# Organizing and Submitting HTC Workloads on the OSPool

OSG Research Facilitation Team

# Overview of the Scaling Up Process

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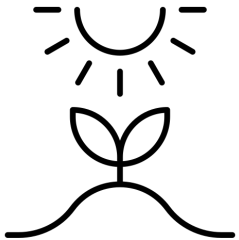
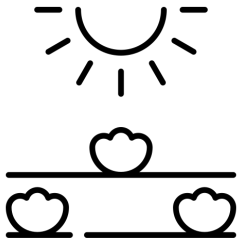
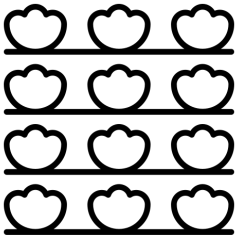
|  Created by Made from the Noun Project |  Created by Made from the Noun Project |  Created by Made from the Noun Project |
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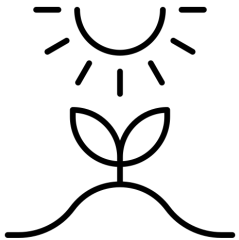
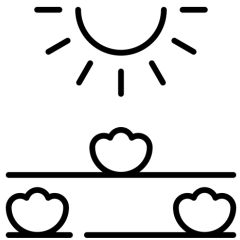
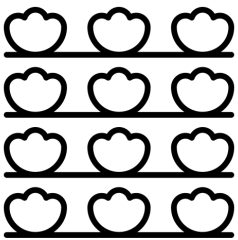
|  Created by Made from the Noun Project |  Created by Made from the Noun Project |  Created by Made from the Noun Project |
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Review Job Components; How to Organize HTC Workload Files

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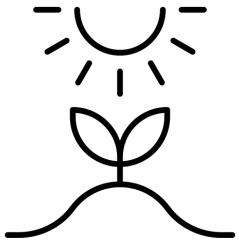
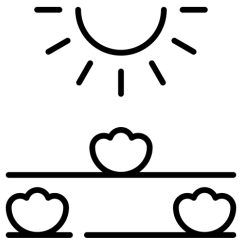
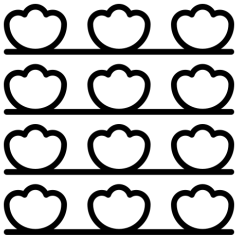
|  Created by Made from the Noun Project |  Created by Made from the Noun Project |  Created by Made from the Noun Project |
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Tips for Scaling Up

# Overview of the Scaling Up Process

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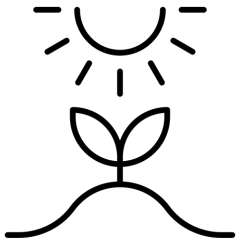
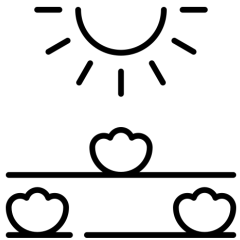
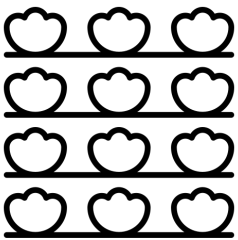
|  Created by Made from the Noun Project |  Created by Made from the Noun Project |  Created by Made from the Noun Project |
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Tools For Monitoring Jobs

# Part 0: Assembling Workload Components

# Recap: HTC Workload Components

What components do you need for an HTC workload (or single job)?

We have talked about all of these things this week!

- Monday: HTCondor Job Submission
  - including coordinating input and output files
- Tuesday: Software
- Wednesday: Data

# Reflection

What are the components you need for your HTC workload?

What results will you generate?

What other files will be generated by HTCondor or the jobs?

# Part I: Organizing HTC Workload Components

# High Throughput Computing (HTC)

One of our favorite HTC examples: baking the world's largest/longest cake

In computational terms: solving a big problem (the world's longest cake) by executing many small, self-contained tasks (individual cakes) and joining them.

