
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           7744567  gpu-h100    runit tkaiser2 PD       0:00      2 (Resources)
```

```
[tkaiser2@kl6 pstream]$sprio -n -l --sort="Y" | head
          JOBID PARTITION     USER  ACCOUNT PRIORITY   AGE        ASSOC      FAIRSHARE  JOBSIZE    PARTITION  QOSNAME    QOS        TRES
        7308137 standard   linzq25    crerp 0.01030294 1.0000000  0.0000000  0.0216014  0.0056273  0.1000000  normal     0.0000000
        7744467 gpu-h100-      cbu   vonset 0.01085842 0.0015129  0.0000000  0.1074309  0.0002063  0.1000000  standby    0.0000000
        7744468 gpu-h100-      cbu   vonset 0.01085842 0.0015129  0.0000000  0.1074309  0.0002063  0.1000000  standby    0.0000000
        7744464 gpu-h100-      cbu   vonset 0.01085843 0.0015146  0.0000000  0.1074309  0.0002063  0.1000000  standby    0.0000000
        7744465 gpu-h100-      cbu   vonset 0.01085843 0.0015146  0.0000000  0.1074309  0.0002063  0.1000000  standby    0.0000000
        7744466 gpu-h100-      cbu   vonset 0.01085843 0.0015146  0.0000000  0.1074309  0.0002063  0.1000000  standby    0.0000000
        7744448 gpu-h100-      cbu   vonset 0.01085849 0.0015228  0.0000000  0.1074309  0.0002063  0.1000000  standby    0.0000000
        7744450 gpu-h100-      cbu   vonset 0.01085849 0.0015228  0.0000000  0.1074309  0.0002063  0.1000000  standby    0.0000000
        7744451 gpu-h100-      cbu   vonset 0.01085849 0.0015228  0.0000000  0.1074309  0.0002063  0.1000000  standby    0.0000000
```

```
[tkaiser2@kl6 pstream]$sprio -n -l --sort="Y" -u $USER | head
          JOBID PARTITION     USER  ACCOUNT PRIORITY   AGE        ASSOC      FAIRSHARE  JOBSIZE    PARTITION  QOSNAME    QOS        TRES
        7744567 gpu-h100  tkaiser2  hpcapps 0.03688496 0.0000000  0.0000000  0.3885369  0.0004087  0.1000000  normal     0.0000000
```

```
[tkaiser2@kl6 pstream]$sprio -n -l | head -1  ;sprio -n -l --sort="Y" | tail
          JOBID PARTITION     USER  ACCOUNT PRIORITY   AGE        ASSOC      FAIRSHARE  JOBSIZE    PARTITION  QOSNAME    QOS        TRES
        7744565 short       jreyna  rescore 0.04172777 0.0000000  0.0000000  0.4409562  0.0002043  0.1000000  normal     0.0000000
        7744553 bigmem      pbrown reedswet 0.04798196 0.0005522  0.0000000  0.5083525  0.0004020  0.1000000  normal     0.0000000
        7744462 bigmem      pbrown reedswet 0.04798883 0.0015170  0.0000000  0.5083525  0.0004020  0.1000000  normal     0.0000000
        7744463 bigmem      pbrown reedswet 0.04798883 0.0015170  0.0000000  0.5083525  0.0004020  0.1000000  normal     0.0000000
        7744460 bigmem      pbrown reedswet 0.04798884 0.0015187  0.0000000  0.5083525  0.0004020  0.1000000  normal     0.0000000
        7744461 bigmem      pbrown reedswet 0.04798884 0.0015187  0.0000000  0.5083525  0.0004020  0.1000000  normal     0.0000000
        7744459 bigmem      pbrown reedswet 0.04798885 0.0015203  0.0000000  0.5083525  0.0004020  0.1000000  normal     0.0000000
        7669804 long      khanwale     nawi 0.05424028 0.2594626  0.0000000  0.3352535  0.0514496  0.1000000  high       1.0000000
        7624973 bigmeml   junchich   tkm4nc 0.06269915 0.5372305  0.0000000  0.6255760  0.0012059  0.1000000  normal     0.0000000
        7744480 gpu-h100-  mvansch questaal 0.08201644 0.0010111  0.0000000  0.8741359  0.0035839  0.1000000  standby    0.0000000
[tkaiser2@kl6 pstream]$
```

The larger the PRIORITY, the higher the job will be positioned in the queue.

Just because a job has a high priority it does not necessarily mean it will start soon.

Priorities

- The larger the PRIORITY, the higher the job will be positioned in the queue.
- Priority is a function of several factors including age and FAIRSHARE.
- https://ni.cmu.edu/computing/knowledge-base/slurm-job-priority-wait-time/
  - Does a good explanation of priorities.
  - However, their weights are much different than NREL'S.
    - Their "FAIRSHARE" is 0.
    - NREL - FAIRSHARE is important: give higher priority to accounts which have not used the machine much recently. Usage has a "half-life."

scancel

- Cancel (kill/stop) your jobs
  - scancel 9382130
    - Kills a particular job(s)
  - scancel -u $USER
    - Kills all of your jobs

sinfo

Show information about partitions and nodes

```
[tkaiser2@vs-login-1 ENV]$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
sm           up 1-00:00:00      1 drain  vs-sm-0016
sm           up 1-00:00:00      4  down  vs-sm-[0001,0024,0028,0032]
sm           up 1-00:00:00      3  drain vs-sm-[0002-0003,0026]
sm           up 1-00:00:00     24   idle vs-sm-[0004-0015,0017-0023,0025,0027,0029-0031]
gpu          up 1-00:00:00      2  drain vs-gpu-[0004,0006]
gpu          up 1-00:00:00      4  alloc vs-gpu-[0001-0003,0005]
lg           up 1-00:00:00      1  alloc vs-lg-0001
lg           up 1-00:00:00      1  down  vs-lg-0004
lg           up 1-00:00:00      2  drain vs-lg-[0010,0017]
lg           up 1-00:00:00     10  alloc vs-lg-[0002-0003,0006-0008,0012-0014,0016,0018]
std          up 1-00:00:00      2  drain vs-std-[0003,0026]
std          up 1-00:00:00      1  drain vs-std-0014
std          up 1-00:00:00     47  alloc vs-std-[0001-0002,0004-0006,0008,0010-0011,0013]
t            up    4:00:00      2  drain vs-t-[0004,0011]
t            up    4:00:00      4  drain vs-t-[0006,0009,0012-0013]
t            up    4:00:00      9   idle vs-t-[0001-0003,0005,0007-0008,0010,0014-0015]
[tkaiser2@vs-login-1 ENV]$
```

This is Vermillion not Kestrel

Kestrel Partitions

Partition Name	Description	Limits	Placement Condition
debug	Nodes dedicated to developing and troubleshooting jobs. Debug nodes with each of the non-standard hardware configurations are available.	- 1 job with a max of 2 nodes per user. - 2 GPUs per user - 1/2 GPU node resources per user (Aurora 1-2 nodes). - 01:00:00 max walltime	-p debug or --partition=debug
short	Nodes that prefer jobs with walltimes <= 4 hours.	2016 nodes total. No limit per user	--time <= 4:00:00 --mem <= 256064 --tmp <= 1700000 [256 nodes]
standard	Nodes that prefer jobs with walltimes <= 2 days	2106 nodes total. 1050 nodes per user	--mem <= 256064 --tmp <= 1700000
long	Nodes that prefer jobs with walltimes > 2 days. Maximum walltime of any job is 10 days	525 nodes total. 252 nodes per user.	--time <= 10-00 --mem <= 256064 --tmp <= 1700000 [256 nodes]
bigmem	Nodes that have 2 TB of RAM and 5.6 TB NVMe local disk.	8 nodes total. 4 nodes per user.	--mem > 256064 --time <= 2-00 --tmp > 1700000
bigmem2	Bigmem nodes that prefer jobs with walltimes > 2 days. Maximum walltime of any job is 10 days.	4 nodes total. 3 nodes per user.	--mem > 256064 --time > 2-00 --tmp > 1700000
hbw	CPU compute nodes with dual network interface cards	512 nodes total. 256 nodes per user. Minimum 2 nodes per job.	-p hbw --time <= 10-00 --nodes >= 2
nvme	CPU compute nodes with 1.7 TB NVMe local drives.	256 nodes total. 128 nodes per user.	-p nvme --time <= 2-00
shared	Nodes that can be shared by multiple users and jobs	64 nodes total. Half of partition per user. 2 days max walltime.	-p shared or --partition=shared
shared1	Nodes that can be shared by multiple users and prefer jobs with walltimes > 2 days.	16 nodes total. 8 nodes per user.	-p shared1 or --partition=shared1
gpu-h100	Shareable GPU nodes with 4 NVIDIA H100 SXM 80GB Computational Accelerators.	130 nodes total. 65 nodes per user.	1 <= --gpus <= 4 --time <= 5-00
gpu-h100s	Shareable GPU nodes that prefer jobs with walltimes <= 4 hours.	130 nodes total. 65 nodes per user.	1 <= --gpus <= 4 --time <= 4:00:00
gpu-h100l	Shareable GPU nodes that prefer jobs with walltimes > 2 days.	26 GPU nodes total. 13 GPU nodes per user.	1 <= --gpus <= 4 --time > 2-00

https://nrel.github.io/HPC/Documentation/Systems/Kestrel/Running/

sinfo

Show information about partitions and nodes

