High Throughput Computing

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Instructor:

RC Homepage: https://www.colorado.edu/rc/

RC Docs: https://curc.readthedocs.io/en/latest/

RC Helpdesk: rc-help@colorado.edu

Course Materials:
https://github.com/ResearchComputing/Supercomputing_Spinup

Survey: http://tinyurl.com/curc-survey18

Login and download course materials

If you have a Summit account:

```
ssh -X <identikey>@login.rc.colorado.edu
```

If you don't have an account:

```
ssh -X user00NN@tlogin1.rc.colorado.edu
```

(for latter case, I will provide you with the "NN" and password)

…Once you are logged in, type the following three commands:

```
cd /scratch/<alpine or summit>/$USER
git clone https://github.com/ResearchComputing/Supercomputing_Spinup.git
```

What is HTC?

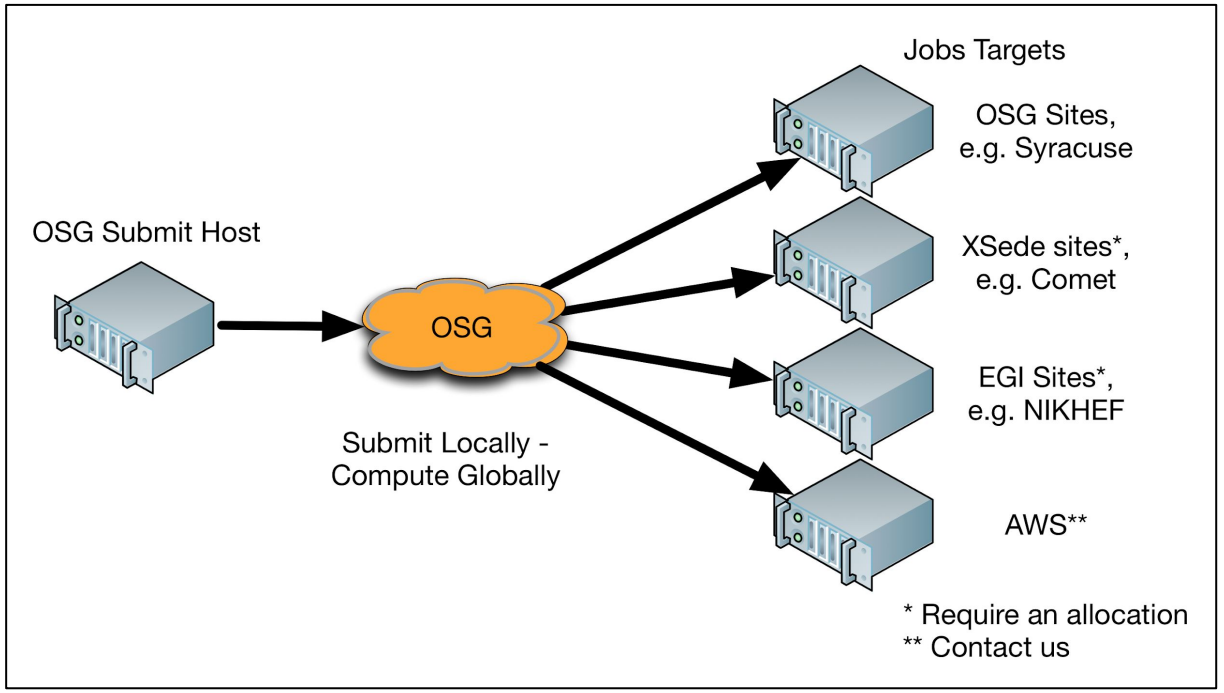
- High throughput computing (HTC) recognizes that most scientists work on research timescales.
- They value how many computing cycles they can get over a period of weeks-to-months rather than a period of hours-to-days.
- Processor speed not a concern – volume is more important.
- Processor type/homogeneity not important either.
- Typical workflow may have hundreds-to-thousands of jobs.
- Often comprised of many serial tasks that can be run independently.
- Goal is to submit lots of jobs with minimal effort and oversight.

http://research.cs.wisc.edu/htcondor/htc.html

Example of ‘pure’ HTC resource

Open Science Grid (OSG)

- NSF/DOE-funded service (free!)
- Open to any U.S.-based researcher
- 125 institutions sharing spare computing cycles
- ~1 Billion core hours per year used
- Can get started quickly. Options for dedicated allocation if needed.
- https://osgconnect.net



https://swc-osg-workshop.github.io/OSG-UserTraining-JLab-2019/materials/AHM/01-IntroGrid.html

Can I do HTC on RMACC Summit?

