# Scientific Workflows at scale using GNU Parallel

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I acknowledge the original developer and maintainer of GNU parallel, **Ole Tange** for the gift of a wonderful tool!

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# Part 1: Overview and Logistics

#### Overview: What shall we learn

- Familiarize with GNU Parallel features
- How to utilize HPC with GNU Parallel
  - Resource Management
  - Working with multicore architectures
- Running workflow tasks asynchronously
  - Data dependencies and Parallelism
- Strategies to run applications and production tasks with GNU Parallel

#### Slides and Practice Data for Download

Slides and practice files available:

github.com/ketancmaheshwari/escience23tut

# tinyurl.com/4v4b8pch



```
/data has data used for exercises.
```

**/src** has code discussed in the tutorial (except the one liners).

#### About You and Me

- Basic exposure to Linux is assumed but feel free to interrupt and ask questions
  - common commands, basic understanding of files and directories, process.
     eg. cd, ls, pwd, cat, date, seq

- About Me
  - Sr. Linux Engineer at Oak Ridge National Laboratory
  - Command line and Linux terminal enthusiast

#### About the Slides

- 8 Parts, each part has 4-10 slides
- Lots of examples in slides
- Summary and Practice Exercises
   We try to solve them here (if time permits)
- Solve it offline if we run out of time
- Plan to publish solutions around Nov 10, 2023, on Github



#### Part 2: Introduction to GNU Parallel

#### What is GNU Parallel

- A terminal tool to parallelize processes
- Easy to install, highly configurable
- Well suited to run many single-core / single-thread tasks on:
  - Compute nodes leveraging multicore architectures
  - Bag of workstations such as testbeds
  - Works well with Resource Managers and Job Schedulers
- Mature (20 years old), Simple and Powerful!

#### Installation

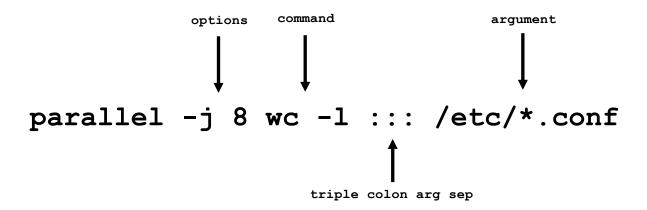
- Download the latest version:
   curl -s https://ftp.gnu.org/gnu/parallel/parallel-latest.tar.bz2
- Untar and cd into it: tar zxf parallel-latest.tar.bz2 cd parallel-20230822
- Install:
  - ./configure --prefix=\$HOME/parallel-install
    make install # needs libevent
- Set PATH and it is ready to go: export PATH=\$HOME/parallel-install/bin:\$PATH which parallel

## Many sources for getting help

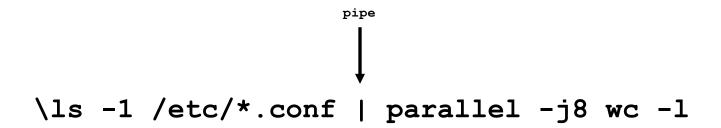
- link to youtube videos by Ole Tange: <a href="www.pi.dk/1">www.pi.dk/1</a>
- www.gnu.org/software/parallel/parallel\_cheat.pdf
- Searching for "gnu parallel" on Hacker news, Reddit, Stack Exchange yields many helpful links

```
man parallel
man parallel_tutorial
parallel --help  # summary of most imp options
parallel --max-line-length-allowed # max size of cmdline
parallel --number-of-cpus && parallel --number-of-cores
```

## Anatomy of a GNU Parallel Command

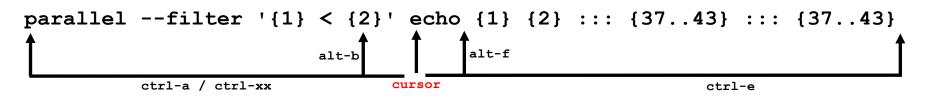


#### Another Form of the same command



## Aside1: Command line Navigation

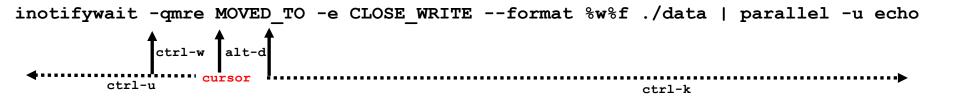
MAC users: terminal pref > profile > keyboard settings > Use option as meta key



ctrl-] <char> moves cursor to 1st occurrence of <char> to right

ctrl-alt-] <char> moves cursor to 1st occurrence of <char> to left

#### Aside2: command line Deletion



use ctrl-y to paste back the deleted

#### **GNU Parallel Alternatives**

• xargs, make -j, find + exec, and others are often cited as alternatives

• A comparison is made and summaries available: gnu.org/software/parallel/parallel alternatives.html

