OSG

Submitting Multiple Jobs With HTCondor

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Agenda

- Motivation for submitting many jobs using a single submit file
- HTCondor submit file options
  - Using variables
  - Modifying the `queue` statement
- Organizational tips for handling many input/output files
  - Submit file options for handing different job structures

Why multiple jobs?

Mei Monte Carlo
Needs to run many random simulations to model particles in a detector

Image credit: The Carpentries Instructor Training

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Why multiple jobs?

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Needs to run many random simulations to model particles in a detector	Testing different design parameters for designing clinical trials.	Applying a quality control / processing pipeline to 20 RNA samples.

When running many jobs we want to avoid:

- starting each job manually
- creating separate submit files for each job

Image credit: The Carpentries Instructor Training

Many jobs, one submit file

HTCondor has several built-in ways to submit many independent jobs from one submit file

Let's review: one job

```
executable = analyze.sh
arguments  = file.in file.out
transfer_input_files = file.in

log    = job.log
output = job.stdout
error  = job.stderr

queue
```

This is the command we want HTCondor to run.

Let's review: one job

```
executable = analyze.sh
arguments  = file.in file.out
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log    = job.log
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queue
```

These are the files we need for the job to run.

Let’s review: one job

```
executable = analyze.sh
arguments  = file.in file.out
transfer_input_files = file.in

log    = job.log
output = job.stdout
error  = job.stderr

queue
```

These files track information about the job.

Let's review: one job

```
executable = analyze.sh
arguments  = file.in file.out
transfer_input_files = file.in

log    = job.log
output = job.stdout
error  = job.stderr

queue
```

The queue term tells HTCondor how many jobs to run.

Submitting Multiple Jobs

When submitting multiple jobs using one submit file, it is helpful to start by thinking about:

1. What is ***constant*** across all jobs?
2. What is ***changing*** from job to job?

Submitting Multiple Jobs

When submitting multiple jobs using one submit file, it is helpful to start by thinking about:

1. What is ***constant*** across all jobs?
2. What is ***changing*** from job to job?

When editing the submit file,
it is helpful to start by editing the **queue** statement.

Variable and queue options

Syntax	List of Values	Variable Name
queue ***N***	Integers: 0 through N-1	$(ProcId)
queue *Var* **matching** *pattern**	List of values that match the wildcard pattern.	$(*Var*) If no variable name is provided, default is $(Item)
queue *Var* **in** (*item1 item2 …*)	List of values within parentheses.	
queue *Var* **from** *list*	List of values from *list*, where each value is on its own line.	

Variable and `queue` options

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Example 1:
Many jobs with <u>named</u> files
`Queue` *`variable`* `from` *`list`*

(e.g. Names like Wisconsin.txt, BiologicalControl.fastq.gz)

Example 1: Many jobs with named files

Scenario: Use an executable to analyze Wisconsin population data

```
$ ./compare_states state.wi.dat out.state.wi.dat
```

```
executable = compare_states
arguments  = state.wi.dat out.state.wi.dat

transfer_input_files = state.wi.dat

queue
```

Example 1: Many jobs with named files

Scenario: Use an executable to analyze Wisconsin population data

Suppose we have data for all 50 states: `state.wi.dat`, `state.mn.dat`, `state.il.dat`, …

Let's use HTCondor to automatically queue a job to analyze each state's data file!

```
e
arguments   = state.wi.dat out.state.wi.dat

transfer_input_files = state.wi.dat

queue
```

Provide a list of values with `queue … from`

One option is to create another file with the list of input files and use the **`queue`** ***`variable`*** **`from`** ***`list`*** syntax.

```
executable = compare_states
arguments  = state.wi.dat out.state.wi.dat

transfer_input_files = state.wi.dat

queue state from state_list.txt
```

File name: state_list.txt

```
state.wi.dat
state.mn.dat
state.il.dat
state.ia.dat
state.mi.dat
```

Which job components vary?