- Not quite at the scale of OSG.
- But you can “wrap up” 100s-to-1000s of jobs and submit them all in one job script to any of the partitions/qos’s on Summit
- Depending on the timescales of your workflow, this might also be called **“many task computing” (MTC)**, which focuses on lots of tasks over shorter timescales.

How can I do HTC/MTC on Summit?

There are two primary ways, and we will cover both today:

1. **Job arrays**
   - Submit one Slurm job script that submits X **jobs simultaneously**
     - Great for lots of tasks that have heterogeneous run times
     - Each job usually runs a serial task but can be a multi-core task if needed
     - Jobs will run as cores become available
     - …works best for longer tasks (> 30 min)
     - Summit limits: Maximum array size of 1000; 100 jobs can run at once in ucb-general

2. **GNU Parallel **or** CURC Load Balancer**
   - Submit one Slurm job script that runs X **tasks** on N requested cores
     - All under one job that works through all X tasks in order, running N at a time (e.g., X=10,000 tasks on N=24 cores)
     - Great for lots of tasks that may have similar run times
     - …works best for shorter tasks (< 30 min)

Job Arrays

- It is easy to adapt an existing job script to run as an array of jobs.
  - Add the following directive: #SBATCH --array=n-N
    - E.g., #SBATCH --array=1-200
    - You can also specify unevenly spaced arrays: #SBATCH –array=1,4,5,9,22
  - You can then just submit your job script and it will run all members from n to N.
  - If your jobs depend on the array index, you can use the environment variable $SLURM_ARRAY_TASK_ID to invoke the present array number.
    - E.g., typing "`python myscript.py file_${SLURM_ARRAY_TASK_ID}.csv`" will run a python script over the array, each time processing a different file.

Example 1: job_array_ex1.sh

```
#!/bin/bash

#SBATCH --job-name=array_ex1
#SBATCH --output=outfiles/array_ex1.%A_%a.out
#SBATCH --partition=shas
#SBATCH --qos=normal
#SBATCH --time=00:00:05
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --array=1-12

# Run your program
echo "################################################"
echo "start array job ${SLURM_ARRAY_TASK_ID}"
echo "This job is performing $SLURM_NTASKS tasks"
echo "This job has reserved $SLURM_CPUS_PER_TASK cores for $SLURM_NTASKS tasks"
JOBMEM=$(echo "scale=2; $SLURM_CPUS_PER_TASK*$SLURM_MEM_PER_CPU/1000" | bc)
echo "Each task has $JOBMEM GB of memory allocated to it"
```

Example 1: job_array_ex1.sh

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#SBATCH --cpus-per-task=1
#SBATCH --array=1-12

# Run your program
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echo "start array job ${SLURM_ARRAY_TASK_ID}"
echo "This job is performing $SLURM_NTASKS tasks"
echo "This job has reserved $SLURM_CPUS_PER_TASK cores for $SLURM_NTASKS tasks"
JOBMEM=$(echo "scale=2; $SLURM_CPUS_PER_TASK*$SLURM_MEM_PER_CPU/1000" | bc)
echo "Each task has $JOBMEM GB of memory allocated to it"
```

Let's run the example:

```
sbatch --reservation=hpc job_array_ex1.sh
```

Example 2: job_array_ex2.sh

- Example 2 is an extension of Example 1
- We load python and R modules and then add lines to call python and R scripts
  - Both scripts read in array-ordered files from the "./infiles" directory as command-line arguments, and print the output to the "./outfiles" directory.

- Examine job_array_ex2.sh

