Snakemake Done Three Ways

HTCondor European Workshop 2025

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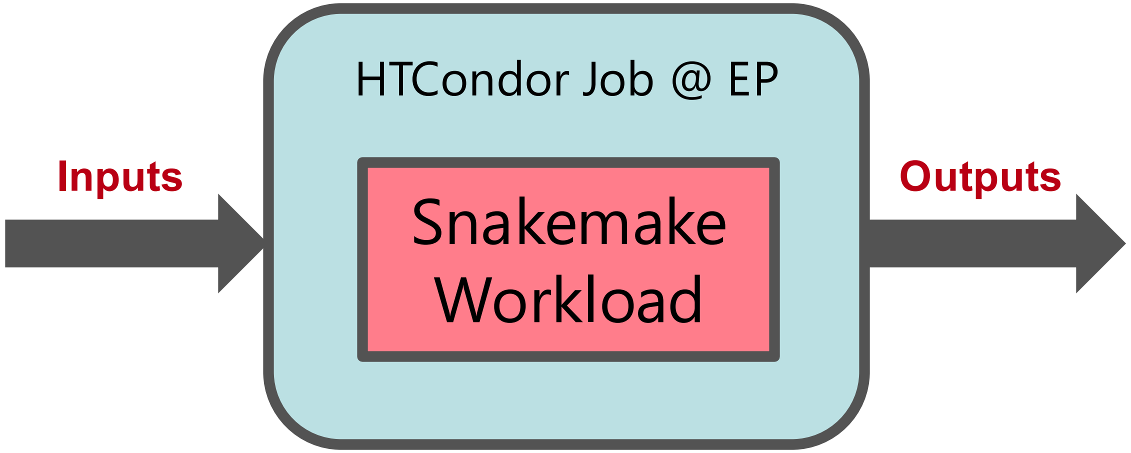
  - SnakeMake
- For as long as there are ~~physicists~~ biologists, there will be new workflow languages! **(arguably, this is a good thing!)**

This talk is about how CHTC approaches users that arrive with The Best workflow language.

Example: Snakemake

Phase I: “I just need to run this one pipeline”

- Never underestimate the power of running an entire pipeline as a single HTCondor job!
  - Pipeline is completely encapsulated in a single HTCondor job.
  - Pipeline has *no* knowledge of HTCondor whatsoever
- Advantages:
  - Simple! Works for nearly any workflow engine.
  - Quickest “time to science” for researchers wanting to run a single pipeline, once.
- Disadvantages:
  - Pipeline needs to fit in a single job!
  - Multiple steps in pipeline may need disparate resource requirements: the “512GB for 5 minutes” problem.



Snakemake invocation example

- For snakemake, this might involve creating a container image with a conda environment installed, the Snakefile, and a script that ultimately invokes