- Now, what parts of our submit file vary depending on the input?
- We want to vary the job's **arguments** and one **input file**.

```
executable = compare_states
arguments  = state.wi.dat out.state.wi.dat

transfer_input_files = state.wi.dat

queue state from state_list.txt
```

Use a custom variable

Replace all our varying components in the submit file with a variable.

```
executable = compare_states
arguments  = $(state) out.$(state)

transfer_input_files = $(state)

queue state from state_list.txt
```

```
state.wi.dat
state.mn.dat
state.il.dat
state.ia.dat
state.mi.dat
```

Use multiple variables with `queue … from`

- The queue from syntax can also support multiple values per job.
- Suppose our command was like this:

```
$ ./compare_states -i [input file] -y [year]
```

File name: state_list.txt

```
state.wi.dat,2010
state.wi.dat,2015
state.mn.dat,2010
state.mn.dat,2015
```

```
executable = compare_states
arguments  = -i $(state) -y $(year)

transfer_input_files = $(state), country.us.dat

queue state,year from state_list.txt
```

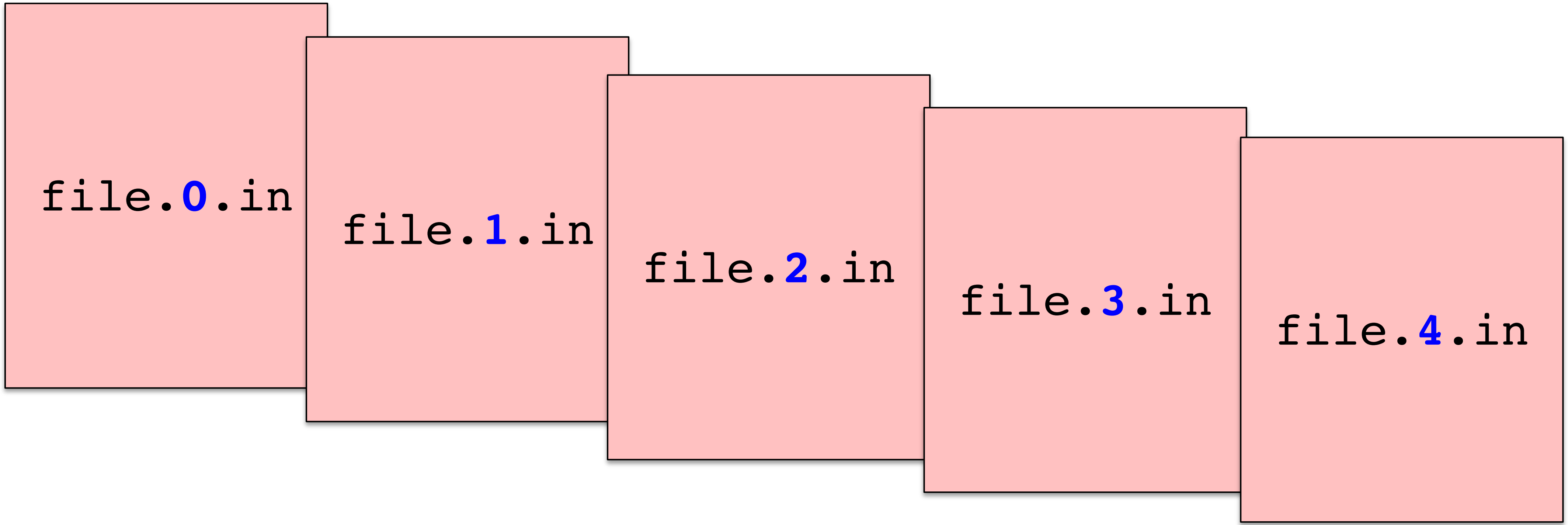
Example 2:

`Queue` *N* with <u>numbered</u> files

(e.g. Names like file.1.txt, sample1.csv)

