

Flux to Great Lakes Training

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<https://www-personal.umich.edu/~mmiranda/GLSlides.pdf>

Outline

What we will cover today:

- High level description of Great Lakes, Lighthouse, & Armis2
- New LMOD software layout
- PBS to Slurm script conversion
- Discuss on demand usage, CPU & RAM
- Hands on examples using Beta:
 - Software modules
 - Finding resources in Slurm
 - Simple Slurm example
 - MPI Slurm example

Clusters

New cluster and changes to existing clusters:

- Great Lakes
 - Slurm and new software layout
 - Standard nodes: Skylake 36 Cores 3.0Ghz, 192GB
 - Large Memory nodes: 1.5 TB
 - GPU nodes: 2 x Tesla V100 16 GB
 - Maximum wall clock time: Two weeks
- Armis2
 - Slurm and new software layout
 - Standard nodes: Haswell
 - ARC-TS will start charging for the service at some point

Lighthouse

- Flux Operating Environment nodes will migrate to Lighthouse
 - Eligible nodes only!
 - Actual compute hardware does not change
- New LMOD software layout
- Will have its own login node: `lighthouse.arc-ts.umich.edu`
- Beta home directories become Lighthouse home directories
- `/scratch`
 - Turbo NFS volume, not Luster
 - Files are auto purged!

Dates:

- August 14, 2019
 - Great Lakes general availability
- November 25, 2019
 - Lighthouse migration must be completed
 - Flux goes offline
 - Billing for Great Lakes starts

Software Module Layout

- The current Flux software layout is flat
 - Everything shows up regardless of whether you can use it or need it!
- New LMOD software layout
 - Tree structure
 - Only software that is truly available to you is visible
 - Cleaner module listing
 - Software collections:
 - Bioinformatics
 - OnCampusAccessOnly
 - RestrictedLicense

/scratch

- Is for active data only.
 - Not for storage
- Data is automatically deleted after 60 days!
 - Files are auto purged!
- Each cluster has its own /scratch system.
 - Armis2 and Lighthouse: Turbo NFS volume, not Lustre
 - Great Lakes: GPFS

Slurm is a scalable cluster management and job scheduling system for Linux clusters.

- Replaces PBS/Torque
- Faster
 - Can start many jobs quickly
 - Can predict job startup time
- Scales better, more jobs
- More flexible
 - Job steps
- Easier to use for simple jobs
 - Does more for you by default
- Complex features for complex jobs

PBS to Slurm

What is the best best way to convert my job submission scripts?

- A few strategies:
 - Rewrite everything from scratch
 - **Rewrite only the preamble and try to reuse the rest.** (recommended)
 - Translate the lines that need to be changed
- This is a chance to learn the best practices.
 - Slurm can work better than PBS but only if used correctly.
 - Accurately request the resources (CPU/RAM) you need.
 - Jobs will start faster
 - More jobs will run
 - Job start prediction will be better

Converting Scripts to Slurm

Rewrite only the preamble and try to reuse the rest.

- 1) Identify what the PBS preamble is requesting:
 - a) How many nodes and CPU-cores are needed?
 - b) How much RAM?
 - c) How much time (wall clock limit)?
 - d) Anything special?
- 2) Write the Slurm preamble.
- 3) Skip the change directory part!
- 4) Copy the actual compute part of the script.
- 5) Test the script.

Converting Scripts to Slurm

```
#### PBS preamble
#PBS -N fmm_test
#PBS -m ae
#PBS -A test_flux
#PBS -q flux
#PBS -l nodes=1:ppn=2,pmem=2000mb
#PBS -l walltime=1:00:00
#PBS -j oe
#PBS -V
#### End PBS preamble
```

What you asked for:

- 1 node with 2 cores
- 2000 MB per core
- 1 hour
 - Usually takes 40 minutes
- Email at end and abort

```
##### Slurm preamble
#SBATCH --job-name=fmm_test
#SBATCH --mail-type=END,FAIL
#SBATCH --account=test
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=2
#SBATCH --mem-per-cpu=2000m
#SBATCH --time=1:00:00
##### End of preamble!
```

```
if [ -s "$PBS_NODEFILE" ] ; then
    echo "Running on"
    uniq -c $PBS_NODEFILE
fi
```

Not needed, but you may want it.

```
if [[ $SLURM_JOB_NODELIST ]] ; then
    echo "Running on"
    scontrol show hostnames $SLURM_JOB_NODELIST
fi
```

```
if [ -d "$PBS_O_WORKDIR" ] ; then
    cd $PBS_O_WORKDIR
    echo "Running from $PBS_O_WORKDIR"
fi
```

Slurm does this for you.

```
# Put your job commands after this line
fmm_engin input.dat output.dat
```

```
# Put your job commands after this line
fmm_engin input.dat output.dat
```

Avoid in Slurm Scripts

It is best to avoid these:

- Always requesting the maximum wall clock time
 - Higher wall clock request will have later start times.
- Always asking for 4000mb per core.
 - You are charged for what you use.
 - What you do not use now may be available for use later.
 - Remember this on demand billing.
- Asking for cores instead of nodes and cores per a node
 - In PBS this is procs=Z instead of nodes=X:ppn=Y, where $Z=X*Y$
 - Job may start faster, but they will run slower!

On Demand

Great Lakes and Armis2 will not have monthly allocation like Flux.

Instead, they will use a model similar to Flux on Demand.

- We do not have the exact pricing, yet.
 - Cost will be based on actual monthly usage.
- Usage is determined by the percentage of the node used by the job.
 - Using all the CPU cores is the same as using all the RAM, that is using the whole node.
- The details are not final at this point.

Questions?

- Keep in mind that the details are not final at this point.
- Any questions on the topics just covered?
 - Clusters: Great Lakes, Armis2, & ect...
 - On Demand
 - Something not mentioned?
- Please hold your detailed questions on the following topics until the end:
 - LMOD Software Modules
 - Slurm and Job Submission
 - PBS to Slurm script conversion

Hands on Examples

- Please login to:
greatlakes.arc-ts.umich.edu
- Link to examples:
<https://www-personal.umich.edu/~mmiranda/GLTutorial.pdf>

Thank You!

- Please contact hpc-support@umich.edu for help.
- Any questions?
You can contact us:
 - coe-research-computing@umich.edu
 - <https://caen.engin.umich.edu/hpc/>