Photos: Arun Sankar via https://www.theguardian.com/world/2020/jan/16/indian-bakers-rise-to-task-of-making-worlds-longest-cake

# High Throughput Computing (HTC)

One of our favorite HTC examples: baking the world's largest/longest cake

**Not pictured:**
How the bakers organized all the inputs (ingredients) and outputs (individual cakes) before they were joined together.

In HTC workload terms: how are you going to organize the components of your workload (software, inputs, outputs) on the Access Point?

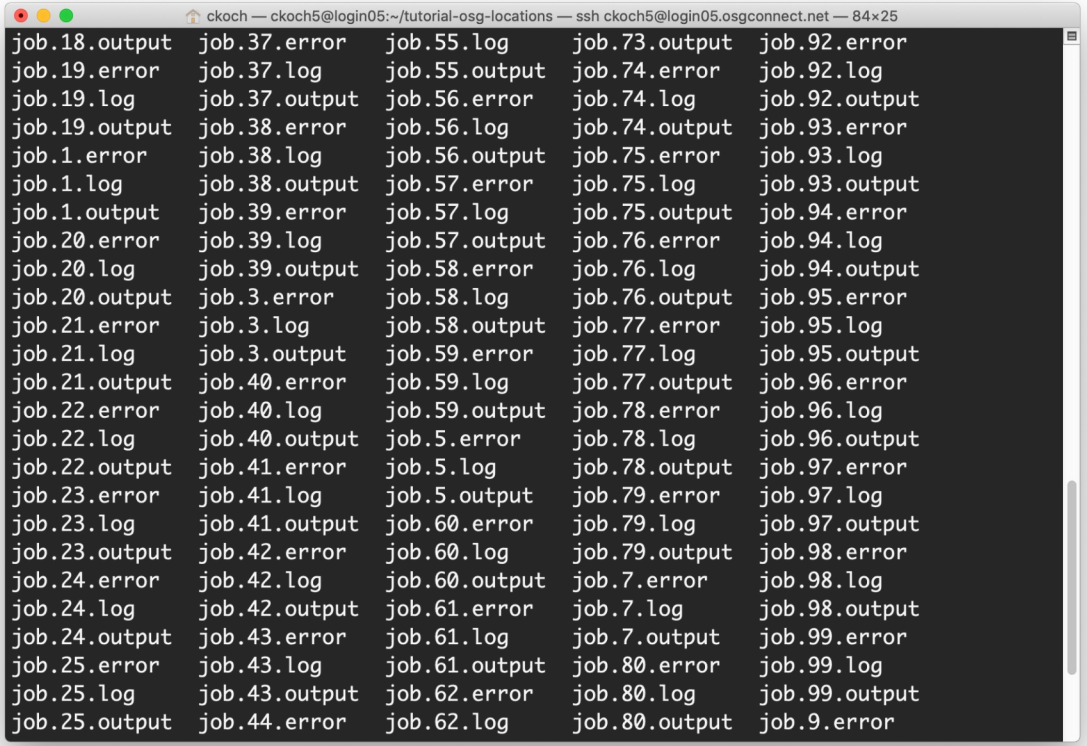
small, self-contained tasks (individual cakes) and joining them.

Photos: Arun Sankar via https://www.theguardian.com/world/2020/jan/16/indian-bakers-rise-to-task-of-making-worlds-longest-cake