List of numerical input values

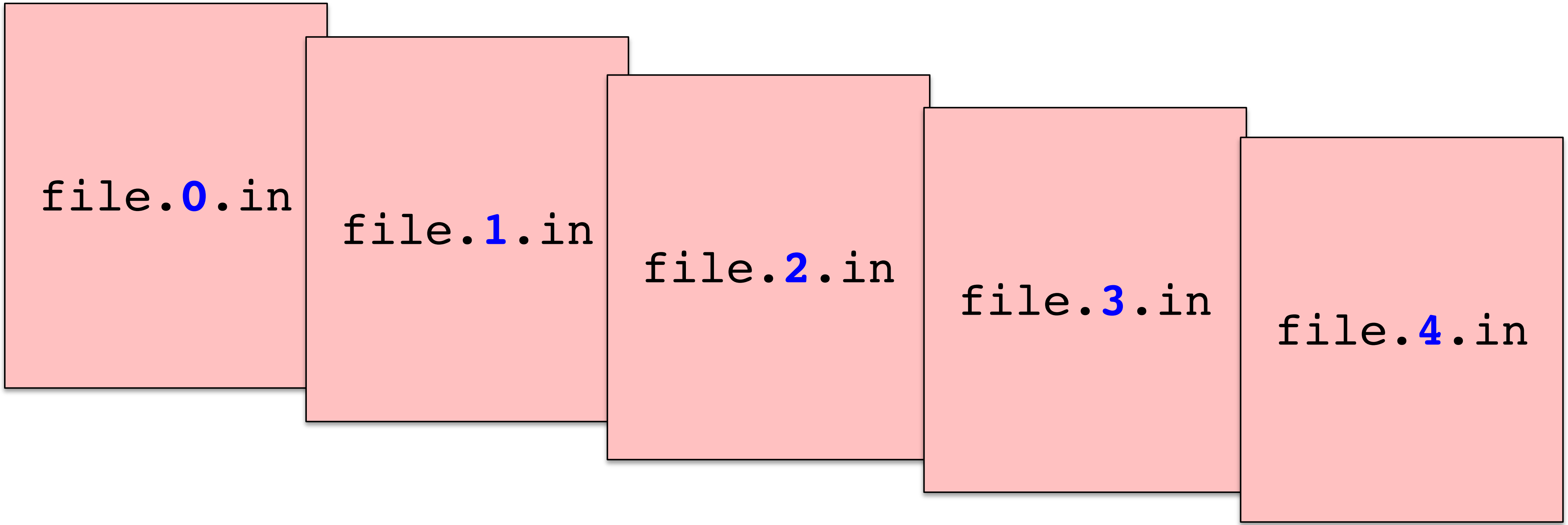
Suppose we have many input files and we want to run one job per input file.



List of numerical input values

Suppose we have many input files and we want to run one job per input file.

We can capture this set of inputs using a **list of integers**.



Provide a list of integer values with `queue N`

```
executable = analyze.sh
arguments  = file.in file.out
transfer_input_files = file.in

log    = job.log
output = job.stdout
error  = job.stderr

queue 5
```

This queue statement will generate a list of integers, 0 - 4

Provide a list of integer values with `queue N`

```
executable = analyze.sh
arguments  = file.in file.out
transfer_input_files = file.in

log    = job.log
output = job.stdout
error  = job.stderr

queue 5
```

If we *only* change our queue statement to queue N, HTCondor will queue N *identical* jobs.

This queue statement will generate a list of integers, 0 - 4

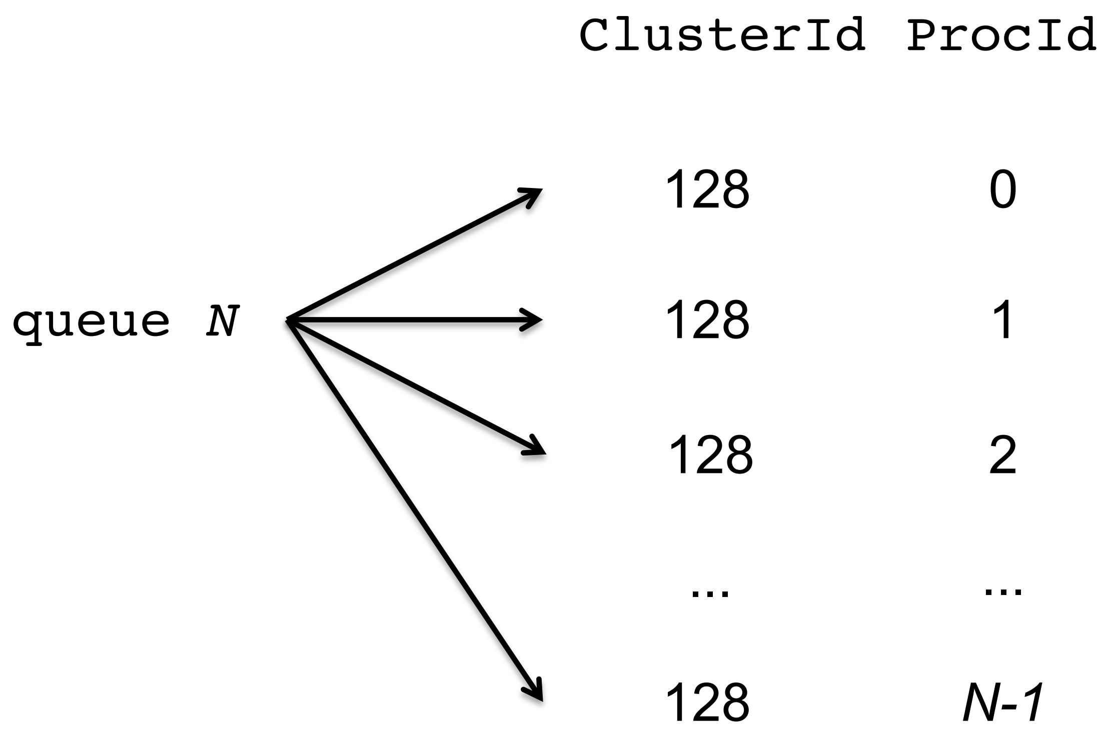
Which job components vary?

```
executable = analyze.sh
arguments  = file.in file.out
transfer_input_files = file.in

log    = job.log
output = job.stdout
error  = job.stderr

queue 5
```