```
[tkaiser2@vs-login-1 ENV]$ sinfo -p lg
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
lg           up 1-00:00:00      1 alloc* vs-lg-0001
lg           up 1-00:00:00      1  down* vs-lg-0004
lg           up 1-00:00:00      4   comp vs-lg-[0005,0009,0011,0015]
lg           up 1-00:00:00      2  drain vs-lg-[0010,0017]
lg           up 1-00:00:00     10  alloc vs-lg-[0002-0003,0006-0008,0012-0014,0016,0018]
[tkaiser2@vs-login-1 ENV]$
[tkaiser2@vs-login-1 ENV]$
[tkaiser2@vs-login-1 ENV]$ sinfo -N -n vs-t-0001
NODELIST   NODES PARTITION STATE
vs-t-0001      1         t idle
[tkaiser2@vs-login-1 ENV]$
[tkaiser2@vs-login-1 ENV]$
[tkaiser2@vs-login-1 ENV]$ sinfo -N  | grep idle    or    (sinfo -N -t idle)
vs-sm-0004       1        sm idle
vs-sm-0005       1        sm idle
vs-sm-0027       1        sm idle
vs-sm-0030       1        sm idle
vs-sm-0031       1        sm idle
vs-t-0001        1         t idle
vs-t-0014        1         t idle
vs-t-0015        1         t idle
[tkaiser2@vs-login-1 ENV]$
```

scontrol

- Many functions, only a few you will most likely ever use:
  - Hold/release a job
    - `scontrol uhold  9382268`
    - `scontrol release  9382268`
  - Get detailed information about a node(s)/job(s)
    - `scontrol show node`
    - `scontrol show job ######`

scontrol show node

```
[tkaiser2@el1 runior]$ scontrol show node r103u01
NodeName=r103u01 Arch=x86_64 CoresPerSocket=18
   CPUAlloc=36 CPUTot=36 CPULoad=26.87
   AvailableFeatures=hy
   ActiveFeatures=hy
   Gres=gpu:v100:2
   NodeAddr=r103u01 NodeHostName=r103u01 Version=21.08.5
   OS=Linux 3.10.0-1062.9.1.el7.x86_64 #1 SMP Fri Dec 6 15:49:49 UTC 2019
   RealMemory=751616 AllocMem=0 FreeMem=718868 Sockets=2 Boards=1
   State=ALLOCATED ThreadsPerCore=1 TmpDisk=24000000
   Weight=1 Owner=N/A MCS_label=N/A
   Partitions=gpu,gpu-stdby,gpul,gpul-stdby,bigscratch
   BootTime=2022-04-07T08:39:15 SlurmdStartTime=2022-04-07T08:44:41
   LastBusyTime=2022-06-02T07:55:17
   CfgTRES=cpu=36,mem=734G,billing=36,gres/gpu=2
   AllocTRES=cpu=36,gres/gpu=2
   CapWatts=n/a
   CurrentWatts=0 AveWatts=0
   ExtSensorsJoules=n/s ExtSensorsWatts=0 ExtSensorsTemp=n/s
```

scontrol show job

```
[tkaiser2@r4i7n35 tkaiser2]$ scontrol show job 9443283
JobId=9443283 JobName=interactive
   UserId=tkaiser2(131364) GroupId=tkaiser2(131364) MCS_label=N/A
   Priority=248099184 Nice=0 Account=hpcapps QOS=normal
   JobState=RUNNING Reason=None Dependency=(null)
   Requeue=0 Restarts=0 BatchFlag=0 Reboot=0 ExitCode=0:0
   RunTime=00:00:17 TimeLimit=01:00:00 TimeMin=N/A
   SubmitTime=2022-06-08T12:28:31 EligibleTime=2022-06-08T12:28:31
   AccrueTime=2022-06-08T12:28:31
   StartTime=2022-06-08T12:28:36 EndTime=2022-06-08T13:28:36 Deadline=N/A
   SuspendTime=None SecsPreSuspend=0 LastSchedEval=2022-06-08T12:28:36 Scheduler=Main
   Partition=debug AllocNode:Sid=el3:27289
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=r4i7n35
   BatchHost=r4i7n35
   NumNodes=1 NumCPUs=36 NumTasks=4 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
   TRES=cpu=36,node=1,billing=36
   Socks/Node=* NtasksPerN:B:S:C=0:0:*:* CoreSpec=*
   MinCPUsNode=1 MinMemoryNode=0 MinTmpDiskNode=0
   Features=[hy|ehy] DelayBoot=00:00:00
   OverSubscribe=NO Contiguous=0 Licenses=(null) Network=(null)
   Command=(null)
   WorkDir=/lustre/eaglefs/scratch/tkaiser2
   Switches=1@2-00:00:00
   Power=
[tkaiser2@r4i7n35 tkaiser2]$
```

scontrol to modify a job

```
todebug ()  {
    scontrol update JobId=$1 TimeLimit=01:00:00
    scontrol update JobId=$1 Partition=debug
}

tolong ()
{
    scontrol update JobId=$1 Partition=long
}

toshort ()
{
    scontrol update JobId=$1 Partition=short
}


to01 ()
{
scontrol update JobId=$1 TimeLimit=00:01:00
}

to05 ()
{
scontrol update JobId=$1 TimeLimit=00:05:00
}

to60 ()
{
scontrol update JobId=$1 TimeLimit=00:60:00
}
```

Here are some functions I have defined to modify jobs.

These are in the "utils" directory; to be discussed shortly.

sacct

```
[tkaiser2@vs-login-1 ENV]$ sacct -S 2025-01-04 -E 2025-01-06 -u $USER
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
50005503     rfm_Hello+        gpu    hpcapps         60  COMPLETED      0:0
50005503.ba+      batch               hpcapps         30  COMPLETED      0:0
50005503.0   HelloTest+               hpcapps         60  COMPLETED      0:0
50005504     rfm_Hello+        gpu    hpcapps         60 CANCELLED+      0:0
50005504.ba+      batch               hpcapps         30  CANCELLED     0:15
50005504.0   HelloTest+               hpcapps         60  CANCELLED     0:15
50005505     rfm_Hello+         lg    hpcapps        120  COMPLETED      0:0
50005505.ba+      batch               hpcapps         60  COMPLETED      0:0
50005505.0   HelloTest+               hpcapps        120  COMPLETED      0:0
50005506     rfm_Hello+         lg    hpcapps        120  COMPLETED      0:0
50005506.ba+      batch               hpcapps         60  COMPLETED      0:0
50005506.0   HelloTest+               hpcapps        120  COMPLETED      0:0
50005507     rfm_Hello+         lg    hpcapps        120  COMPLETED      0:0
50005507.ba+      batch               hpcapps         60  COMPLETED      0:0
50005507.0   HelloTest+               hpcapps        120  COMPLETED      0:0
50005508     rfm_Hello+         lg    hpcapps        120  COMPLETED      0:0
50005508.ba+      batch               hpcapps         60  COMPLETED      0:0
50005508.0   HelloTest+               hpcapps        120  COMPLETED      0:0
[tkaiser2@vs-login-1 ENV]$
```

Show history of my jobs between January 4 and January 6

sacct

- Like most commands sacct has a format option
- Things important to me:
  - JobID
  - Start
  - Nodelist
  - Starting directory
- I have a bash function (recent) that
  - Takes days range (not date)
    - Calls sacct with the above requested
    - Does some filtering

recent - sacct

