# 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

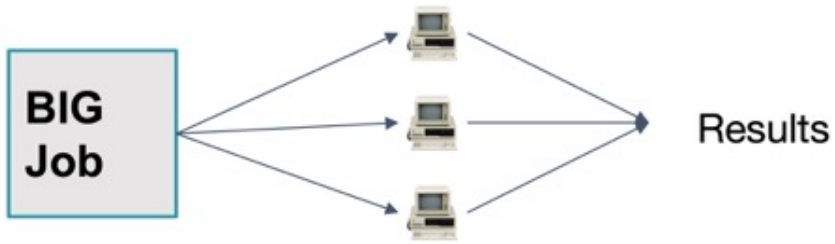
**Slides**
https://github.com/ResearchComputing/easy_parallelization_htc_primer

# 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

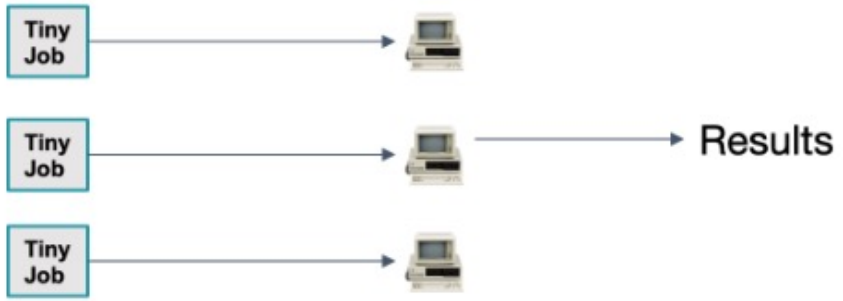
# What is High Throughput Computing (HTC)?

## Internal parallelization




Example: Climate Model

## External parallelization




Example: Image processing

**This is HTC!**

# 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 |

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 :*

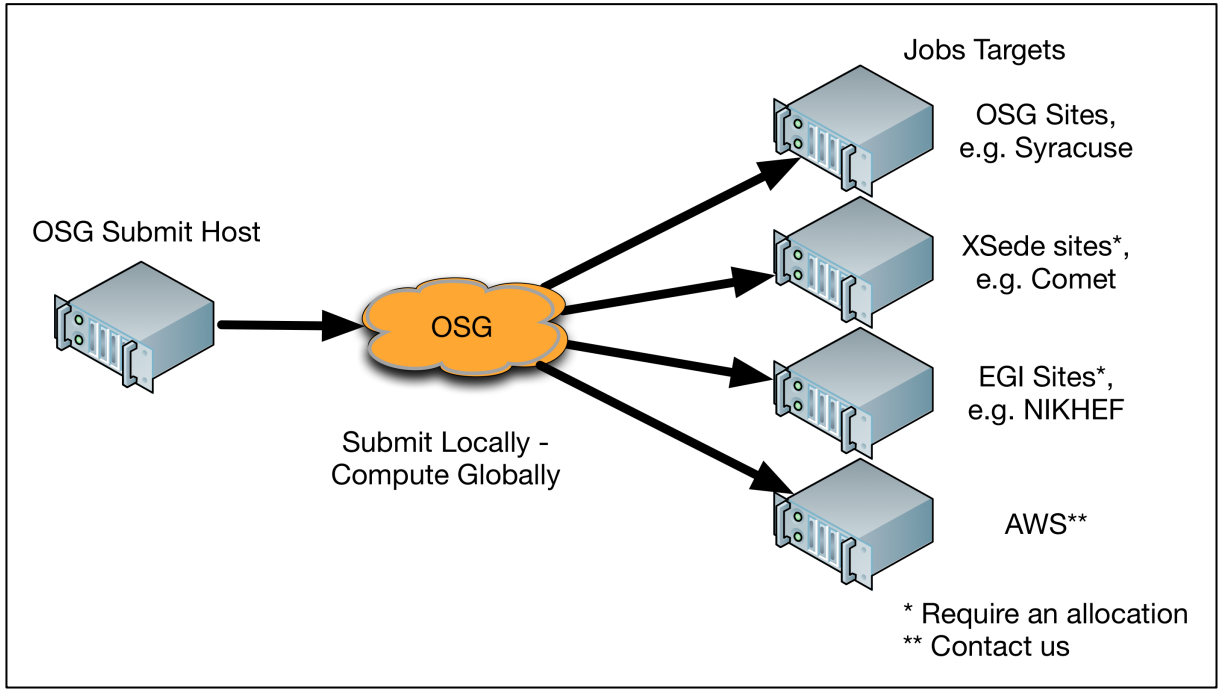
```
]$ sbatch –reservation=htc
cars_mpg_gnuparallel.sh
```

*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
```

# 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