The arguments for our command and the input files would be different for each job.

We might also want to differentiate these job files.

HTCondor Automatic Variables



	ClusterId	ProcId
`queue` *N*	128	0
	128	1
	128	2
	...	...
	128	*N-1*

Each job's `ClusterId` and `ProcId` can be accessed inside the submit file using:

`$(ClusterId)`

`$(ProcId)`

* May also see `$(Cluster)`, `$(Process)` in documentation

Use $(ProcID) as the variable

```
executable = analyze.sh
arguments  = file.$(ProcID).in file.$(ProcID).out
transfer_input_files = file$(ProcID).in

log    = job.$(ProcID).log
output = job.$(ProcID).stdout
error  = job.$(ProcID).stderr

queue 5
```

The default variable representing the changing numbers in our list is `$(ProcID)`

Submitting Jobs

Jobs in the queue will be grouped in batches
(default: cluster number)

```
$ condor_submit job.submit
Submitting job(s).
5 job(s) submitted to cluster 128.
```

```
$ condor_q
-- Schedd: submit-1.chtc.wisc.edu : <128.104.101.92:9618?... @ 05/09/19 10:35:54
OWNER  BATCH_NAME    SUBMITTED    DONE    RUN    IDLE  TOTAL  JOB_IDS
alice  ID: 128       5/9  11:03      _      _      5      5   128.0-4

5 jobs; 0 completed, 0 removed, 5 idle, 0 running, 0 held, 0 suspended
```

To see individual jobs, use:
condor_q -nobatch

Other options: `queue N`

Can I start from 1 instead of 0?

- Yes! These two lines increment the $(ProcId) variable

```
tempProc = $(ProcId) + 1
newProc = $INT(tempProc)
```

- You would use the second variable name $(newProc) in your submit file

Can I create a certain number of digits (i.e. 000, 001 instead of 0,1)?

- Yes, this syntax will make $(ProcId) have a certain number of digits

```
$INT(ProcId,%03)
```

Other Options for Submitting Multiple Jobs

Variable and `queue` options

Syntax	List of Values	Variable Name
queue *N*	Integers: 0 through N-1	$(ProcId)
➡ queue *Var* matching *pattern**	List of values that match the wildcard pattern.	$(*Var*) If no variable name is provided, default is $(Item)
queue *Var* in (*item1 item2* …)	List of values within parentheses.	
queue *Var* from *list.txt*	List of values from *list.txt*, where each value is on its own line.	

Other options: `queue ... matching`

`Queue matching` has options to select only files or directories

```
queue infile matching files *.dat
```

```
queue indirs matching dirs job*
```

If you have questions about which queue statement would work best for *your* workflow, don't hesitate to reach out to OSG staff this week!

Queue options, pros and cons

`queue` ***`N`***	- Simple, good for multiple jobs that only require a numerical index.
`queue matching` ***`pattern*`***	- Natural nested looping, minimal programming, use optional "files" and "dirs" keywords to only match files or directories - Requires good naming conventions.
`queue in (`*`list`*`)`	- All information contained in a single file, reproducible - Harder to automate submit file creation
`queue from` ***`file`***	- Supports multiple variables, highly modular (easy to use one submit file for many job batches), reproducible - Additional file needed

Organization

(more on this later!)