```
[tkaiser2@vs-login-1 ENV]$ recent 4 1
50022417 2022-05-31T12:18:06  vs-sm-0025   /home/tkaiser2
50022418 2022-05-31T12:22:11  vs-sm-0025   /home/tkaiser2
50022433 2022-06-01T14:30:09  None assigned    /projects/hpcapps/tkaiser2/runior
50022434 2022-06-01T14:30:38  None assigned    /projects/hpcapps/tkaiser2/runior
50022435 2022-06-01T14:31:26  vs-sm-[0017-0020]/projects/hpcapps/tkaiser2/runior
50022436 2022-06-01T14:33:51  vs-sm-[0017-0020]/projects/hpcapps/tkaiser2/runior
50022437 2022-06-01T14:37:40  vs-sm-[0017-0020]/projects/hpcapps/tkaiser2/runior
50022438 2022-06-01T14:39:13  vs-sm-[0017-0020]/projects/hpcapps/tkaiser2/runior
50022439 2022-06-01T14:42:13  vs-sm-[0029-0030]/projects/hpcapps/tkaiser2/runior
50022440 2022-06-01T14:44:31  vs-sm-[0030-0031]/projects/hpcapps/tkaiser2/runior
50022441 2022-06-01T14:46:29  vs-sm-[0030-0031]/projects/hpcapps/tkaiser2/runior
50022442 2022-06-01T14:50:40  vs-sm-[0030-0031]/projects/hpcapps/tkaiser2/runior
50022443 2022-06-01T14:54:33  vs-sm-[0030-0031]/projects/hpcapps/tkaiser2/runior
50022444 2022-06-01T14:58:43  vs-sm-[0030-0031]/projects/hpcapps/tkaiser2/runior
50022445 2022-06-01T15:06:47  vs-sm-[0030-0031]/projects/hpcapps/tkaiser2/runior
50022446 2022-06-02T14:47:12  None assigned    /projects/hpcapps/tkaiser2/runior
50022447 2022-06-01T16:29:33  vs-sm-[0029-0030]/projects/hpcapps/tkaiser2/runior
50022448 2022-06-01T16:31:14  vs-sm-[0017-0018]/projects/hpcapps/tkaiser2/runior
50022449 2022-06-01T16:33:26  vs-sm-0025   /projects/hpcapps/tkaiser2/runior
[tkaiser2@vs-login-1 ENV]$
```

Recent is function I defined. Source is in the examples.

saccntmgr

Another command with many functions but you will most likely only use it to find out what accounts you have on a machine

```
[thk2@el1 ENV]$ sacctmgr show associations user=$USER format=account%15
        Account
---------------
        hpcapps
    continental
       mobility
           msoc
            wks
       naermpcm
[thk2@el1 ENV]$
```

```
alias accounts='sacctmgr show associations user=$USER format=account%15'
```

salloc

- salloc
  - Used to allocate resources for a job in an interactive mode. Typically this is used to allocate resources and spawn a shell. The shell is then used to execute srun commands to launch parallel tasks.

```
salloc --nodes=2 --ntasks=72 --time=01:00:00 --partition=debug --account=hpcapps
```

Running Interactively

- Sometimes you want to grab a node or nodes and run commands
- Almost like running on login node except you are actually logged in to a compute node and you have access to all of the nodes you have allocated
- After you get started you can run simple commands or run in parallel with srun
- The command to do this is salloc
- Note: The way this works has recently changed

Grab nodes and run with salloc

```
[thk@el1 ~]$ salloc --nodes=2 --ntasks=72 --time=01:00:00 --partition=debug --account=hpcapps
salloc: Pending job allocation 9382710
salloc: job 9382710 queued and waiting for resources
salloc: job 9382710 has been allocated resources
salloc: Granted job allocation 9382710
salloc: Waiting for resource configuration
salloc: Nodes r102u[34-35] are ready for job
[thk@r102u34 ~]$
[thk@r102u34 ~]$
[thk@r102u34 ~]$ printenv  SLURM_NODELIST
r102u[34-35]
[thk@r102u34 ~]$
[thk@r102u34 ~]$
[thk@r102u34 ~]$ srun -n 4 --distribution=block -l  hostname
1: r102u34
0: r102u34
2: r102u35
3: r102u35
[thk@r102u34 ~]$
```

Some Notes:

- Interactive (salloc) session: .bashrc gets sourced
  - Your environment looks like a new login shell
  - Will be extra variables for SLURM
  - Setting you changed after getting on Kestrel will not be on the login nodes
- sbatch: .bashrc does not get sourced
  - Environment defined on submitting node more or less gets passed as is
  - Module "counts" will change

More sbatch /salloc options

- Any option specified with #sbatch can be overwritten with an option on the command line
  - `sbatch --time=1-00:00:00 my script`
- You can ask for nodes with a specific amount of memory, scratch disk, gpus
  - --x Request that a specific list of hosts **not** be included for your job
  - These options are specific to Kestrel but other machines will have similar options
    - --mem=700000 700 Gbytes (big memory nodes)
    - --tmp=1500000 1.5 Tbytes of scratch
    - On Kestrel, setting specifics can put you in different partitions

Directory for today...

```
[tkaiser2@kl1 slurm25]$ls -Rr
.:
utils  slurm1  slurm0  pstream.c  mstream.cu  mpmd  makefile  gpu  doall
array  affinity

./utils:
tymer  slurmnodes  onnodes  ongpus  myalias  doall  allow

./slurm1:
script  makefile

./slurm0:
script  makefile  docommand

./mpmd:
script  mlist.py  makefile  hellof.f90  helloc.c

./gpu:
mstream.cu  makefile  doit  dogpu

./array:
uselist  usedirs  useboth  tymer  setarray.py  makefile  invertp.py  invertc.c
doit  doboth  bot.tgz

./affinity:
makefile  doaff  break
[tkaiser2@kl1 slurm25]$
```

What's in the utils dir

source utils/myalias

- Get a nice node list for a job
  - **thenodes**
- Show your accounts
  - **accounts**
- Show information about a job
  - **showjob**
- Show what I have in the queue
  - **sq**
- Print a clean module list in load order
  - **mylist**
- Show my recent jobs
  - **recent**
- Show my recent jobs with run time
  - **recentt**
- Show a list of nodes scheduled to soon (maybe) be used
  - **pnodes**
- Do a salloc of various flavors
  - **alloc**
- Send a job to debug, long, short, set time to 1, 5, 60 minutes
  - **todebug**

What's in the utils dir

```
[tkaiser2@kl1 utils]$onnodes -h
./onnodes [JOB_ID ...]
  OR
./ongpus [JOB_ID ...]
 For each specified or running JOB
  For each NODE of the JOB
    Show what user has running on each core
    If NODE has GPUs show what is running on the GPUs
    Must be called as ongpus to get gpu info
```

```
[tkaiser2@kl1 utils]$slurmnodes -h
USAGE:
slurmnodes compressed node list + -Fattribute1,attribute2,...
Where a compressed node list is of the form:
     x1002c4s5b1n1,x1002c5s2b0n0,x1002c5s5b1n0,x1002c6s3b1n[0-1]

Without any inputs:
default node is x1000c0s0b0n1
default attributes are: ['CPUAlloc', 'CPULoad', 'FreeMem']

all is a valid input for both nodes and attributes

Examples:
     Get the state of all nodes
slurmnodes all -FState

     Get a list of attributes
slurmnodes  -Fall
     OR
slurmnodes  -F
```

```
[tkaiser2@kl1 utils]$tymer -h

USAGE:

./tymer  [file] [comment]

With no input on the command line prints
time in seconds and date to the screen.

With a file name on the command line it reads
the file, if it exists, and prints a delta time
from the last time this program updated the file
and appends the time information to the file.

Note: file can be /dev/null or ""

If the file does not exist it creates it and
write the current time information.
You can add optional comments that will be added
to the end of the line.

tymer can be called as a function:
from tymer import *
tymer()                          prints to stdout
tymer("file")                    prints to file
tymer("-i")                      use an internal file for saving time
tymer(["file","comments"])       prints to file with comments
tymer(["","comments"])           prints to stdout with comments
tymer(["/dev/null","comments"])prints to stdout with comments
```

```
[tkaiser2@kl1 7802275]$allow
Generate a task/thread mask for srun
```

Slurm array jobs

- Slurm allows array jobs:

Job arrays offer a mechanism for submitting and managing collections of similar jobs quickly and easily. All jobs must have the same initial options (e.g. size, time limit, etc.), however it is possible to change some of these options after the job has begun execution using the command specifying the *JobID* of the array or individual *ArrayJobID*.

Job arrays will have two additional environment variable set. **SLURM_ARRAY_JOB_ID** will be set to the first job ID of the array. **SLURM_ARRAY_TASK_ID** will be set to the job array index value. For example a job submission of this sort:

sbatch --array=1-3 some_script
will generate a job array containing three jobs. If the sbatch command responds
Submitted batch job 36
then the environment variables will be set as follows:

```
SLURM_JOBID=36
SLURM_ARRAY_JOB_ID=36
SLURM_ARRAY_TASK_ID=1

SLURM_JOBID=37
SLURM_ARRAY_JOB_ID=36
SLURM_ARRAY_TASK_ID=2

SLURM_JOBID=38
SLURM_ARRAY_JOB_ID=36
SLURM_ARRAY_TASK_ID=3
```

Apology

- Our example is complex
- It could be a talk unto itself
- Goal is not complete understanding
- Show what is possible
- You can dig through the example and use it as a basis for your work.

Slurm array jobs

```
[joeuser@lognode memory]$ sbatch --nodelist=node002 --array=1-4 array
Submitted batch job 11968


[joeuser@lognode memory]$ squeue -u joeuser
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           11968_1     debug   hybrid  joeuser  R       0:05      1 node002
           11968_2     debug   hybrid  joeuser  R       0:05      1 node002
           11968_3     debug   hybrid  joeuser  R       0:05      1 node002
           11968_4     debug   hybrid  joeuser  R       0:05      1 node002
```

Here we run 4 jobs on the same node producing:

```
[joeuser@lognode memory]$ ls -lt | head
total 12768
-rw-rw-r-- 1 joeuser joeuser   1791 Sep 11 14:50 stderr.11968
-rw-rw-r-- 1 joeuser joeuser    803 Sep 11 14:50 stderr.11970
-rw-rw-r-- 1 joeuser joeuser    803 Sep 11 14:50 stderr.11971
-rw-rw-r-- 1 joeuser joeuser    803 Sep 11 14:50 stderr.11969
-rw-rw-r-- 1 joeuser joeuser   2763 Sep 11 14:50 fillmemc.sinput1.output.11968.11968.1
-rw-rw-r-- 1 joeuser joeuser   2763 Sep 11 14:50 fillmemc.sinput4.output.11971.11968.4
-rw-rw-r-- 1 joeuser joeuser   2763 Sep 11 14:50 fillmemc.sinput2.output.11969.11968.2
-rw-rw-r-- 1 joeuser joeuser   2763 Sep 11 14:50 fillmemc.sinput3.output.11970.11968.3
```

A set of array jobs can run on the same node or many different nodes.

On Kestrel running in the shared partition will "allow" subjobs to run on the same node at the same time but other considerations might prevent it. `export SBATCH_PARTITION=shared`

Our Array Job Example Overview

- Standard header
- We want to share a node for multiple instances so we set the memory for a node
- We created a directory hierarchy with a directory for each job and under that a directory for each subjob
- Gets different inputs for each subjob. We show how to do that in two different ways.
- Run our program

Array Job Example

- Our program does 4 matrix inversions (twice so you should end up with the same matrices with which you started)
- The "array" aspect of this example is that each subjob will invert a different set of matrices.
- The program takes an input from the command line of the form
  - 10 20 30 40 200
- The first 4 integers give the diagonal values for the matrices and the last value is the size
- The program returns times and errors for the inversions

Array Job Example

- We run two different ways
  - Input for each run is in a separate directory
    - Our script selects a directory
    - Each instance will read data from a different directory
  - There is a single input files
    - Our script selects a line from the input
    - Each instance will use a different line of input

Array Job Example

- Recall that when you run an array job you get both
  - $SLURM_ARRAY_JOB_ID
    - Like the normal SLURM_JOB_ID ,say 2197923
  - $SLURM_ARRAY_TASK_ID
    - Numbers in the range n1 to n2; the array values set on your sbatch line. Example 1-24
      - sbatch --array=1-24 array.job

Array Job Example

- Our script sets

```
export JOB_ID=$SLURM_ARRAY_JOB_ID
export SUB_ID=$SLURM_ARRAY_TASK_ID
```

- and uses these values to create a main directory for all our jobs and a sub directory for each subjob

Our script(s) in details

```
#!/bin/bash -e
#SBATCH --job-name="array_job"
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=4
#SBATCH --time=00:05:00
###### sending output to /dev/null will suppress it
###### this is a good idea for array jobs lest it
###### create extra output for each subjob
##SBATCH -o /dev/null
##SBATCH --exclusive=user
##SBATCH --account=hpcapps

#SBATCH --mem=5G

#----------------------
# example invocation
# sbatch --array=1-24 array_simple
```

For Kestrel don't use exclusive

mem is what is required for each subjob.
If this is not set your subjobs might not be able to share cores on a node

```
module load python

export OMP_NUM_THREADS=4

#run with either the C or python version of our program
#export EXE=invertp.py
export EXE=invertc


# go to our starting directory
cd $SLURM_SUBMIT_DIR

# get the JOB and SUBJOB ID
if [[ $SLURM_ARRAY_JOB_ID ]] ; then
        export JOB_ID=$SLURM_ARRAY_JOB_ID
        export SUB_ID=$SLURM_ARRAY_TASK_ID
else
        export JOB_ID=$SLURM_JOB_ID
        export SUB_ID=1
fi
```

We will use
$SLURM_ARRAY_JOB_ID
and $SLURM_ARRAY_TASK_ID
to use as directory names.
$SLURM_ARRAY_TASK_ID
Will also be used to grab the correct line from our input.

```
# make a top level directory for the job
# if it does not already exist
mkdir -p $JOB_ID
cd $JOB_ID

# make a directory for the subjob and go there
mkdir -p $SUB_ID
cd $SUB_ID

# Make a copy of our script
cat $0 > myscript

# Get the name of our LIST, default to list
if [ -z ${LIST+x} ]; then echo "LIST is unset"; export LIST=list ; else echo "LIST is set to '$LIST'"; fi
```

We are creating a directory for each job and subjob.

Directory $JOB_ID

Subdirectories
$JOB_ID/$SUB_ID

Get the name of our file list or assume it is “list”

Example #1
Data is in a directory

```
# Here we assume that our LIST is is a set of directories
# under a "main" directory "inputs" each containing data sets.
# For our current program we require each directory contain an
# input file myinput.
#
# We get the directory from the list
   dir=`head -n $SUB_ID $SLURM_SUBMIT_DIR/$LIST | tail -1`

# Copy our input from the directory
   cp -r $SLURM_SUBMIT_DIR/inputs/$dir/* .
   printenv > envs

# Run our job
   hostname > node
   echo $SLURM_SUBMIT_DIR/inputs/$dir > directory

   $SLURM_SUBMIT_DIR/tymer timer start_time
   $SLURM_SUBMIT_DIR/$EXE `cat myinput` > output
   $SLURM_SUBMIT_DIR/tymer timer end_time
```

Example #2
Each line contains input

```
# Here we assume that our each line of our LIST contains
# data for our program.
#
# Grab the line
    export input=`head -n $SUB_ID $SLURM_SUBMIT_DIR/$LIST | tail -1`
    printenv > envs

# Run our job
   hostname > node

   $SLURM_SUBMIT_DIR/tymer timer start_time
   echo $input > myinput
   eval $SLURM_SUBMIT_DIR/$EXE `cat myinput` > output
   $SLURM_SUBMIT_DIR/tymer timer end_time
```

Our makefile

```
[timk@colostate.edu@login12 array]$ vi makefile

all:invertc input

invertc:invertc.c
        gcc -O3 -fopenmp invertc.c -o invertc

input:setarray.py
        rm -rf in_list list inputs
        ./setarray.py 100

clean:
        rm -rf invertc in_list dir_list inputs

backup:
        tar -czf array.tgz array.job  doit invertc.c makefile setarray.py tymer invertp.py bot
```

The makefile does two things. It builds the matrix inversion program invertc and runs the python program setarry.py.

The python program creates our input files “in_list” and “dir_list” and a directory “inputs.”

The directory “inputs” contains 100 subdirectories each with input for our program. The file dir_list contains a list of these directories.

The file in_list contains 100 lines of input for our program, one line per iteration.

```
[timk@colostate.edu@shas0136 array]$ cat doit
# make our program and data set
make clean
make

#run assuming each line of "in_list" contains our input
export LIST=in_list
sbatch --array=1-24   usedirs
sbatch --array=25-48  usedirs

#run assuming data in in directories specified in "dir_list"
export LIST=dir_list
export USEDIRS=yes
sbatch --array=1-24   uselist
sbatch --array=25-48  uselist

unset LIST
unset USEDIRS
```

The file doit runs make to create our program and data sets. It also will submit our batch script as an array

It also will submit our batch script 4 times. Each submission will have 24 subjobs.

For our first set of submissions we assume that our data is in a set of directories

For the second two we assume our input is all in the single file in_list

```
source doit
rm -rf invertc in_list dir_list inputs slurm*out
gcc -O3 -fopenmp invertc.c -o invertc
rm -rf in_list dir_list inputs
./setarray.py 100
Submitted batch job 7749134
Submitted batch job 7749135
Submitted batch job 7749136
Submitted batch job 7749137
[tkaiser2@kl6 array]$
```

We source the file which builds the program and submits our jobs.

makefile

```
[tkaiser2@kl6 array]$cat makefile
all:invertc input

invertc:invertc.c
    gcc -O3 -fopenmp invertc.c -o invertc

# Our python program creates a file in_list that
# contains 100 lines of input, one for each run
# and a diredctory "inputs" that contains 100
# subdirectories each with an input file. The
# file dir_list contains a list of the directories

input:setarray.py
    rm -rf in_list dir_list inputs
    ./setarray.py 100

clean:
    rm -rf invertc in_list dir_list inputs slurm*out

backup:
    tar -czf array.tgz bot doseperate dotogether invertc.c invertp.py makefile setarray.py tymer useboth usedirs uselist
```

Data sets

```
[tkaiser2@kl6 array]$head -5 in_list
74 50 62 29 400
66 13 7 69 400
60 36 88 84 400
17 84 19 57 400
42 38 14 91 400
[tkaiser2@kl6 array]$

[tkaiser2@kl6 array]$head -5 dir_list
set001
set002
set003
set004
set005

[tkaiser2@kl6 array]$cat inputs/set001/myinput
63 67 47 55 200
[tkaiser2@kl6 array]$cat inputs/set005/myinput
44 65 99 50 200
[tkaiser2@kl6 array]$
```