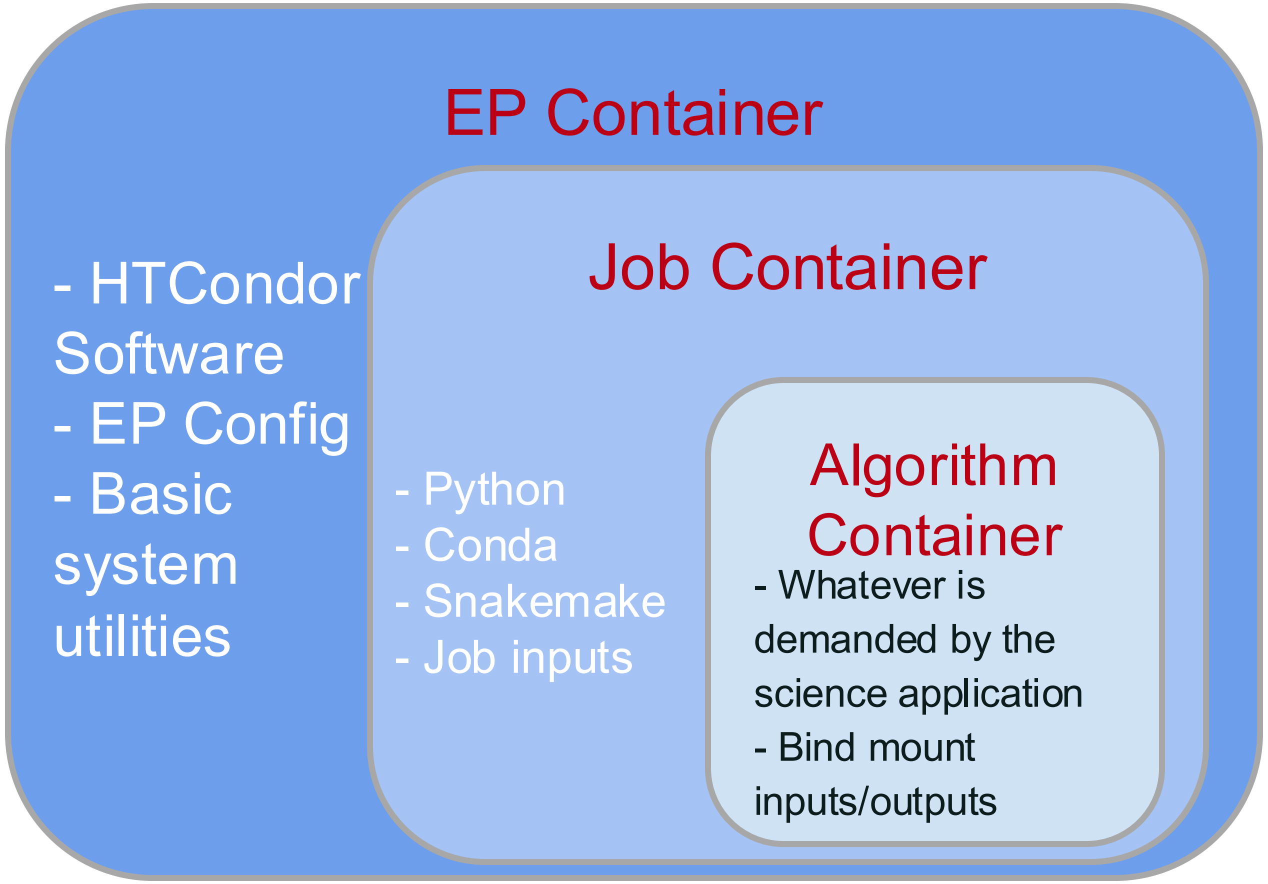
snakemake <output file>

- Snakemake will construct a DAG and, ideally, create the prescribed output file that HTCondor will send back to the AP.
- What can possibly go wrong?

Nested

Containers!

Example challenge: Nested Containers in the OSPool



EP Container

- HTCondor Software
- EP Config
- Basic system utilities

Job Container

- Python
- Conda
- Snakemake
- Job inputs

Algorithm Container

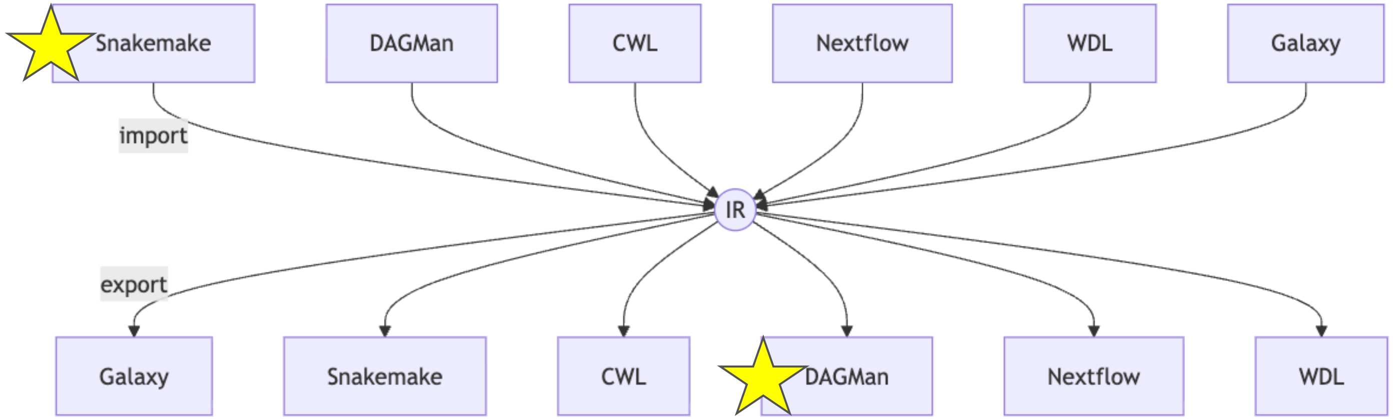
- Whatever is demanded by the science application
- Bind mount inputs/outputs

When running unprivileged (in a glidein), the Snakemake community’s frequent use of containers can cause triply-nested containers!