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Organization

```
12181445_0.err  16058473_0.err  17381628_0.err  18159900_0.err  5175744_0.err  7266263_0.err
12181445_0.log  16058473_0.log  17381628_0.log  18159900_0.log  5175744_0.log  7266263_0.log
12181445_0.out  16058473_0.out  17381628_0.out  18159900_0.out  5175744_0.out  7266263_0.out
13609567_0.err  16060330_0.err  17381640_0.err  3446080_0.err   5176204_0.err  7266267_0.err
13609567_0.log  16060330_0.log  17381640_0.log  3446080_0.log   5176204_0.log  7266267_0.log
13609567_0.out  16060330_0.out  17381640_0.out  3446080_0.out   5176204_0.out  7266267_0.out
13612268_0.err  16254074_0.err  17381665_0.err  3446306_0.err   5295132_0.err  7937420_0.err
13612268_0.log  16254074_0.log  17381665_0.log  3446306_0.log   5295132_0.log  7937420_0.log
13612268_0.out  16254074_0.out  17381665_0.out  3446306_0.out   5295132_0.out  7937420_0.out
13630381_0.err  17134215_0.err  17381676_0.err  4347054_0.err   5318339_0.err  8779997_0.err
13630381_0.log  17134215_0.log  17381676_0.log  4347054_0.log   5318339_0.log  8779997_0.log
13630381_0.out  17134215_0.out  17381676_0.out  4347054_0.out   5318339_0.out  8779997_0.out
```

Many jobs means many files.

Tip: Organize with Directories

```
executable = analyze.sh
transfer_input_files = input/file$(ProcID).in,
                       shared/

log    = logs/job.$(ProcID).log
output = output/job.$(ProcID).stdout
error  = error/job.$(ProcID).stderr

queue 5
```

```
submit_dir/
  jobs.submit
  analyze.sh
  shared/
    script1.sh
    reference.dat
  input/
    file0.in
    ...
  logs/
    job.0.log
    ...
  output/
    job.0.stdout
    ...
  error/
    job.0.stderr
    ...
```

Tip: Organize with Directories

```
executable = analyze.sh
transfer_input_files = input/file$(ProcID).in,
                       shared/

log    = logs/job.$(ProcID).log
output = output/job.$(ProcID).stdout
error  = error/job.$(ProcID).stderr

queue 5
```

Transfer an entire directory (**shared**)
or just the contents of a directory (**shared/**)

```
submit_dir/
  jobs.submit
  analyze.sh
  shared/
    script1.sh
    reference.dat
  input/
    file0.in
    ...
  logs/
    job.0.log
    ...
  output/
    job.0.stdout
    ...
  error/
    job.0.stderr
    ...
```

Submit File Options for Organizing Files

Syntax	Purpose	Features
`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** - Used to avoid having to write some paths in other submit file values
`Transfer_output_remaps = “`**`file1.out`**`=path/to/`**`file1.out;`** **`file2.out`**`=path/to/`**`renamedFile2`**`.out”`	Used to save output files to a specific path and using a certain name	- Used to save output files to a **specific folder** - Used to **rename** output files to avoid writing over existing files

Job-specific directories with `initialdir`

- Use `initialdir` to set the submission directory.
- All output files will be saved back to this directory.

```
executable = analyze.sh
transfer_input_files = file.in
initialdir = job$(ProcId)

output = job.stdout
error  = job.stderr

queue 5
```

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

```
submit_dir/
  jobs.submit
  analyze.sh
  job0/
    file.in
    job.stdout
    job.stderr
  job1/
    file.in
    job.stdout
    job.stderr
  job2/
    ...
```

Send output to a specific directory

- **Reminder**: by default, HTCondor transfers all files back to the submission directory
- Use `transfer_output_remaps` to save output files to a specific path and using a certain name to avoid a cluttered workspace/ writing over other files

```
submit_dir/
  jobs.submit
  analyze.sh
  input/
    file.in
  output/
    file.out
```

```
executable             = analyze.sh
arguments              = file.in file.out

transfer_input_files   = input/file.in
transfer_output_remaps = “file.out=output/file.out”

queue
```

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Questions?

Additional Slides of Interest

Case Study 1

Mei Monte Carlo
Needs to run many random simulations to model particles in a detector

What varies?

- Not much – just needs an index to keep simulation results separate.

Use `queue N`

- Simple, built-in
- No need for specific input values

Case Study 2

Tamara Trials
Testing different design parameters for designing clinical trials.

What varies?

- Five parameter combinations per job
- Parameters are given as arguments to the executable

Use `queue … from`

- queue from can accommodate multiple values per job
- Easy to re-run combinations that fail by using subset of original list

Case Study 3

Ben Bioinformatics

Applying a quality control / processing pipeline to 20 RNA samples.

What varies?

- Each job analyzes one sample; each sample consists of two fastq files in a folder with a standard prefix.

Use `queue … matching`

- Folders have a standard prefix, input files have standard suffix, easy to pattern match

Good alternative: `queue … from`

- Provide list of folder names/file prefixes, construct paths in the submit file.