```
more job_array_ex2.sh
```

- Run job_array_ex2.sh

```
sbatch --reservation=hpc job_array_ex2.sh
```

GNU Parallel

- GNU parallel is a shell tool for executing tasks in parallel using one or more computers.
  - In it's simplest form, GNU parallel is a parallel replacement of a do or for loop.
- Options to specify how many tasks should run in parallel, display output in order, delay starts, limit resources and more!
- Let's get started with some command line examples. Start an interactive job:
  - `sinteractive --reservation=hpc --ntasks=8`
  - `ml gnu_parallel`

GNU Parallel Useful Options

- View what commands parallel will run without executing them:
  - `seq 10 | parallel --dry-run echo {}`
- Limit number of tasks running at one time:
  - `seq 10 | parallel -j 2 echo {}`
- Stagger start times for processes to avoid I/O overload:
  - `seq 10 | parallel --delay 2.0 echo {}`
- See all the options:
  - `man parallel`

Let's try working with files

- Let's run our python script on all of the input files in ./infiles:
  - `find infiles/*.txt | parallel python python_array_test.py {}`

- Or we can read the commands and arguments from a file
  - `find infiles/*.txt | parallel --dry-run python python_array_test.py {} > commands.txt`
  - `parallel < commands.txt`

Example: gnu_parallel_ex1.sh

- Job script is similar to job scripts for job arrays except:
  - Does not have the #SBATCH --array=n-N flag
  - Requires loading the gnu_parallel module
  - You will likely increase --ntasks because you want to spread tasks across many cores
  - All standard output goes to a single *.out file (unless you redirect output)

- This example does the same tasks as job_array_ex2.sh:
  - We load python and R modules call python and R scripts
    - Both scripts read in files from the "./infiles" directory as command-line arguments, and print the output to the "./outfiles" directory.

- Examine job script

```
more gnu_parallel_ex1.sh
```

- Run job script

```
sbatch --reservation=hpc gnu_parallel_ex1.sh
```

CURC Load Balancer

- In-house tool for executing tasks in parallel using one or more RMACC Summit nodes.

- Very simple to use:
  - Step 1: Create file that lists tasks you want to run
    - One task per line
    - If multiple commands per task can separate each command with semi-colin ";"
    - …or if each task is a complex list of commands, can create a bash script for each task
  - Step 2: load modules and execute using "`mpirun lb commands.txt`"

- Let's try an example…

Example: load_balance_ex1.sh

- Job script is similar to job scripts for job arrays except:
  - Does not have the #SBATCH --array=n-N flag
  - Requires loading the intel, impi and loadbalance modules
  - You will likely increase --ntasks because you want to spread tasks across many cores
  - All standard output goes to a single *.out file (unless you redirect output)

- This example does the same tasks as gnu_parallel_ex1.sh:
  - We load python and R modules call python and R scripts
    - Both scripts read in files from the "./infiles" directory as command-line arguments, and print the output to the "./outfiles" directory.
    - We will reuse the "commands.txt" file we created during the gnu parallel exercises.

- Examine job script

```
more load_balance_ex1.sh
```

- Run job script

```
sbatch --reservation=hpc load_balance_ex1.sh
```

Which HTC/MTC tool should I use?

	Job Arrays	GNU Parallel	Load Balancer
Job length?	Best for tasks > 30 min	Best for tasks < 30 min	Best for tasks < 30 min
Where can I use?	RMACC Summit, other HPC resources	RMACC Summit or your laptop/desktop	RMACC Summit, other HPC resources
Max jobs in queue?	1000 (per array)	No	No
Max cores per job?	None; works well one one or multiple nodes	None but works best on one node/machine	None; works well one one or multiple nodes
Max cores per task?	None	None but most commonly used for serial tasks	None but most commonly used for serial tasks
Does it reserve a controller core?	No	No	Yes
Other features?	Easy to adapt a "regular" job script to accommodate job arrays	Great for replacing/speeding up loops; Can pick up where you left off if job times out; commonly found on any HPC system	Works well for input files with heterogeneous names ; easy to set up multi-node jobs

Other HTC/MTC resources

- On Blanca: If you belong to a group with a Blanca node, this is a fantastic place to do HTC/MTC!

- On OSG (if you grow beyond Summit)

  https://opensciencegrid.org/about/introduction/

  (Need help getting started on OSG? Contact me)

Thank you!

- We'd love your feedback: http://tinyurl.com/curc-survey18
- CURC Load Balancer documentation
  https://curc.readthedocs.io/en/latest/software/loadbalancer.html
- GNU Parallel documentation
  https://curc.readthedocs.io/en/latest/software/GNUParallel.html
  https://www.gnu.org/software/parallel/parallel_tutorial.html
- Slurm job arrays
  https://slurm.schedmd.com/job_array.html