• An insightful read, though it may or may not be unbiased! ©



## Part 3: Features and Examples - I

#### Basic Syntax and Semantics

```
Triple colon: Run <command> in parallel for each of the input parameters:
parallel [options] <command> ::: <args>
Quad colon: Run <command> in parallel for each line in input file; -a is alternative syntax to
quad colon
parallel [options] <command> :::: <input file>
parallel [options] -a <input file> <command>
Semantics: Run <command1> in parallel for each line of the standard output from
<command0> as arg
<command0> | parallel [options] <command1>
```

#### Examples

• Triple colon:

```
parallel echo ::: {1..4}
parallel du -h ::: */*
May use -NO when no commands have no arguments (still need to provide :::)
parallel -NO date ::: xyz
```

Quadruple colon:

```
parallel echo :::: /etc/passwd
parallel -a /etc/passwd echo # same as above
```

Another example of the pipe form:

```
find /somedir/subdir -iname '*.txt' -print | parallel echo
"File: "
```

#### Examples

```
• With multiple ::: all combinations will be generated
    parallel echo ::: A B C ::: 1 2 3
    is equivalent to a nested for loop:
    for i in A B C; do
      for j in 1 2 3; do
         echo $i $j
      done
    done
 • --link to map the args 1:1:
    parallel --link echo ::: A B C ::: 1 2 3
```

#### Examples

• Use { [n] } to put nth set of arguments in multiple commands / args:

```
parallel "mkdir -p /tmp/dir.{1} ; fallocate -l 1K
/tmp/dir.{1}/file.{2}" ::: {1..4} ::: {a..d}
```

Other patterns may be put in {} to treat args in special ways: {.} remove extension, eg. /tmp/afile.txt --> /tmp/afile {/} extracts just the filename, eg. /tmp/afile.txt --> afile.txt {#} sequence number of the job {%} slot number of the job parallel echo "sequence {#} slot {%}" ::: {1..100} parallel echo {2.} {1} ::: 1 2 ::: afile.txt bpic.png

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# Highly Configurable I

- --keep-order/-k will ensure the output order is preserved
   parallel -k "sleep {}; echo {}" ::: {5..1}
- --jobs/-j to control the job slots (limited by available cores)
   parallel -j 2 echo ::: 5 4 3 1 2
   0 means as many jobs as possible, default is all cores on a machine. May be provided as %.
   Silently ignores if value is greater than cores available.
- ¬N to limit the arguments received at a time

```
parallel -N3 echo ::: {A..F}
A B C
D E F
```

# Highly Configurable II

- --timeout: kill a job if it takes more than a certain time (sec)
   parallel --timeout 1000 ./runtask ::: {1..100}
   may be specified as a percentage value of the median runtime (<100% won't make sense)
   parallel --timeout 200% ./runtask ::: {1..100}</li>
- --progress, --eta, --bar: show progress of a run, in terms of estimated time, tasks, nodes etc.
- --wd <dirlocation>: provide a working directory (cwd) for commands
- --dry-run: show what will run in standard output but will not run anything, very useful

#### Checkpoint and Resume

```
--joblog, --resume: Allows for monitoring progress, checkpointing
and resuming an interrupted / partially failed run
```

```
parallel -j 16 -N 100 --joblog /tmp/job.log --resume
gzip {} :::: filelist.txt
```

Additionally, --retry-failed (reads from log) and --resume-failed (resumes afresh) to try failed jobs again.

# Saving Output in Files, Variables, Databases

```
    Outputs may be saved in files:

 parallel --files echo ::: A B C # will be saved in /tmp

    Saving output in CSV file:

 parallel --results my.csv echo ::: A B ::: C D

    Saving to an SQL database:

 DBURL=sqlite3://mydatabase; TABLE=$DBURL/mytable
 parallel --sqlandworker $TABLE echo ::: A B ::: C D

    Saving to shell variables:

 env parallel --install # activate parset, restart shell
 parset myvar1,myvar2 -j2 echo ::: a b
 echo $myvar1 $myvar2
```

# Config Profiles I

• Specific configuration profiles may be saved in files and used in combinations:

/etc/parallel/config for systemwide configuration
~/.parallel/config for user-level configuration which will override
systemwide:

```
$ cat ~/.parallel/savesql
--sqlandworker sqlite3://user:passwd@host:9900/mydatabase/mytable
-N256
```

```
parallel --profile savesql <analytics_process> ::: <1m args>
```

#### Multiple Config Profiles may be used together

```
• cat ~/.parallel/benice
    --nice 17
    -N100
    --timeout 300%
• cat ~/.parallel/dryv
    --vv # useful when used with ssh
    --dry-run
• parallel --profile benice --profile dryv <heavy_process> ::: <args>
```

#### Quick Exercise: Prime numbers over Partitions

```
Consider the following C code that prints the prime
numbers between a range given as arguments:
#include <stdio.h>
#include <stdlib.h>
int main(int argc, char* argv[]){
 int flag, i, j;
 int num1 = atoi(argv[1]);
int num2 = atoi(argv[2]);
  for(i=num1+1; i<num2; ++i){
   flag=0;
   for(j=2; j<=i/2; ++j){
     if(i\%j=0){
      flag=1;
      break:
   if(flag==0) printf("%d\n",i);
return 0;
```

- Save the program as prime.c
- Compile as make prime
- Test: ./prime 1 10
- Run ./prime in parallel to find prime numbers between 1 and 1000 by running 10 instances by providing argument pairs: 1 100, 101 200, ..., 901 1000
- Hint1: use the bash curly brace expression creatively to obtain the ranges {min..max..step} ☺
- Hint2: use --link flag to ensure the provided arguments match 1-1
- Hint3: use --dry-run first to ensure correct invocation

# Part 4: Features and Examples - II

#### Resource Management

- --load: To avoid overloading systems, look at the load before starting another job.
  - parallel --load 100% echo ::: "Load less than 1 job per CPU"
- --noswap: Check if the system is swapping and run only when not. parallel --noswap echo ::: "System is not swapping now"
- --memfree: Run only when enough memory is free.

  parallel --memfree 1G --retries 5 echo ::: "1G is free now."

  note: max memory is the "available" on the **free** command
- --delay <x.y> adds x.y sec delay in dispatching tasks to prevent overwhelming the system

#### Combine Data and GNU Parallel in One Script

With the --shebang flag like so:
 #!/usr/bin/parallel --shebang -r echo
 data\_item1
 data\_item2
 data\_item3
 Parallelize existing scripts with --shebang-wrap
 #!/usr/bin/parallel --shebang-wrap /bin/bash

```
chmod u+x parbash.sh
./parbash.sh 1 2 3
```

echo "Arguments \$@"

# Working with Remote Systems over SSH

General Syntax:
 parallel -S server1, server2 commands flags ::: args

• Example:

```
parallel -S u@vm1.org,u@vm2.org "hostname; echo {}" ::: foo bar --sshloginfile flag allows to read the remote ssh config from a file, eg. .ssh/config
```

 Remote ssh hosts may be divided into groups and jobs may be selectively run on them:

```
parallel --hostgroup -S @grp1/$server1 -S @grp2/$server2 \
  echo {} ::: run_on_grp1@grp1 run_on_grp2@grp2
```

# GNU parallel can transfer data to / from remote

• --transferfile to transfer files. Uses rsync to do transfer • --return to return files from remote via rsync • --cleanup to remove files from remote once job is done echo "This is input file" > input file parallel -S remote server --transferfile {} cat ::: input file echo "This is input file" > input file parallel -S \$remote server1 --transferfile {} --return  $\{\}.out cat \{\} ">" \{\}.out ::: input file$ • --trc to combine the three options (--transferfile, --return, and --cleanup)

# Real-World Examples working with ssh I

```
• parallel -S
  rage1, rage4, rage7, rage8, rage9, rage10, rage11, rage12
  ${scan_cmd} ::: \
  ${scan_path}/{44..51} \
  >> scanperf.8proc.8node.out

• parallel -S rage4 --jobs 30 'nats -s rage2:4222 \
  pub migration.files.request --count 1 \
  "{\"path\": \"/lustre/crius/migagenttests/{1}/file.{2}\\"}"'\
  ::: {0..63} ::: {1..3000}
```

# Real-world examples working with ssh II

```
parallel -S rage4 --jobs 30 "touch -d '-1 week'\
/lustre/crius/{1}/file.{2}" ::: {0..63} ::: {1..3000}
parallel -k -S \
rage1, rage2, rage4, rage5, rage6, rage7, rage8, rage9 \
/lustre/crius/scripts/measure_lfsfind.sh ::: {28..35} \
>> lfsfindperf.8proc.8node.out
```