```
[tkaiser2@kl6 array]$ls slurm-774929*
slurm-7749293_10.out  slurm-7749293_23.out  slurm-7749294_29.out  slurm-7749294_43.out  slurm-7749295_18.out  slurm-7749295_8.out   slurm-7749296_37.out
slurm-7749293_11.out  slurm-7749293_24.out  slurm-7749294_30.out  slurm-7749294_44.out  slurm-7749295_19.out  slurm-7749295_9.out   slurm-7749296_38.out
slurm-7749293_12.out  slurm-7749293_2.out   slurm-7749294_31.out  slurm-7749294_45.out  slurm-7749295_1.out   slurm-7749296_25.out  slurm-7749296_39.out
slurm-7749293_13.out  slurm-7749293_3.out   slurm-7749294_32.out  slurm-7749294_46.out  slurm-7749295_20.out  slurm-7749296_26.out  slurm-7749296_40.out
slurm-7749293_14.out  slurm-7749293_4.out   slurm-7749294_33.out  slurm-7749294_47.out  slurm-7749295_21.out  slurm-7749296_27.out  slurm-7749296_41.out
slurm-7749293_15.out  slurm-7749293_5.out   slurm-7749294_34.out  slurm-7749294_48.out  slurm-7749295_22.out  slurm-7749296_28.out  slurm-7749296_42.out
slurm-7749293_16.out  slurm-7749293_6.out   slurm-7749294_35.out  slurm-7749295_10.out  slurm-7749295_23.out  slurm-7749296_29.out  slurm-7749296_43.out
slurm-7749293_17.out  slurm-7749293_7.out   slurm-7749294_36.out  slurm-7749295_11.out  slurm-7749295_24.out  slurm-7749296_30.out  slurm-7749296_44.out
slurm-7749293_18.out  slurm-7749293_8.out   slurm-7749294_37.out  slurm-7749295_12.out  slurm-7749295_2.out   slurm-7749296_31.out  slurm-7749296_45.out
slurm-7749293_19.out  slurm-7749293_9.out   slurm-7749294_38.out  slurm-7749295_13.out  slurm-7749295_3.out   slurm-7749296_32.out  slurm-7749296_46.out
slurm-7749293_1.out   slurm-7749294_25.out  slurm-7749294_39.out  slurm-7749295_14.out  slurm-7749295_4.out   slurm-7749296_33.out  slurm-7749296_47.out
slurm-7749293_20.out  slurm-7749294_26.out  slurm-7749294_40.out  slurm-7749295_15.out  slurm-7749295_5.out   slurm-7749296_34.out  slurm-7749296_48.out
slurm-7749293_21.out  slurm-7749294_27.out  slurm-7749294_41.out  slurm-7749295_16.out  slurm-7749295_6.out   slurm-7749296_35.out
slurm-7749293_22.out  slurm-7749294_28.out  slurm-7749294_42.out  slurm-7749295_17.out  slurm-7749295_7.out   slurm-7749296_36.out

[tkaiser2@kl6 array]$cat slurm-7749294_36.out
LIST is set to 'dir_list'
1743539148.516247 Tue Apr  1 14:25:48 2025      0.000      0.000 start_time
1743539148.576869 Tue Apr  1 14:25:48 2025      0.061      0.061 end_time
[tkaiser2@kl6 array]$

[tkaiser2@kl6 array]$ls 7*
7749293:
1  10  11  12  13  14  15  16  17  18  19  2  20  21  22  23  24  3  4  5  6  7  8  9

7749294:
25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41  42  43  44  45  46  47  48

7749295:
1  10  11  12  13  14  15  16  17  18  19  2  20  21  22  23  24  3  4  5  6  7  8  9

7749296:
25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41  42  43  44  45  46  47  48

[tkaiser2@kl6 array]$ls 7749293/1
directory  envs  myinput  myscript  node  output  timer

[tkaiser2@kl6 array]$cat 7749293/1/output
45 56 19 17 200
section 1 start time= 0.00016499   end time=  0.0090261  error= 4.21146e-11
section 2 start time= 0.00016713   end time=  0.0094981  error= 2.35085e-11
section 3 start time= 0.00016904   end time=  0.0093021  error= 3.41071e-10
section 4 start time= 0.00016904   end time=  0.0093081  error= 4.80289e-11

[tkaiser2@kl6 array]$ls 7749295/1
envs  myinput  myscript  node  output  timer

[tkaiser2@kl6 array]$cat 7749295/1/output
48 12 38 77 400
section 1 start time= 0.00024509   end time=   0.073825  error= 1.78e-10
section 2 start time= 0.00024605   end time=   0.074992  error= 1.76297e-09
section 3 start time= 0.00024891   end time=   0.074665  error= 7.64311e-11
section 4 start time= 0.00024891   end time=   0.073795  error= 4.19306e-10
[tkaiser2@kl6 array]$
```

When finished we get 4 top level directories, each with 24 subdirectories.

```
[timk@colostate.edu@shas0136 test]$ ls 2197925
25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41  42  43  44  45  46  47  48

[timk@colostate.edu@shas0136 test]$ ls 2197925/25
directory  envs  myinput  myscript  node  output  timer

[timk@colostate.edu@shas0136 test]$ cat 2197925/25/directory
/projects/timk@colostate.edu/test/inputs/set024

[timk@colostate.edu@shas0136 test]$ cat 2197925/25/myinput
10 84 20 50 200

[timk@colostate.edu@shas0136 test]$ cat 2197925/25/output
10 84 20 50 200
section 1 start time= 5.7936e-05   end time=   0.019413  error= 3.87013e-12
section 2 start time= 5.7936e-05   end time=   0.019923  error= 9.82607e-12
section 3 start time=   0.019456   end time=   0.038625  error= 4.5729e-12
section 4 start time=   0.019967   end time=   0.039389  error= 6.69376e-12


[timk@colostate.edu@shas0137 test]$ cat 2197925/25/timer
1555962929.441435 Mon Apr 22 13:55:29 2019      0.000      0.000 start_time
1555962929.523498 Mon Apr 22 13:55:29 2019      0.082      0.082 end_time
[timk@colostate.edu@shas0137 test]$
```

Each sub directory contains the output from a single run. Here we have the output from the set of runs where our input came from a set of directories.

```
[timk@colostate.edu@shas0136 test]$ ls 2197922
1  10  11  12  13  14  15  16  17  18  19  2  20  21  22  23  24  3  4  5  6  7  8  9

[timk@colostate.edu@shas0136 test]$ ls 2197922/1
envs  input  myscript  node  output  timer

[timk@colostate.edu@shas0136 test]$ cat 2197922/1/input
87 94 27 17 400

[timk@colostate.edu@shas0136 test]$ cat 2197922/1/output
87 94 27 17 400
section 1 start time= 6.2943e-05   end time=    0.15121  error= 4.31382e-11
section 2 start time= 6.2943e-05   end time=    0.15126  error= 1.53059e-11
section 3 start time=    0.15138   end time=    0.30201  error= 3.08275e-11
section 4 start time=    0.15144   end time=    0.30183  error= 2.21327e-11
```

Here we have the output from the set of runs where our input came from lines in a file.

Ask for GPU nodes

--partition=gpu-h100 --gres=gpu:h100:4

```
[tkaiser2@kl1 slurm25]$cat dogpu
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=8
#SBATCH --time=00:02:00
#SBATCH --partition=gpu-h100
#SBATCH --gres=gpu:h100:4

# What node(s) are we on?
echo $SLURM_NODELIST

# What partition
echo $SLURM_JOB_PARTITION

# GPU information
nvidia-smi -L
```

```
[tkaiser2@kl1 slurm25]$cat slurm-7583410.out
x3100c0s21b0n0
gpu-h100
GPU 0: NVIDIA H100 80GB HBM3 (UUID: GPU-96224b76-119e-b3d5-bcf1-de1c07aaac45)
GPU 1: NVIDIA H100 80GB HBM3 (UUID: GPU-e6b0d645-48b9-0341-0b87-b8ae88ac0761)
GPU 2: NVIDIA H100 80GB HBM3 (UUID: GPU-c1fb2da2-5567-abdb-1b1b-039ef0062f7b)
GPU 3: NVIDIA H100 80GB HBM3 (UUID: GPU-e5172eda-9fd6-954e-0d21-31b1afb358f1)
[tkaiser2@kl1 slurm25]$
```

```
[tkaiser2@kl1 slurm25]$cat nogres
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=8
#SBATCH --time=00:02:00
#SBATCH --partition=gpu-h100
########     #SBATCH --gres=gpu:h100:4 ########

# What node(s) are we on?
echo $SLURM_NODELIST

# What partition
echo $SLURM_JOB_PARTITION

# GPU information
nvidia-smi -L
```

```
[tkaiser2@kl1 slurm25]$cat slurm-7583402.out
x3100c0s13b0n0
gpu-h100
No devices found.
[tkaiser2@kl1 slurm25]$
```

If you land on a node that has GPUs but don't specify the --gres option you will not see the GPUs.

As of 06/09/22 on Vermilion gres in not currently required/supported

Ask for GPU nodes

--gres=gpu:h100:4