- Docker is not your friend, but Apptainer is!
- Users may need to convert their Docker images to an Apptainer .sif file.
  - N.b.: A very opaque, difficult environment to develop in!
- **The secret**: starting apptainer from "unpacked" .sif images (`--sandbox`)
- Fewer issues when the Snakemake workload is not itself using containers – but we don’t get to control that!

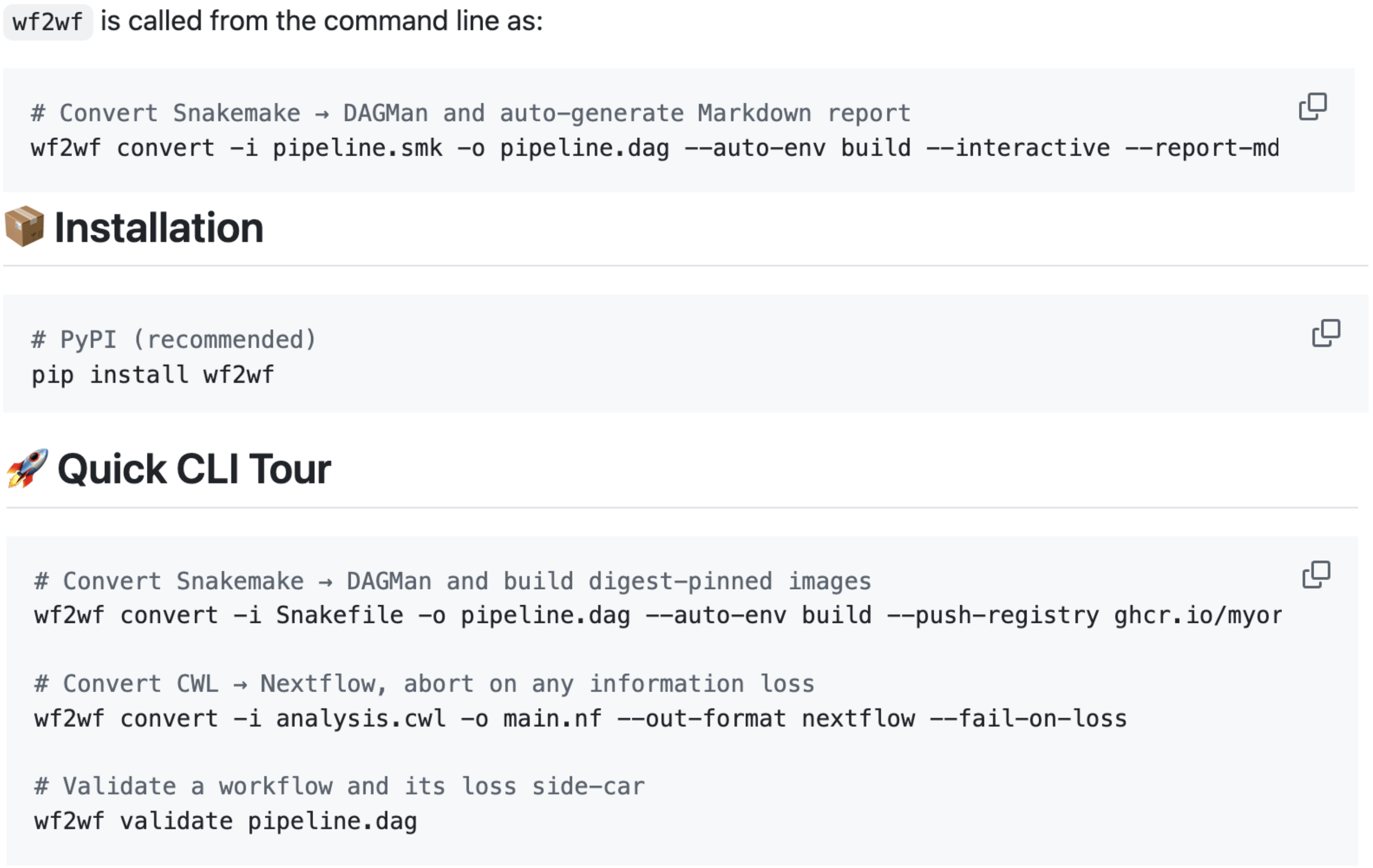
Phase II: “This postdoc joined my lab…”