#### PoliMOR: A Policy Engine "Made-to-Order" for Automated and **Scalable Data Management in Lustre**

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#### **ABSTRACT**

Modern supercomputing systems are increasingly reliant on hierarchical, multi-tiered file and storage system architectures due to tems, data management services are required to maintain healthy utilization, performance, and capacity levels. We present PoliMOR.

management challenging. Data management practices must minimize wastefulness of storage resources, promote fair usage, and satisfy application I/O needs (ideally in a systematic and automated cost-performance-capacity trade-ofton an are sented sat PDS\\Word 2.30 at nS (tas 2s 3 nay include purging old files to recover disk space, staging data to a tier with higher performance, or migrating data to tape. Sites could potentially handle some of these

# The Pipe Mode to Process Large Data I

• When data is sent over a Linux pipe to parallel command, it is treated as **arguments** for command to run:

```
cat data.txt | parallel echo
```

• In the pipe mode, the data is delivered to the parallel command as standard input aka **stdin**:

```
cat data.txt | parallel --pipe wc -l
```

• The "--pipe" input may be controlled for block-size / number of lines and number of jobs:

```
cat data.txt |\
  parallel --pipe --block 2M -j4 --round-robin wc -l
```

# The Pipe Mode to Process Large Data II [1]

- --pipepart may be used when using large data. Same as pipe but faster, has a few limitations [2]
- --recend <string> splits record at this string
- --line-buffer may be used to buffer output by line

- [1] thenybble.de/posts/json-analysis/
- [2] www.gnu.org/software/parallel/parallel\_design.html#pipepart-vs-pipe

### Part 5: HPC and GNU Parallel

# A SLURM Workload Manager Primer I

- salloc
   Obtain a job allocation.
- sbatch
   Submit a batch script for later execution.
- srun
  Obtain a job allocation (as needed) and execute an application. Option we

will use: --wait=0 means do not terminate other tasks if one finishes

- squeue
   View information about jobs.
- sinfo
  View information about nodes and partitions.

# A SLURM Workload Manager Primer II

- At runtime, SLURM offers several environment variables that could be leveraged to steer executions:
  - \$SLURM\_NTASKS
    Same as -n, -ntasks. The number of tasks.
  - \$SLURM\_CPUS\_PER\_TASK Number of CPUs per task.
  - \$SLURM\_NODEID
     The node id of the current node. Starts from 0.
  - \$SLURM\_NNODES
    Total nodes allocated to current job.
  - \$SLURM\_NODELIST
     A list of nodes allocated to current job.

# srun parallel vs parallel srun?

```
srun="srun --exclusive -N1 -n1 -c1"
parallel -j $SLURM_NTASKS "$srun ./runtask.sh {1}" :::
{1...112}

VS
srun --ntasks-per-node=1 parallel -j $cores_per_node
app_invocation
Consensus: srun ... parallel ....
Reasons:
```

- 1. Higher overhead in invoking multiple srun allocations
- 2. Leveraging SLURM's srun and environment variables

### Working with HPC Schedulers: SLURM, 1 node

```
#!/bin/bash
                                    code in Github: src/singlenode
#SBATCH -J singlenode
#SBATCH -o %x-%j.out
#SBATCH -e %x-%j.err
#SBATCH -t 0:10:00
#SBATCH -N 1
srun parallel --jobs 8 ./payload.sh argument {} ::::
input.txt
```

# Using --dry-run to generate parallel commands

```
#SBATCH --job-name=parallel job
#SBATCH ...
find infiles/*.txt | parallel --dry-run ./process data {}
>commands.txt
##OR
find infiles/*.txt | parallel --dry-run Rscript
R array test.R {} >commands.txt
parallel -j $SLURM NTASKS < commands.txt
```

#### Multinode Execution in SLURM

```
#SBATCH -J multinode

#SBATCH -o %x-%j.out

#SBATCH -e %x-%j.err

#SBATCH -t 0:20:00

#SBATCH -p batch

#SBATCH -N 4
```