```
[tkaiser2@kl1 slurm25]$cat dogpu
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=8
#SBATCH --time=00:02:00
#SBATCH --partition=gpu-h100
#SBATCH --gres=gpu:h100:4

# What node(s) are we on?
echo $SLURM_NODELIST

# What partition
echo $SLURM_JOB_PARTITION

# GPU information
nvidia-smi -L
```

```
[tkaiser2@kl1 slurm25]$cat slurm-7583410.out
x3100c0s21b0n0
gpu-h100
GPU 0: NVIDIA H100 80GB HBM3 (UUID: GPU-96224b76-119e-b3d5-bcf1-de1c07aaac45)
GPU 1: NVIDIA H100 80GB HBM3 (UUID: GPU-e6b0d645-48b9-0341-0b87-b8ae88ac0761)
GPU 2: NVIDIA H100 80GB HBM3 (UUID: GPU-c1fb2da2-5567-abdb-1b1b-039ef0062f7b)
GPU 3: NVIDIA H100 80GB HBM3 (UUID: GPU-e5172eda-9fd6-954e-0d21-31b1afb358f1)
[tkaiser2@kl1 slurm25]$
```

```
[tkaiser2@kl1 slurm25]$cat nogres
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=8
#SBATCH --time=00:02:00
#SBATCH --partition=gpu-h100
########     #SBATCH --gres=gpu:h100:4 ########

# What node(s) are we on?
echo $SLURM_NODELIST

# What partition
echo $SLURM_JOB_PARTITION

# GPU information
nvidia-smi -L
```

```
[tkaiser2@kl1 slurm25]$cat slurm-7583402.out
x3100c0s13b0n0
gpu-h100
No devices found.
[tkaiser2@kl1 slurm25]$
```

If you land on a node that has GPUs but don't specify the --gres command you will not see the GPUs.

As of 06/09/22 on Vermilion gres in not currently required/supported

GPU Example

```
#!/bin/bash
#SBATCH --job-name="gpu_job"
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=4
#SBATCH --time=00:02:00
#SBATCH --partition=gpu-h100
#SBATCH --gres=gpu:h100:4
#SBATCH --exclusive=user
#SBATCH –account=hpcapps

# Check we are launching from a GPU node

if echo $SLURM_SUBMIT_HOST | egrep "kl5|kl6" > /dev/null  ; then : ; else echo Run script from a GPU node;  echo  exit ; fi

mkdir $SLURM_JOBID
cp  mstream.cu makefile doit dogpu  $SLURM_JOBID
cd $SLURM_JOBID


nvidia-smi -L > gpuinfo


# Run a mpi/cuda version of the stream bechnmark
ml PrgEnv-nvhpc
CC mstream.cu -o mstream
srun -n 4 ./mstream -n 5000 > mstream.out


mv slurm-$SLURM_JOBID.out .
```

Two additions:

- Check we are launching from a GPU node
- Run a “mpi/cuda” version of the stream benchmark
- Our "doit" script will login into a gpu node and launches from there

gpu

GPU Example

```
template <typename T>
__global__ void STREAM_Copy(T const * __restrict__ const a, T * __restrict__ const b, long len)
{
    long idx = (long)threadIdx.x + (long)blockIdx.x * (long)blockDim.x;
    if (idx < len)
        b[idx] = a[idx];
}

template <typename T>
__global__ void STREAM_Scale(T const * __restrict__ const a, T * __restrict__ const b, T scale,  long len)
{
    long idx = (long)threadIdx.x + (long)blockIdx.x * (long)blockDim.x;
    if (idx < len)
        b[idx] = scale * a[idx];
}

template <typename T>
__global__ void STREAM_Add(T const * __restrict__ const a, T const * __restrict__ const b, T * __restrict__ const c, long len)
{
    long idx = (long)threadIdx.x + (long)blockIdx.x * (long)blockDim.x;
    if (idx < len)
        c[idx] = a[idx] + b[idx];
}

template <typename T>
__global__ void STREAM_Triad(T const * __restrict__ a, T const * __restrict__ b, T * __restrict__ const c, T scalar, long len)
{
    long idx = (long)threadIdx.x + (long)blockIdx.x * (long)blockDim.x;
    if (idx < len)
        c[idx] = a[idx] + scalar * b[idx];
}
```

Output

```
[tkaiser2@kl1 7764252]$ls
dogpu  doit  gpuinfo  makefile  mstream  mstream.cu  mstream.out  strm.0000  strm.0001  strm.0002  strm.0003

[tkaiser2@kl1 7764252]$cat strm.0000
 STREAM Benchmark implementation in CUDA on device 0 of x3103c0s9b0n0
 Device name: NVIDIA H100 80GB HBM3
 Array elements 5000 Array size (double precision) =   0.04 MB
 Total memory for 3 arrays =   0.00 GB
 NTIMES 200000
 using 192 threads per block, 27 blocks
 output in IEC units (KiB = 1024 B)

Function      Rate (GiB/s)  Avg time(s)  Min time(s)  Max time(s)
-----------------------------------------------------------------
Copy:          10.7759      0.00000736   0.00000691   0.00014782
Scale:         10.7759      0.00000734   0.00000691   0.00015306
Add:           16.1638      0.00000734   0.00000691   0.00004506
Triad:         16.1638      0.00000737   0.00000691   0.00005603
 Total time       5.91 seconds
STREAM Benchmark implementation in CUDA on device 1 of x3103c0s9b0n0
Device name: NVIDIA H100 80GB HBM3
Array elements 5000 Array size (double precision) =   0.04 MB
Total memory for 3 arrays =   0.00 GB
NTIMES 200000
using 192 threads per block, 27 blocks
output in IEC units (KiB = 1024 B)
```

We run 4 MPI tasks/per node and each task "hits" one GPU

```
[tkaiser2@kl1 7764252]$cat strm.0003
 STREAM Benchmark implementation in CUDA on device 3 of x3103c0s9b0n0
 Device name: NVIDIA H100 80GB HBM3
 Array elements 5000 Array size (double precision) =   0.04 MB
 Total memory for 3 arrays =   0.00 GB
 NTIMES 200000
 using 192 threads per block, 27 blocks
 output in IEC units (KiB = 1024 B)

Function      Rate (GiB/s)  Avg time(s)  Min time(s)  Max time(s)
-----------------------------------------------------------------
Copy:          12.5000      0.00000716   0.00000596   0.00003409
Scale:         12.5000      0.00000713   0.00000596   0.00003409
Add:           18.7500      0.00000714   0.00000596   0.00003815
Triad:         18.7500      0.00000718   0.00000596   0.00005794
 Total time       5.75 seconds
[tkaiser2@kl1 7764252]$
```

Shared partition

```
[tkaiser2@kl1 slurm25]$salloc  --nodes=1 --time=01:00 --account=hpcapps --partition=shared --tasks-per-node=4
. . .
. . .
[tkaiser2@x1008c0s0b1n1 slurm25]$printenv | grep SLURM | grep "NODE="
SLURM_TASKS_PER_NODE=4
SLURM_STEP_TASKS_PER_NODE=1
SLURM_NTASKS_PER_NODE=4
SLURM_JOB_CPUS_PER_NODE=4
SLURM_CPUS_ON_NODE=4
```

```
[tkaiser2@kl1 slurm25]$salloc  --nodes=1 --time=01:00 --account=hpcapps --partition=shared --tasks-per-node=4 --cpus-per-task=2
. . .
. . .
[tkaiser2@x1008c0s0b1n1 slurm25]$printenv | grep SLURM | grep "NODE="
SLURM_TASKS_PER_NODE=4
SLURM_STEP_TASKS_PER_NODE=1
SLURM_NTASKS_PER_NODE=4
SLURM_JOB_CPUS_PER_NODE=8
SLURM_CPUS_ON_NODE=8
```

You only get “charged” for what you use.

Shared partition

```
[tkaiser2@kl1 slurm25]$salloc  --nodes=1 --time=01:00:00 --account=hpcapps --partition=shared
--tasks-per-node=4
. .
. . .
[tkaiser2@x1008c0s0b1n1 slurm25]$/home/tkaiser2/hog
     1 ::          0.1630130       0.1630130      6.587
     2 ::          0.3267691       0.1637561      6.557
     3 ::          0.4938800       0.1671109      6.425
Killed
```

```
salloc  --nodes=1 --time=01:00:00 --account=hpcapps --partition=shared
--tasks-per-node=4 --cpus-per-task=2
. . .
. . .
[tkaiser2@x1008c0s0b1n1 slurm25]$/home/tkaiser2/hog
     1 ::          0.1458972       0.1458972      7.360
     2 ::          0.2909060       0.1450088      7.405
     3 ::          0.4365361       0.1456301      7.373
     4 ::          0.5813200       0.1447840      7.416
     5 ::          0.7271311       0.1458111      7.364
     6 ::          0.8707340       0.1436028      7.477
     7 ::          1.0156901       0.1449561      7.407
Killed
```