# Why organize?

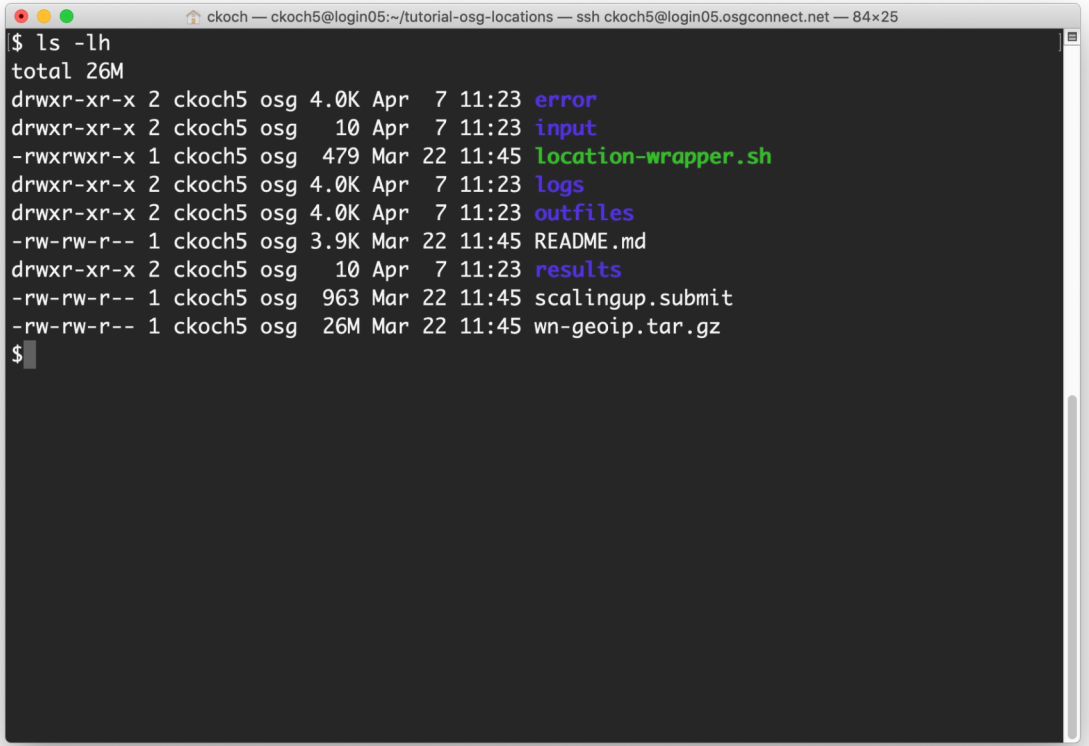
By default, HTCondor writes all job files (input, output, HTCondor logs, etc.) back to the same place, which means your home directory can look something like this:

*This makes it hard to find things!*



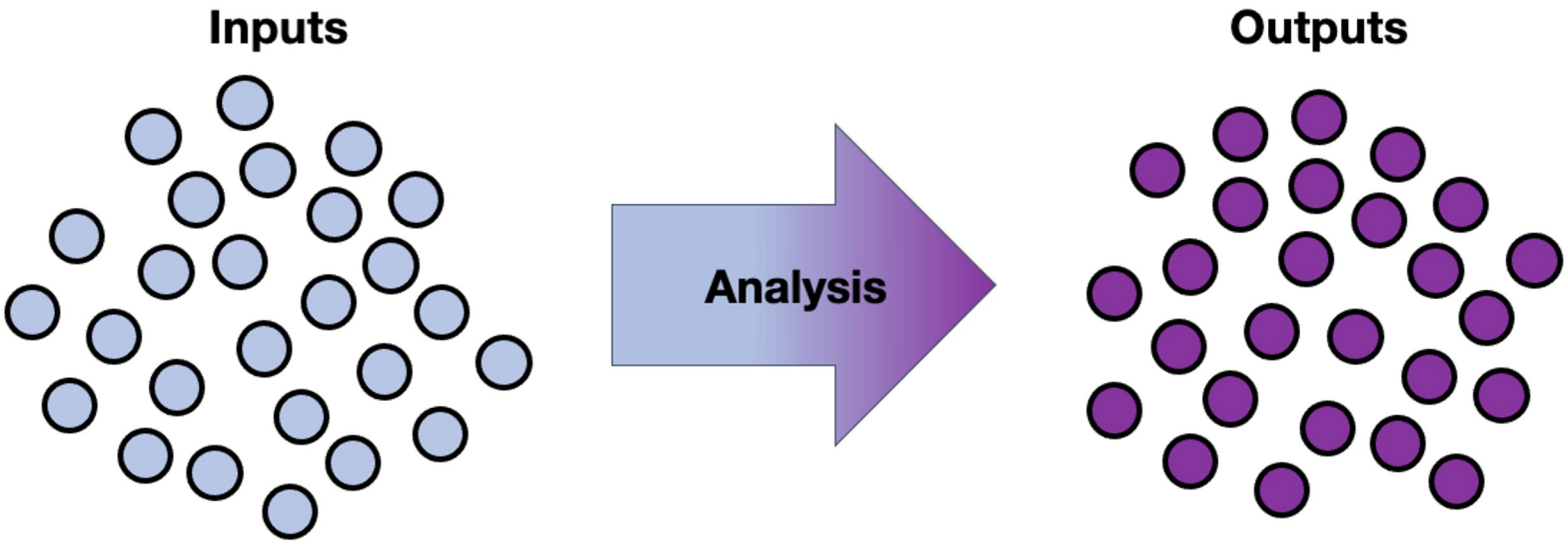

# Why organize?

We can improve our workflow by intentionally organizing our input and output files on the Access Point.




# HTC Workloads as Input/Output Sets

The next example will model workloads that use many input files to produce many output files.



# Example: Text Analysis






Book text to analyze

Python script that counts the frequency of different words

Output counts of different words in book

```
$ ./wordcount.py Dracula.txt
```

open book by Soremba from the Noun Project
PY File by Arthur Shlain from the Noun Project
Number by Travis Avery from the Noun Project

# Organizational Plan For Our Files

```
wordcount.sub
wordcount.py
input/
        Dracula.txt
        ...
output/
        count.Dracula.txt
```

We will assume that we want to put our input files (books) in one folder, and our output files (word counts) in another folder.

# Organizational Plan For Our Files

```
wordcount.sub
wordcount.py
input/
        Dracula.txt
        ...
output/
        count.Dracula.txt
        ...
log/
  job.0.log
  ...
errout/
  job.0.out
  job.0.err
  ...
```

There are ***additional*** files that will be produced by the job as well that we should consider – the HTCondor log, stdout and stderr. We'll put these into two folders.

# Coordinate HTCondor and File Structure

```
wordcount.sub
wordcount.py
input/
        Dracula.txt
        ...
output/
        count.Dracula.txt
        ...
log/
        job.0.log
        ...
errout/
        job.0.out
        job.0.err
        ...
```

```
# submit file name: wordcount.submit
executable = wordcount.py
arguments = Dracula.txt

transfer_input_files = inputs/Dracula.txt
transfer_output_remaps =
 "count.Dracula.txt=outputs/count.Dracula.txt"

log = logs/$(ProcId).log
error = errout/$(ProcId).err
output = errout/$(ProcId).out

queue 1
```

# HTCondor Options for Organizing Files

| | | |
|---|---|---|
| `Transfer_output_remaps = “file1.out=path/to/file1.out; file2.out=path/to/renamedFile2.out”` | Used to save output files in a specific path and using a certain name | - Used to save output files to a **specific folder**<br>- Used to **rename** output files to avoid writing over existing files |
| `Initialdir = path/to/initialDirectory` | Sets the submission directory for each job. When set, this is becomes the base path where output files will be saved. | - Used to submit multiple jobs from **different directories**<br>- Used to avoid having to write some paths in other submit file values |

**More Information:** https://htcondor.readthedocs.io/en/latest/users-manual/file-transfer.html

# Return Output to Specified Directory with InitialDir

```
submission_dir/
        job.sub
        exec.py
        Shared_vars.txt
        results/
                input.txt
                output.txt
                job.err
                job.log
                job.out
```

```
# File name: job.sub
executable = exec.py

initialdir = results
transfer_input_files = input.txt,
  ../shared_vars.txt

log = job.log
out = job.out
error = job.err

queue 1
```