- The “all-in-one” is great for the “I wanted to re-run this one workload I read in a paper”.
  - Not great for producing science of your own (what happens when reviewers ask you to re-run multiple results quickly?).
- What about the “postdoc using Snakemake joined my lab” case? Assumptions:
  - Locally, you use a native HTCondor workflow such as DAGman.
  - Postdoc used Snakemake because that’s what the former lab used, not because they are a Snakemake enthusiast.
  - Approach: Conversion!
- Case study: wf2wf utility. See https://github.com/csmcal/wf2wf
  - Goal: convert between workflow description formats



Converting between Workflow Languages

- The wf2wf utility *converts* a given workflow between formats.
- Once done, we assume you tweak/change/tinker with the destination format (DAGMan!).
- Challenges:
  - **Lossy translation**. Anyone who uses Google Translate understands that automatic translation is not perfect!
    - A <u>human</u> is needed to review the result.
  - **One-time-nature**. Good for moving into a new ecosystem.



`wf2wf` is called from the command line as:

```
# Convert Snakemake → DAGMan and auto-generate Markdown report
wf2wf convert -i pipeline.smk -o pipeline.dag --auto-env build --interactive --report-md
```

📦 Installation

```
# PyPI (recommended)
pip install wf2wf
```

🚀 Quick CLI Tour

```
# Convert Snakemake → DAGMan and build digest-pinned images
wf2wf convert -i Snakefile -o pipeline.dag --auto-env build --push-registry ghcr.io/myor

# Convert CWL → Nextflow, abort on any information loss
wf2wf convert -i analysis.cwl -o main.nf --out-format nextflow --fail-on-loss

# Validate a workflow and its loss side-car
wf2wf validate pipeline.dag
```

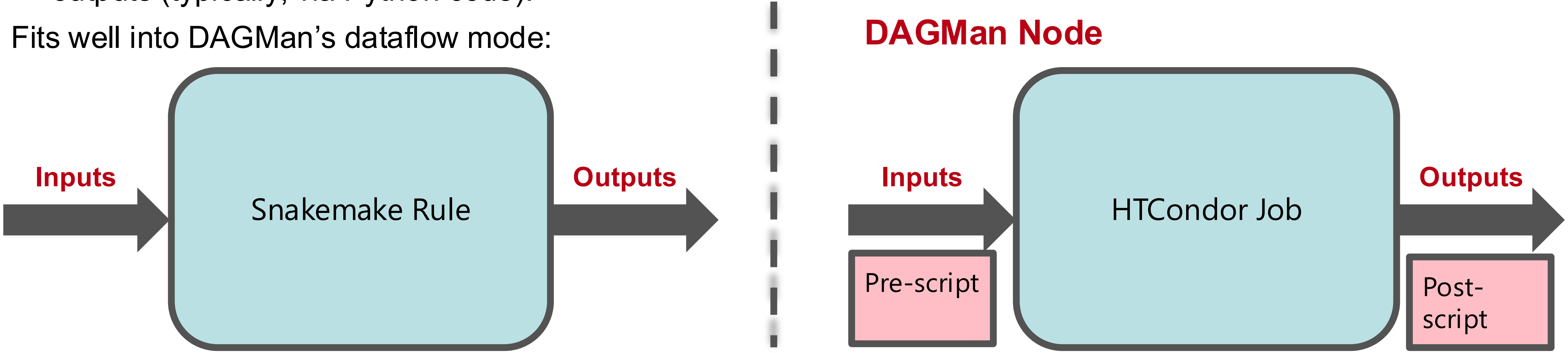
Phase III: The True Believer

- What happens when the ~~user~~ postdoc is not migrating between ecosystems but wants to work in Snakemake?
  - Valid! This may be due to expertise (“this is what I know”), passion (“I am a core Snakemake developer”), or the community (“Journal reviewers requested we publish workloads using Snakemake”).
  - We are not interested in a conversion requiring human touch-up but core HTCondor/Snakemake integration.

- Lesson learned from prior projects: HTCondor’s best analogy is *not* SLURM but AWS. That is:
  - Each workflow engine has a set of plugins for different “execution environments”.
  - The “batch system-like” plugin interface (i.e., SLURM) almost always assumes a shared filesystem.
  - HTCondor prefers to have **no** shared filesystem.
  - Thus: look for executions environments that work with AWS which rarely has a shared filesystem between worker (nodes / VMs / containers).