```
[tkaiser2@kl1 slurm25]$salloc  --nodes=1 --time=01:00:00 --account=hpcapps --partition=shared
                               --tasks-per-node=4 --cpus-per-task=2 --mem=16000
. . .
. . .
[tkaiser2@x1008c0s0b1n1 slurm25]$/home/tkaiser2/hog
     1 ::          0.1295950       0.1295950      8.285
     2 ::          0.2586551       0.1290600      8.320
     3 ::          0.3880930       0.1294379      8.295
     4 ::          0.5172129       0.1291199      8.316
     5 ::          0.6463461       0.1291332      8.315
     6 ::          0.7754819       0.1291358      8.315
     7 ::          0.9048121       0.1293302      8.302
     8 ::          1.0338349       0.1290228      8.322
     9 ::          1.1628139       0.1289790      8.325
    10 ::          1.2923260       0.1295121      8.291
    11 ::          1.4220200       0.1296940      8.279
    12 ::          1.5522740       0.1302540      8.243
    13 ::          1.6825619       0.1302879      8.241
    14 ::          1.8127539       0.1301920      8.247
    15 ::          1.9497881       0.1370342      7.836
Killed
```

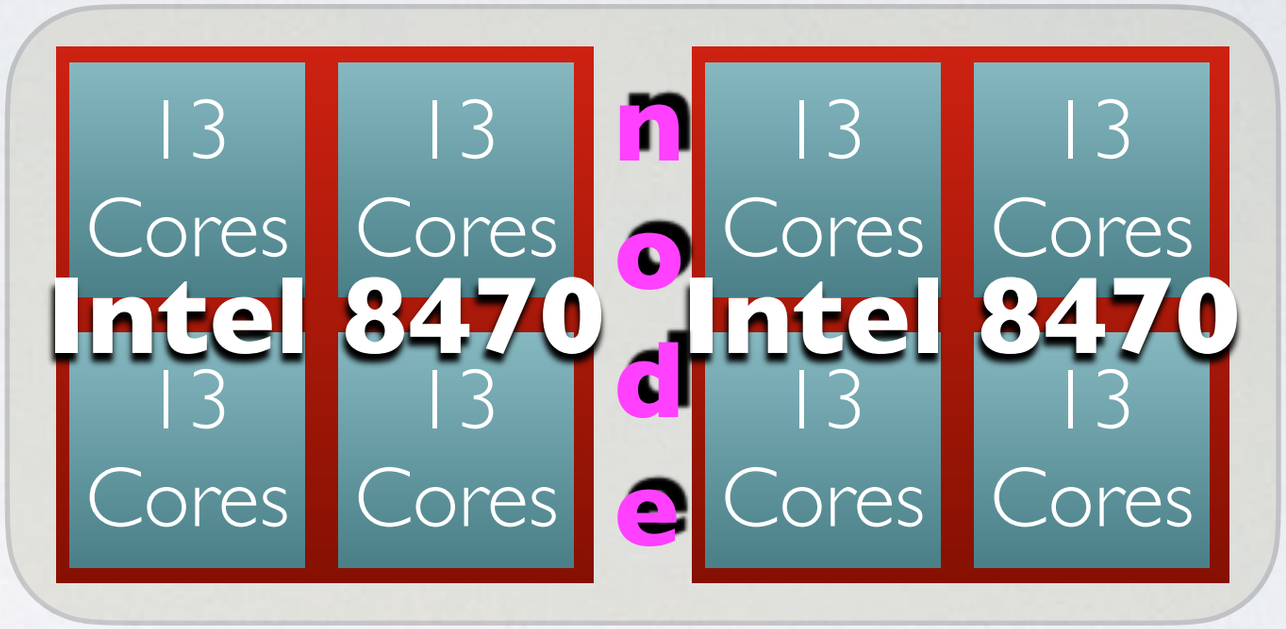
In shared, by default, you get 1GB of memory for each core requested

We're running a code that just keeps asking for more memory!

(We're trained experts. Don't try this at home)

AFFINITY & WHY IMPORTANT

- Affinity - mapping of threads/tasks to cores
- Kestrel 104 cores/node
    - 2 chips (Intel 8470)
        - 52 cores each
        - 4 "tiles" with 13 cores each



- **Worst case: Multiple threads/tasks can end up on the same core potentially reducing performance by 2X or maybe much more**
- Also: You may want to put threads/tasks on particular tiles to maximize communications or memory access
- Possible to have different MPI tasks to have different # threads

0-12	26-38
13-25	39-51

52-64	78-90
65-77	91-103

Affinity

- Mapping of tasks and threads to cores
- If you have two or more tasks or threads on the same core performance can tank.
- Our example code, pstream.c is designed to show mappings of tasks/threads to cores
- Mappings are effected by environmental variables and command line arguments
- Desired mappings can be application specific
- Default mappings might not be very good

Our script for affinity testing

```
#!/usr/bin/bash
#SBATCH --job-name="affinity"
#SBATCH --nodes=1
#SBATCH --exclusive
#SBATCH --export=ALL
#SBATCH --time=00:10:00
#SBATCH --partition=short

# Select MPI version based on the variable MYMPI, default to intel-oneapi-mpi
if [ -z "${MYMPI+x}" ]; then export MYMPI=intel-oneapi-mpi ; fi

# Setup
export BASE=$SLURM_SUBMIT_DIR
mkdir -p $BASE/$SLURM_JOB_ID
cd $BASE/$SLURM_JOB_ID

# Save info
cat $0   > $SLURM_JOB_ID.script
printenv > $SLURM_JOB_ID.env

# Get and build glorified "Hello World"
curl -s https://raw.githubusercontent.com/timkphd/examples/master/hybrid/pstream.c -o pstream.c
module load $MYMPI
echo MYMPI $MYMPI
echo MPI= `which mpicc`
mpicc -fopenmp pstream.c -o pstream

for nmpi in 1 2 4 8 13 26 52 104 ; do
   for nthreads in  2 4 8 13 ; do
     cores=`echo "$nmpi*$nthreads" | bc`
     if [ "$cores" -le "104" ] ; then
        echo Running on a total of $cores cores
        export OMP_NUM_THREADS=$nthreads
        export OMP_PROC_BIND=spread
        # The last column of output from pstream is the core on which a task/thread is run

        srun --cpu-bind=v --threads-per-core=1 --cpus-per-task=$nthreads --ntasks $nmpi ./pstream -F -D -t 2 > ${nmpi}_${nthreads}
# If we don't use the extra settings some tasks/threads will get mapped to the same cores and you'll see FAILED
       #srun --cpu-bind=v                                                --ntasks $nmpi ./pstream -F -D -t 2 > ${nmpi}_${nthreads}
        # We grab the core #s.  There should be unique set and the size should be equal to $cores
        used=`cat  ${nmpi}_${nthreads} | grep ^0 | awk '{print $6}' | sort -u | wc -l`
        if [ "$cores" -eq "$used" ] ; then
                echo SUCCESS ${nmpi}_${nthreads}
        else
                echo FAILED ${nmpi}_${nthreads}
        fi
     fi
    done
done
cp $SLURM_SUBMIT_DIR/slurm-$SLURM_JOB_ID.* .
```

On our run line we add:

--cpu-bind=v --threads-per-core=1 --cpus-per-task=$nthreads

--cpu-bind=v produces a “verbose” output mappings

affinity

Output from one of the runs

Core on which a task/thread is running

```
[tkaiser2@kl1 7772992]$cat 2_4
MPI VERSION Intel(R) MPI Library 2021.12 for Linux* OS

task     thread              node name  first task    # on node  core
0001     0000          x1001c0s3b0n1        0000          0001  0052
0001     0003          x1001c0s3b0n1        0000          0001  0055
0001     0002          x1001c0s3b0n1        0000          0001  0054
0001     0001          x1001c0s3b0n1        0000          0001  0053
0000     0000          x1001c0s3b0n1        0000          0000  0000
0000     0001          x1001c0s3b0n1        0000          0000  0001
0000     0003          x1001c0s3b0n1        0000          0000  0003
0000     0002          x1001c0s3b0n1        0000          0000  0002
total time      3.545
[tkaiser2@kl1 7772992]$
```

affinity

Output from a “broken” run