# Separate Jobs with InitialDir

```
submission_dir/
        job.submit
        analyze.exe
        job0/
                file.in job.log job.err
                file.out job.out
        job1/
                file.in job.log job.err
                file.out job.out
        job2/
                file.in job.log job.err
                file.out job.out
```

```
# File name = job.submit

executable = analyze.exe
initialdir = job$(ProcId)

arguments = file.in file.out
transfer_input_files = file.in

log = job.log
error = job.err
output = job.out

queue 3
```

Executable should be in the directory with the submit file, *not* in the individual job directories

# Organizing Larger Data Files

If we had larger data files, they need to be organized separately. On OSG Connect, the place for these files is the “/public” folder

Files that belong in /public:

- Input: > 100Mb per file per job
- Output: > 1GB per file per job

Once inputs and outputs are placed in the right location, use the appropriate HTCondor file transfer options to move the data to jobs.

# Reflection

How big are the files in my input / output sets?

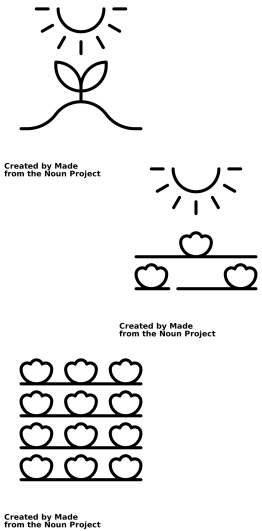
What organizational strategy makes sense for the next steps in my analysis?

- Do you want inputs in one folder and outputs in another folder? Use `transfer_output_remaps`.
- Do you have many outputs for each job that you'd like to group together, but keep separate from other job outputs? Do you want to keep inputs/outputs for the same job together? Maybe use `initialdir`.

How do you want to organize the HTCondor/system files?

# Part II: Scaling Up

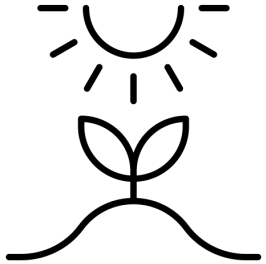
# Overview of the Scaling Up Process




1. **Run a single job:** For each job type, get a test job working reliably & tune resource needs
2. **Test a small workload:** Scale up to ~10 jobs, checking reliability & Access Point resource demand
3. **Scale up:** Continue scaling up in 10–100× increments, checking for & fixing issues

# Stage 1: Get One Job Running

**You know how to do this!** 😊



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- Gather executable, inputs, arguments, etc.*
- Estimate initial resource needs*
- Write a submit file
- Submit!
- Review all outputs, including log, output, and error files
- Check actual resource usage and update resource needs*
- Repeat until (fairly) accurate and reliable

* More details on next slides

# Stage 1: Tips for Initial Test Jobs

- Test one of each kind of job you will run (e.g., prep, simulation, analysis)
- Select smaller data sets or subsets of data for your first test jobs
- Pick test jobs that will reproduce results from elsewhere, if possible
- Name files carefully to help identify which results go with which tests
- Make sure you understand and can run your software
  - Software — executable, dependencies, maybe a wrapper script to prepare environment
  - Command-line arguments
  - Input files

# Stage 1: Estimating Initial Resource Needs

**CPU**

- By default, start with 1
- Unless you know for sure that you executable uses a certain number > 1

**Memory**

- Start with the total memory available on laptop or where it ran before
- It’s ok if this is a lot the first time, you will fine-tune later

**Disk**

- Estimate (as best you can) and sum sizes of: executable (+ environment), input files, output files, temporary files, standard output/error

# Stage 1: Run, Refine, Repeat

**After running a test job:**

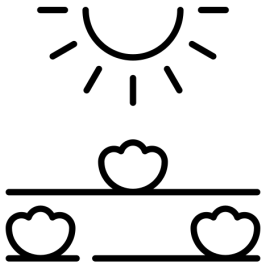
- Check logs and output for errors, warning, holds, etc.
- Check HTCondor job log for actual resource usage
- Fix issues, update resource needs, run 1 job again!
- Good opportunity to check “fit” of jobs to HTC and maybe adjust

```
005 (1234.000.000) 2022-07-28 09:12:34 Job terminated.
    (1) Normal termination (return value 0)
[...]
    Partitionable Resources :    Usage  Request Allocated
       Cpus                 :                1         1
       Disk (KB)            :       40       30   4203309
       Memory (MB)          :        1        1         1
```