#!/bin/bash

code in Github: src/multinode

srun --no-kill --ntasks-per-node=1 --wait=0 driver.sh \$1

# Driver and Payload codes

```
# Deliver tasks depending on the nodeid
cat $1 |
awk -v NNODE="$SLURM_NNODES" -v NODEID="$SLURM_NODEID" \
'NR % NNODE == NODEID' |
parallel ./payload.sh argument_{}}
```

```
#!/bin/bash
H="$(hostname)"
echo "This is the payload script. \
$1 is the argument passed to it. Ran on machine $H."
```

# Part 6: Asynchronous Workflow Execution

# Asynchronous Execution of Workflows



#### proc1.sh:

#!/bin/bash

sleep \$(shuf -i 20-60 -n 1)

shuf \$1 > ./out/proc\_\$(basename \$1)

echo "./out/proc\_\$(basename \$1)" >> jobqueue

#### proc2.sh:

#!/bin/bash

shuf \$1 > ./out/f\_\$(basename \$1) echo "Done for \$1"

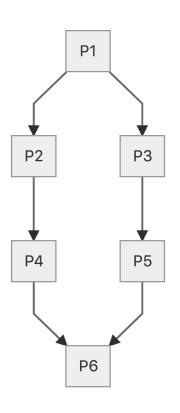
#### workflow.sh:

#!/bin/bash

parallel ./proc1.sh {} ::: ./inputs/\*.txt &

>jobqueue; tail -n+0 -f jobqueue | parallel -u ./proc2.sh {}

# A DAG Workflow Example



- Six processes
- Data dependencies
- May work independently with file inputs
- Branch Parallelism
- Asynchronous execution desired when multiple inputs

# Sequential Bash Script Representation for one set of inputs

```
#!/bin/bash
#p1.sh
if test "$#" != 2 ; then
    echo "wrong
invocation..exiting."
    exit 3
fi
if [ -f "$2" ] ; then
    rm -v "$2"
fi
cat $1 >> $2 || exit
echo "processed by p1" >> $2
echo "$2" >> ./q.p1
```

```
#!/bin/bash
p1/p1.sh inputs/in1.txt
p1/out1.txt
p2/p2.sh p1/out1.txt p2/out2.txt
p3/p3.sh p1/out1.txt p3/out3.txt
p4/p4.sh p2/out2.txt p4/out4.txt
p5/p5.sh p3/out3.txt p5/out5.txt
p6/p6.sh p4/out4.txt p5/out5.txt
outputs/out6.txt
```

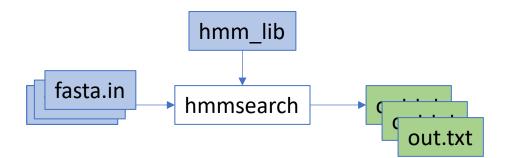
#### **GNU Parallel version**

```
#!/bin/bash
mkdir -p p{1..5}/outdir outputs
parallel --link p1/p1.sh {1} {2} ::: inputs/in{1..6}.txt :::
p1/outdir/out{1..6}.txt &
touch q.p1 ; tail -n+0 -f q.p1 | parallel -u --link p2/p2.sh {1} {2} :::: - :::
p2/outdir/out{1..6}.txt &
touch q.p1 ; tail -n+0 -f q.p1 | parallel -u --link p3/p3.sh {1} {2} :::: - :::
p3/outdir/out{1..6}.txt &
touch q.p2; tail -n+0 -f q.p2 | parallel -u --link p4/p4.sh {1} {2} :::: - :::
p4/outdir/out{1..6}.txt &
touch q.p3; tail -n+0 -f q.p3 | parallel -u --link p5/p5.sh {1} {2} :::: - :::
p5/outdir/out{1..6}.txt &
(stdbuf -oL paste <(touch q.p4 ; tail -n+0 -f q.p4) <(touch q.p5 ; tail -n+0 -f
q.p5)) | parallel -u --link p6/p6.sh :::: - ::: outputs/out{1..6}.txt
```

# Part 7: A Real Application

# A Real Application: Bioinformatics

- HMMER3 Takes a protein sequence and compares it to a probabilistic profile that describes a protein domain.
- It reports when there is a statistically significant likelihood that the protein and the domain share the same evolutionary origin.
- This basic comparison is repeated for all combinations of many protein sequences and many domains.