```
MPI VERSION MPI VERSION    : CRAY MPICH version 8.1.28.15 (ANL base 3.4a2)
MPI BUILD INFO : Wed Nov 15 21:00 2023 (git hash 1cde46f)

task    thread             node name  first task    # on node  core
0000      0000         x1003c0s0b1n0        0000         0000  0000
0001      0000         x1003c0s0b1n0        0000         0001  0000
0002      0000         x1003c0s0b1n0        0000         0002  0000
0003      0000         x1003c0s0b1n0        0000         0003  0000
0000      0001         x1003c0s0b1n0        0000         0000  0052
0001      0001         x1003c0s0b1n0        0000         0001  0052
0002      0001         x1003c0s0b1n0        0000         0002  0052
0003      0001         x1003c0s0b1n0        0000         0003  0052
total time      2.928
```

All tasks/threads end up on core 0 or 52.

affinity

Results

--threads-per-core=1 --cpus-per-task=$nthreads

MPI tasks _ Threads	With extra options	Time (sec)	Without extra options	Time (sec)	Slowdown
1_2	SUCCESS	5.26	SUCCESS	5.25	1.0
1_4	SUCCESS	3.54	SUCCESS	3.55	1.0
1_8	SUCCESS	2.72	SUCCESS	2.73	1.0
1_13	SUCCESS	2.31	SUCCESS	2.30	1.0
2_2	SUCCESS	5.26	SUCCESS	5.26	1.0
2_4	SUCCESS	3.55	SUCCESS	3.55	1.0
2_8	SUCCESS	2.73	SUCCESS	2.73	1.0
2_13	SUCCESS	2.31	SUCCESS	2.31	1.0
4_2	SUCCESS	5.26	**FAILED**	14.22	2.7
4_4	SUCCESS	3.55	**FAILED**	7.35	2.1
4_8	SUCCESS	2.74	**FAILED**	5.69	2.1
4_13	SUCCESS	2.38	**FAILED**	3.88	1.6
8_2	SUCCESS	5.27	**FAILED**	28.23	5.4
8_4	SUCCESS	3.57	**FAILED**	14.56	4.1
8_8	SUCCESS	2.96	**FAILED**	7.66	2.6
8_13	SUCCESS	2.55	**FAILED**	5.10	2.0
13_2	SUCCESS	5.29	**FAILED**	46.06	8.7
13_4	SUCCESS	3.79	**FAILED**	23.77	6.3
13_8	SUCCESS	2.94	**FAILED**	12.42	4.2
26_2	SUCCESS	5.46	**FAILED**	91.56	16.8
26_4	SUCCESS	3.44	**FAILED**	47.72	13.9
52_2	SUCCESS	4.57	**FAILED**	183.78	40.3

Affinity Settings

- srun options that effect affinity
  - https://slurm.schedmd.com/mc_support.html#srun_lowlevelmc
  - --cpu-bind
  - --cpus-per-task
  - --distribution
  - --ntasks-per-core
  - --ntasks-per-socket
  - --threads-per-core
- Openmp variables that effect affinity
  - OMP_NUM_THREADS
  - OMP_PROC_BIND
  - OMP_PLACES

What's a Reservation

- Nodes can be set aside, temporarily, for use for a particular purpose or set of people
- Only "special" people can assess these nodes
  - --reservation=rrrr
  - export SBATCH_RESERVATION=rrrr
- Can still access other nodes/partitions
- Sometimes used to "drain" nodes.

man pages

- All of the commands from today have man pages
  - man sbatch
  - man squeue
  - man srun
  - man sinfo
  - man scancel
  - man sacctmgr

https://slurm.schedmd.com/quickstart.html

Some Links

- https://www.nrel.gov/hpc/
  - NREL's HPC docs front page
- https://github.com/NREL/HPC/tree/master/slurm
  - My slurm script examples (old but still might be useful)
- https://nrel.github.io/HPC/Documentation/Slurm/batch_jobs/
  - Local slum info with script tutorial
- https://nrel.github.io/HPC/Documentation/Systems/
  - Systems page
- https://slurm.schedmd.com/quickstart.html
  - Slurm Docs
- https://nrel.github.io/HPC/Documentation/Systems/Kestrel/Environments/gpubuildandrun/
  - Building and running go Kestrel's GPU nodes
- https://github.com/timkphd/examples/tree/master/workshop/2025/slurm
  - Public copy of examples

Different # tasks on each node

```
[tkaiser2@x1004c6s0b0n1 mpmd]$cat ./mlist.py
#!/usr/bin/env python3
# usage
# scontrol show hostnames | ./mlist.py  4 2 6
import sys
node_list = sys.stdin.read()
node_list=node_list.split()
k=0
nnodes=len(node_list)
for n in sys.argv[1:]:
    for j in range(0,int(n)):
        print(node_list[k % nnodes])
    k=k+1
```

1. Create a node list file "hlist" containing a node for each task
2. Export SLURM_HOSTFILE to tell run to use it
3. srun as normal

```
[tkaiser2@x1004c6s0b0n1 mpmd]$scontrol show hostnames | ./mlist.py  4 2 6 4 > hlist
[tkaiser2@x1004c6s0b0n1 mpmd]$cat hlist
x1004c6s0b0n1
x1004c6s0b0n1
x1004c6s0b0n1
x1004c6s0b0n1
x1004c6s4b1n0
x1004c6s4b1n0
x1004c6s0b0n1
x1004c6s0b0n1
x1004c6s0b0n1
x1004c6s0b0n1
x1004c6s0b0n1
x1004c6s0b0n1
x1004c6s0b0n1
x1004c6s4b1n0
x1004c6s4b1n0
x1004c6s4b1n0
x1004c6s4b1n0
```

```
[tkaiser2@x1004c6s0b0n1 mpmd]$tasks=`wc -l hlist | cut -f 1 -d" "`
[tkaiser2@x1004c6s0b0n1 mpmd]$echo $tasks
16

[tkaiser2@x1004c6s0b0n1 mpmd]$export SLURM_HOSTFILE=hlist

[tkaiser2@x1004c6s0b0n1 mpmd]$srun -n $tasks ./helloc > output

[tkaiser2@x1004c6s0b0n1 mpmd]$grep Hello output | sort -nk5,5
 Hello from x1004c6s0b0n1 (C) 0 of 16
 Hello from x1004c6s0b0n1 (C) 1 of 16
 Hello from x1004c6s0b0n1 (C) 2 of 16
 Hello from x1004c6s0b0n1 (C) 3 of 16
 Hello from x1004c6s4b1n0 (C) 4 of 16
 Hello from x1004c6s4b1n0 (C) 5 of 16
 Hello from x1004c6s0b0n1 (C) 6 of 16
 Hello from x1004c6s0b0n1 (C) 7 of 16
 Hello from x1004c6s0b0n1 (C) 8 of 16
 Hello from x1004c6s0b0n1 (C) 9 of 16
 Hello from x1004c6s0b0n1 (C) 10 of 16
 Hello from x1004c6s0b0n1 (C) 11 of 16
 Hello from x1004c6s4b1n0 (C) 12 of 16
 Hello from x1004c6s4b1n0 (C) 13 of 16
 Hello from x1004c6s4b1n0 (C) 14 of 16
 Hello from x1004c6s4b1n0 (C) 15 of 16
[tkaiser2@x1004c6s0b0n1 mpmd]$
```

MPMD - different apps for various tasks

```
[tkaiser2@x1001c1s0b1n0 mpmd]$scontrol show hostnames | ./mlist.py  4 2 6 4 > hlist
[tkaiser2@x1001c1s0b1n0 mpmd]$ export SLURM_HOSTFILE=hlist
```

```
[tkaiser2@x1001c1s0b1n0 mpmd]$cat apps
0-5 ./helloF
6-8   ./helloc
9   ./helloF
10    ./helloc
11  ./helloF
12-15 ./helloc
```

```
[tkaiser2@x1001c1s0b1n0 mpmd]$srun -n 16 --multi-prog apps
```

Sorted output

```
Hello from x1001c1s0b1n0 (F)           0  of          16
Hello from x1001c1s0b1n0 (F)           1  of          16
Hello from x1001c1s0b1n0 (F)           2  of          16
Hello from x1001c1s0b1n0 (F)           3  of          16
Hello from x1001c1s1b0n0 (F)           4  of          16
Hello from x1001c1s1b0n0 (F)           5  of          16
Hello from x1001c1s0b1n0 (C) 6 of 16
Hello from x1001c1s0b1n0 (C) 7 of 16
Hello from x1001c1s0b1n0 (C) 8 of 16
Hello from x1001c1s0b1n0 (F)           9  of          16
Hello from x1001c1s0b1n0 (C) 10 of 16
Hello from x1001c1s0b1n0 (F)          11  of          16
Hello from x1001c1s1b0n0 (C) 12 of 16
Hello from x1001c1s1b0n0 (C) 13 of 16
Hello from x1001c1s1b0n0 (C) 14 of 16
Hello from x1001c1s1b0n0 (C) 15 of 16
```

1. Here we also use a host list file but that is not required
2. Create an "apps" file that contains a numbered list of the app for each task
3. srun with --multi-prog apps
4. No arguments after this new option
5. If you need arguments for your app they go in the "apps" file
6. Broken for Cray MPICH

Slurm Basics

June 3, 2025

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Setup On Kestrel..

ssh kestrel.nrel.gov

```
cd /scratch/$USER
mkdir slurm25
cd slurm25
tar -xzf /scratch/tkaiser2/shared/slurm25/slurm25.tgz

export SLURM_ACCOUNT=YOUR_ACCOUNT
export SALLOC_ACCOUNT=$SLURM_ACCOUNT
export SBATCH_ACCOUNT=$SLURM_ACCOUNT
```

. ./doall

To get the results without running...

```
tar -xzf /scratch/tkaiser2/shared/slurm25/run25.tgz
```