# Stage 2: Scale To About 10 Jobs

**For each kind of job, once you have 1 job working, try about 10**

- Try a representative variety of arguments and input files
- Start developing methods for checking results of *all* jobs
- Estimate total resource needs for the Access Point itself
- **Repeat tests** at this scale until issues are fixed & resources are accurate



# Stage 2: Try Various Inputs

**For Stage 1, the suggestion was to keep things short and simple**

- For Stage 2, it is time to explore the entire range of inputs to your jobs
  - Different command-line arguments; e.g., start, middle, and end of parameter sweep
  - Different input files; e.g., small, medium, and large — whatever makes sense for you
- As you explore, you may find that per-job resource needs vary
- Set your resource requests a bit higher than maximum observed usage
  - For example, if 10 test jobs used between 938 MB – 1.23 GB of memory, update your submit file to request 1.5 GB memory
- After any changes, run the same test again and re-evaluate

# Stage 2: Checking Results of Multiple Jobs

**Start developing methods for checking the results of multiple jobs**

- Output from your executable (i.e., your research results)
- Debugging output: standard output and error files, executable logs, etc.
- HTCondor job log file (`log = xxx` in your submit file)

**This may be one of the most overlooked aspects of scaling up!**

- Checking 1 job is easy; checking 10 is tedious; checking 1000s by hand? 😭
- Techniques include:
  - Sampling
  - Developing tools to automate (see Part III)
- Sounds a bit like research, right? You know how to do that…

# Stage 2: Estimate Access Point Needs

**Do not forget about your Access Point – it is a shared resource, too!**

- Storage space for files
  - Based on a run of 10 jobs, estimate total number and size of all files for full production
  - Do you have enough storage space on the Access Point? If not, what options exist?
  - Review the Data lecture for more suggestions
- Number of running jobs
  - In theory, how many jobs could you have running at once?
  - Each running job uses some CPU and memory on the Access Point itself
  - If submitting over 10,000 jobs consider limiting (*throttling*) running and idle jobs on Access Point

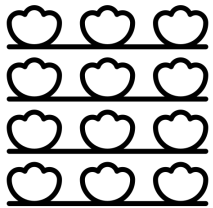
# Stage 3: Iterate in Steps of 10–100×

**By now, you have tested tens of jobs, maybe in a workflow; what next?**

- Continue scaling up in increments of 10–100 times the number of jobs
- All the considerations from Stage 2 apply at each increment
- Be sure to find, understand, and hopefully fix issues before moving on

**As you scale up, a challenge is to distinguish among:**

- Real issues with your jobs, workflow, resource requests, etc.
- Real issues with certain subsets of your jobs
- Temporary issues with the HTC infrastructure itself
- Bugs and other longer-lasting issues with the infrastructure
- We can help! Email us with support requests if you get stuck.



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# Reflection

Where are you in the scaling up process?

What are three things you should consider in your current stage?

# Other Thoughts: What's Your Context?

**Major considerations** (details vary a lot!):

- Computational workflow: Automate running of different jobs in order
- Technical workflow: Management of runs, files, etc.
- Research workflow: Revisit goals, scale, and how computing fits

# Other Thoughts: Computational Workflows

- Do you have different kinds of jobs that need to be run in a specific order to implement your overall computational goal?
- If so, you may be able to use HTCondor DAGMan (or other tools) to automate parts or all of the whole process.
- Attend the optional DAGMan lecture later today if you think this situation applies to you!
- **Test computational workflows with few jobs of each type, just as you would in Stage 2.**

# Other Thoughts: Technical Workflow Considerations

- How will you get the necessary files to the Access Point and, if needed, OSDF Origin?
- How will you manage individual sets of runs? For example, how will you organize files (see earlier)? If you need to rerun jobs, how will you keep track of each run?
- How will you move results off of the Access Point (which is temporary storage **only**)? Do you have a place to archive results? How will it be organized?