# Download App Package and Data

- Download the hmmsearch package: <a href="hmmer.org/download.html">hmmer.org/download.html</a> wget http://eddylab.org/software/hmmer/hmmer-3.4.tar.gz
- Download the protein HMM searchable library here:
   wget ftp.ebi.ac.uk/pub/databases/Pfam/current\_release/Pfam-A.hmm.dat.gz
- Download the fasta file:
   wget
   https://ftp.uniprot.org/pub/databases/uniprot/current\_releas
   e/knowledgebase/complete/uniprot sprot.fasta.gz

# Install the hmmsearch package

```
• tar zxf hmmer-3.4.tar.qz
cd hmmer-3.4/
• ./configure --prefix=$PWD/install
 ... output ...
 HMMER configuration:
  compiler: qcc -03 -pthread
  host: x86 64-pc-linux-gnu
  linker:
  libraries: -lpthread
  DP implementation: sse
• make -j install # hmmer will be installed.
```

# gunzip and split the Fasta File

```
qunzip uniprot sprot.fasta.gz
awk -v chunksize=$(grep ">" uniprot sprot.fasta -c)
'BEGIN{n=0; chunksize=int(chunksize/256)+1 }
/^>/ {
       if(n%chunksize==0){
         file=sprintf("uniprot %d.fasta",1+(n%256));
       print >> file; n++; next;
{ print >> file; }' < uniprot sprot.fasta
```

# Part 8: Putting it all Together

#### HMMSearch Command line

```
hmmsearch --cpu 8 --noali -o output.txt \
                             Pfam-A.hmm input.fasta
ls | head -3
uniprot 100.fasta
uniprot 101.fasta
uniprot 102.fasta
find $PWD -type f | grep fasta > inputs.txt
```

# First Approach: srun ... parallel

```
srun --no-kill --ntasks-per-node=1 --wait=0

parallel -j 8 $HOME/hmmer-3.3/install/bin/hmmsearch
--cpu 4 --noali -o {//}/output_{{/}}.txt

$SCRATCH/Pfam-A.hmm {} :::: inputs.txt
```

# Second Approach: Distribute Tasks

```
#driver.sh
cat inputs.txt |awk -v NNODE="$SLURM NNODES" -v
NODEID="$SLURM NODEID" \ 'NR % NNODE == NODEID' |
parallel ./pay\overline{1}oad.sh {}
#payload.sh [untested]
$HOME/hmmer-3.3/install/bin/hmmsearch
--cpu 4 --noali -o {//}/output {/}.txt
$SCRATCH/Pfam-A.hmm $1
```

## Summary

- GNU Parallel is an effective tool that could be useful in day-to-day tasks on the terminal as well as for larger workflows
- Many options to choose from to customize a parallel operation
- Very handy for quick prototyping
- May be well suited for some production level work

### Practice and Exercises: Titanic Data Challenge

#### Data: in Github, Titanic.csv

- Problem 1. What characteristics are shared by all passengers whose fare is
   0?
- Problem 2. How many married women over age 50 embarked in Cherbourg?
   (Married women are denoted by "Mrs.")
- Problem 3. Which embarkation city had the highest-paying passengers on average?
- Problem 4. What is the most common last name among passengers? What is the average number of passengers per last name?
- Problem 5. What's the survival rate for passengers in the three different classes, i.e., what fraction of passengers in each class survived?

# [longer] Practice and Exercises : MIT Datacenter Challenge

- dcc.mit.edu A 2.6T dataset pertaining to cluster operations
- 900K+ files, 2.6m+ lines of CSV data.
- Partial data available on Github at data/datacenter-challenge
- Although geared towards AI based models, GNU Parallel could help gain insight on patterns from existing data
- Scheduling Characterization
- Workload Characterization
- File System Characterization
- Error Characterization

## Credits, references and resources

- gnu.org/software/parallel
- rcc.uchicago.edu/documentation/ build/html/running-jobs/srun-parallel/index.html
- <u>ulhpc-tutorials.readthedocs.io/en/latest/sequential/basics</u>
- docs.ycrc.yale.edu/clusters-at-yale/guides/parallel
- www.vanderbilt.edu/accre/documentation/parallel
- docs-research-it.berkeley.edu/services/high-performance-computing/user-guide/runningyour-jobs/gnu-parallel
- omgenomics.com/parallel
- curc.readthedocs.io/en/latest/software/GNUParallel.html
- thenybble.de/posts/json-analysis
- stackoverflow.com/questions/tagged/gnu-parallel
- unix.stackexchange.com/questions/tagged/gnu-parallel

### Other Possible Venues to look for challenges

- data/sales-data.csv: ~10K lines of sales data (mock)
- annas-blog.org/worldcat-scrape.html
- smc-datachallenge.ornl.gov
- www.reddit.com/r/DataHoarder

# Thank you for your time and attention Questions?

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