RC Primer: Incredibly Easy Parallelization with High Throughput Computing

Research Computing
UNIVERSITY OF COLORADO BOULDER

Incredibly Easy Parallelization with High Throughput Computing

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- Website: www.rc.colorado.edu/rc
- Documentation: https://curc.readthedocs.io
- Helpdesk: rc-help@colorado.edu
- Survey: http://tinyurl.com/curc-survey18

Slides
https://github.com/ResearchComputing/easy_parallelization_htc_primer

Meet the User Support Team

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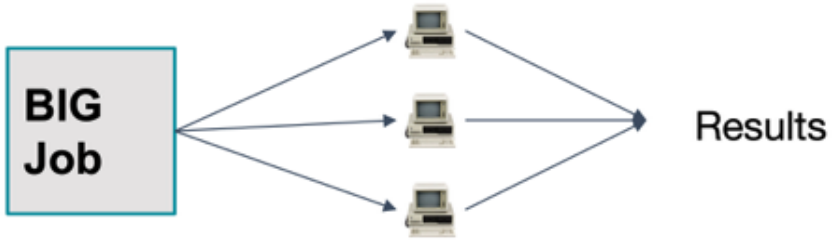
Learning Objectives and Outline

- Introduction to high throughput computing (HTC)
- HTC method 1: Job Arrays
- HTC method 2: Load Balancer
- HTC method 3: GNU Parallel
- Open Science Grid

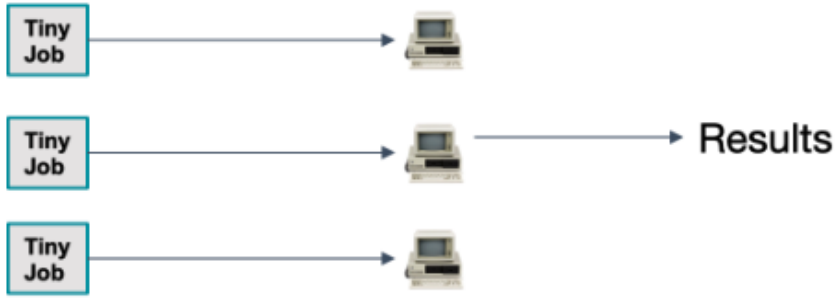
What is High Throughput Computing (HTC)?

Internal parallelization



Example: Climate Model

External parallelization



Example: Image processing

This is HTC!

Concept review

Three HTC methods for Alpine

	Job Arrays	Load Balancer	GNU Parallel
Job length?	Best for tasks > 10 min	Best for tasks < 30 min	Best for tasks < 30 min
Where can I use?	Alpine, other HPC resources	Alpine, other HPC resources	Alpine or your laptop/desktop
Max jobs in queue?	1000 across all arrays/jobs; each array member counts as a job	No	No
Max cores per job?	None; works well on one or multiple nodes	None; works well on one or multiple nodes	None but works best on one node/machine
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	Yes	No
Other features?	Easy to adapt a "regular" job script to accommodate job arrays	Works well for input files with heterogeneous names ; easy to set up multi-node jobs	Great for replacing/speeding up loops; Can pick up where you left off if job times out

Concept review

Now let’s try some examples….

Logging into CU Research Computing

login to CURC via your terminal:

```
$ ssh monaghaa@login.rc.colorado.edu
```

…or login to CURC via your browser:

https://ondemand-rmacc.rc.colorado.edu

(once logged in, navigate to **Clusters -> Alpine shell**)

Additional information:
https://curc.readthedocs.io/en/latest/access/logging-in.html
https://curc.readthedocs.io/en/latest/gateways/OnDemand.html

Download the example files

```
]$ cd /scratch/alpine/$USER
]$ git clone https://github.com/ResearchComputing/easy_parallelization_htc_primer
]$ cd easy_parallelization_htc_primer/examples
]$ ls
cars_mpg_array.sh       cars_mpg_input_args_array.txt          cars_mpg_input_commands_lb.txt  cars_mpg.py
cars_mpg_gnuparallel.sh  cars_mpg_input_commands_gnuparallel.txt  cars_mpg_lb.sh

]$ cat cars_mpg.py
import sys

car=sys.argv[1]
mpg=sys.argv[2]

print("The " + car + " gets " + mpg + " mpg.")
```

Method 1 Example: Job Arrays

To run this example :

```
]$ sbatch –reservation=htc
cars_mpg_array.sh
```

cars_mpg_array.sh (job script)

```
#!/bin/bash
#SBATCH --time=00:00:10
#SBATCH --partition=amilan
#SBATCH --qos=normal
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --job-name=cars
#SBATCH --output=cars.%A_%a.out
#SBATCH --array=1-5

# load anaconda python
source /curc/sw/anaconda/default

# run workflow
python cars_mpg.py $(sed -n "${SLURM_ARRAY_TASK_ID}p" cars_mpg_input_args_array.txt)
```