# Other Thoughts: Research Workflow Considerations

**Now that you have run some jobs:**

- Consider the balance between human effort (yours!) and computer time; will the use of HTC actually save you time in the long run and improve your research?
- Estimate how much total calendar time it will take your computational work to complete. Do you have enough time before your next deadline?
- Could you do even more? If things are going well, could you expand your research questions by using more computing? Think big!

# Part III: Tools for Monitoring

# Tools for Learning About Jobs

**HTCondor's job attribute information**

- Accessed via `condor_q`, or `condor_history`

**Files**

- HTCondor log files
- Standard error/standard output files

# Job Attributes with condor_q

HTCondor stores a list of information about each job.

This information is stored in this format:

- `AttributeName = value`

You can find a list of attributes for a single job by running:

- `condor_q -l JobID`

You can print out specific attributes by using the “format” or “auto-format” flags with an HTCondor command:

- `condor_q -af Attribute1 Attribute2`
- adds job number: `condor_q -af:j Attribute1 Attribute2`

# Interesting Job Attributes

- Job identifying information
  - ClusterID
  - ProcID
  - Cmd
  - Arguments
  - UserLog
- Where it ran
  - LastRemoteHost
  - MATCH_EXP_JOBGLIDEIN_ResourceName
- Resource Request and Usage
  - RequestCpus (Memory, Disk)
  - MemoryProvisioned (Disk)
  - CPUsUsage (MemoryDisk)
- Timing
  - EnteredCurrentStatus
  - QDate

# Interesting Job Attributes

- Codes
  - JobStatus
  - ExitCode
  - HoldReasonCode
  - HoldReasonSubCode,
  - NumHoldsByReason
- Counts
  - NumJobStarts
  - NumShadowStarts
  - NumSystemHolds,

# Checking Completed Jobs

- condor_history
  - Contains finalized job attributes for completed jobs
    - some have different names (HoldReason --> LastHoldReason)
  - Easy to use constrain and to display values (like condor_q)
  - Can be slow to search (latest first) and may drop old records quickly
- HTCondor job log files (log = xxx in submit)
  - Contain a lot of information
  - That is both a blessing and a curse
  - Somewhat easy to parse — or use HTCondor Python bindings to help

# HTCondor Job Log Files

- One big, combined file, or one per job? Your preference, really
- With tens or hundreds of jobs (& more), not practical to review manually
- Can try to use the grep command-line tool to find specific lines

# HTCondor Job Log Files: Terminations

**To find when every job ended:**

```
$ grep '^005' LOGS
```

(*LOGS* can be one file, a list of files, or a glob (using *) of files)

**To find termination codes (exit codes) for every job:**

```
$ grep termination LOGS
```

(will not show job IDs, though)

**To get counts by termination code:**

```
$ grep termination LOGS | sort | uniq -c
```

# HTCondor Job Log Files: Resource Lines

**To get memory resource lines:**

```
$ grep -h 'Memory (MB) *:' LOGS >
memory_resources.txt
```

**To get disk resource lines:**

```
$ grep -h 'Disk (KB) *:' LOGS > disk_resources.txt
```

Import the resulting files into Excel (with some attention to import options)

**For file transfers:**

```
$ grep -h 'Total Bytes Sent By Job' LOGS
$ grep -h 'Total Bytes Received By Job' LOGS
```

# HTCondor Job Log Files: Checking on Holds

**To view all job holds, their reasons, and related codes:**

```
$ grep -h -A 2 '^012' LOGS
```

(Omit the -h option to see log filenames for each hit.)

**Note:** The OSPool may automatically release (rerun) some held jobs; if you don't look for them explicitly, you may never know those holds occurred