Only request resources for 1 member

This flag makes the array

cars_mpg_args_array.txt
(arguments)

```
mustang 25
pinto 30
chevette 33
nova 21
cutlass 23
```

Method 2 Example: Load Balancer

To run this example :

```
]$ sbatch –reservation=htc cars_mpg_lb.sh
```

cars_mpg_lb.sh (job script)

```
#!/bin/bash
#SBATCH --time=00:00:10
#SBATCH --partition=amilan
#SBATCH --qos=normal
#SBATCH --nodes=1   # optional
#SBATCH --ntasks=6
#SBATCH --job-name=cars
#SBATCH --output=cars.%j.out


# load loadbalancer and anaconda python
module purge
module load loadbalance
source /curc/sw/anaconda/default

# run workflow
mpirun lb cars_mpg_input_commands_lb.txt
```

Request resources for all members

Load the 'loadbalance' module

cars_mpg_commands_lb.txt (arguments)

```
python cars_mpg.py mustang 25
python cars_mpg.py pinto 30
python cars_mpg.py chevette 33
python cars_mpg.py nova 21
python cars_mpg.py cutlass 23
```

Method 3 Example: GNU Parallel

cars_mpg_gnuparallel.sh (job script)

```
#!/bin/bash
#SBATCH --time=00:00:10
#SBATCH --partition=amilan
#SBATCH --qos=normal
#SBATCH --nodes=1   # optional
#SBATCH --ntasks=5
#SBATCH --job-name=cars
#SBATCH --output=cars.%j.out


# load gnu parallel and anaconda python
module purge
module load gnu_parallel
source /curc/sw/anaconda/default

# run workflow
parallel -j $SLURM_NTASKS < cars_mpg_input_commands_gnuparallel.txt
```

Request resources for all members

Load the 'gnu_parallel' module

To run this example :

```
]$ sbatch –reservation=htc
cars_mpg_gnuparallel.sh
```

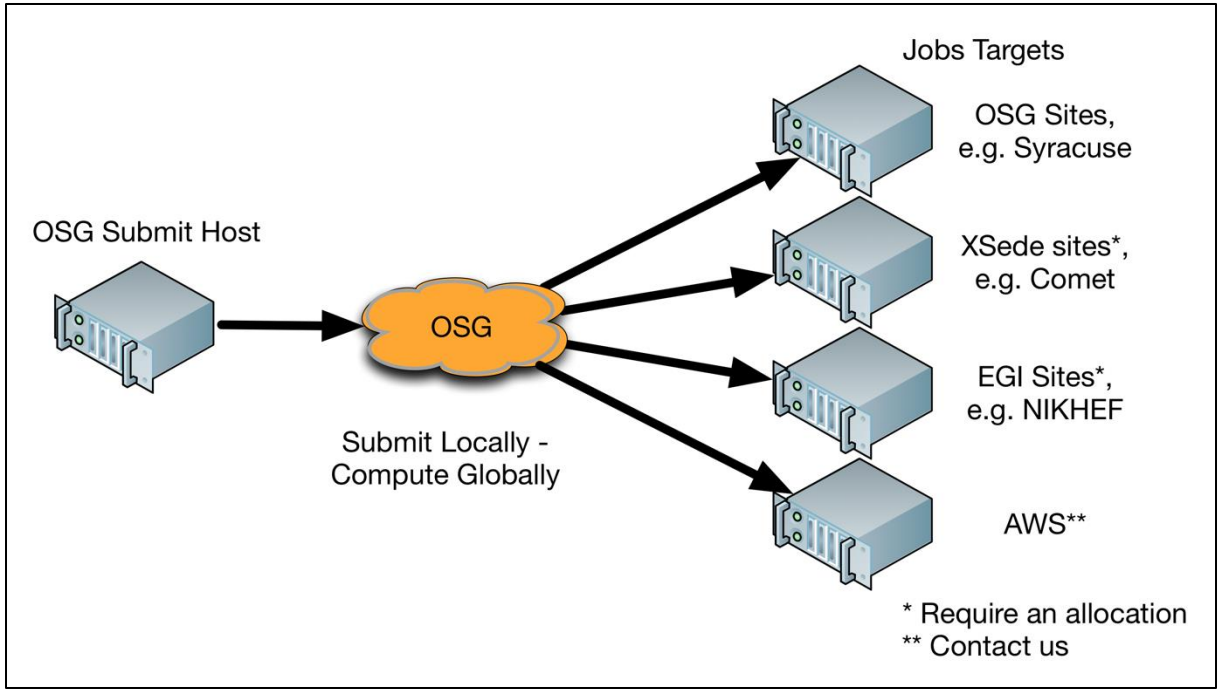
cars_mpg_commands_gnuparallel.txt (arguments)

```
python cars_mpg.py mustang 25
python cars_mpg.py pinto 30
python cars_mpg.py chevette 33
python cars_mpg.py nova 21
python cars_mpg.py cutlass 23
```

Concept review

A Community HTC Resource beyond Alpine: 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



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

Thank you!

Survey and feedback

http://tinyurl.com/curc-survey18