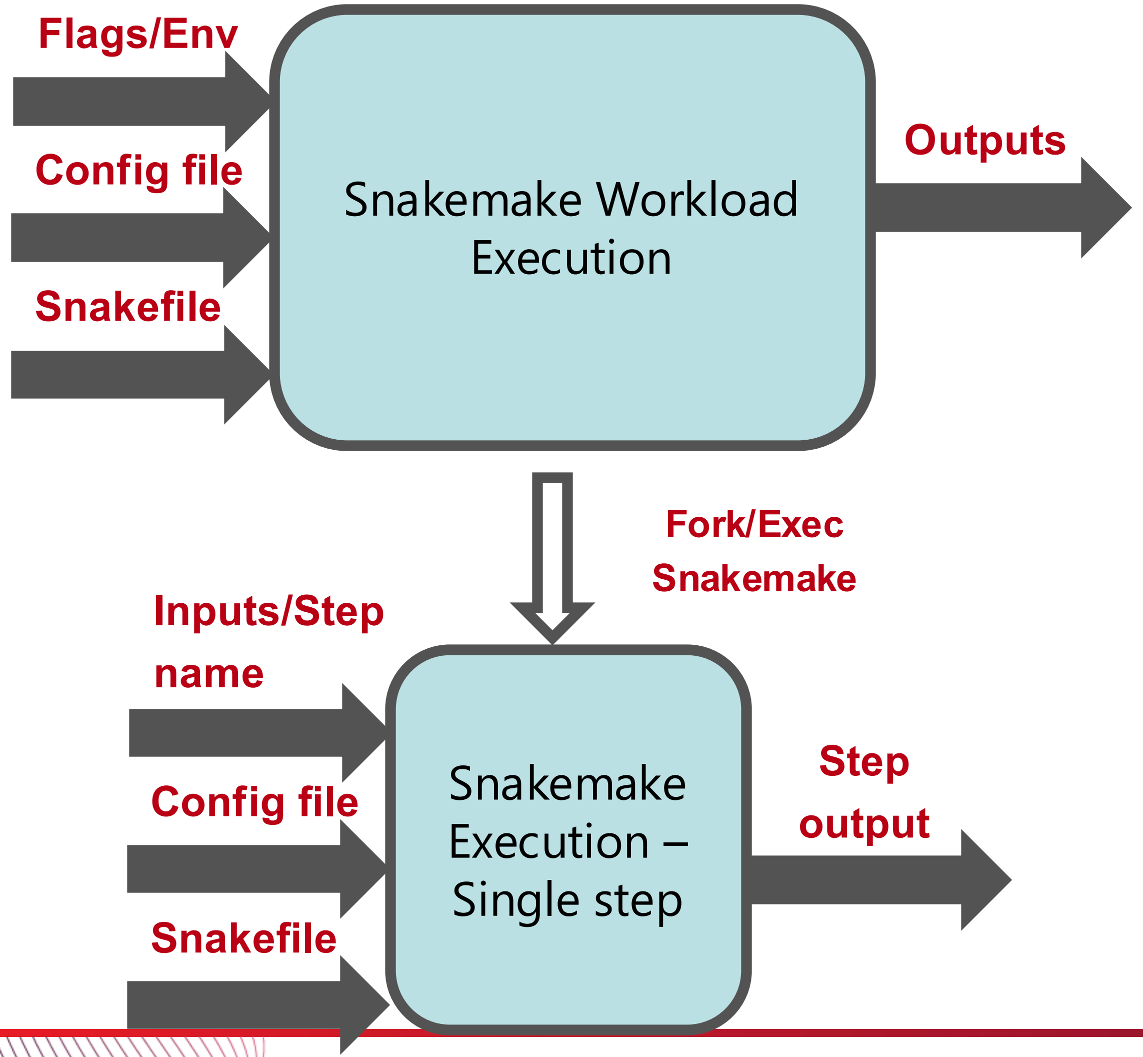
The Snakemake example

- It's all in the name: Snakemake.
  - Snake: Workflow description language is largely in Python, interspersed with YAML. Familiar to a "python native".
  - **Make**: Core concept is that of a Unix Makefile: each rule describes the **inputs**, **outputs**, and how to create the outputs (typically, via Python code).
- Fits well into DAGMan's dataflow mode:



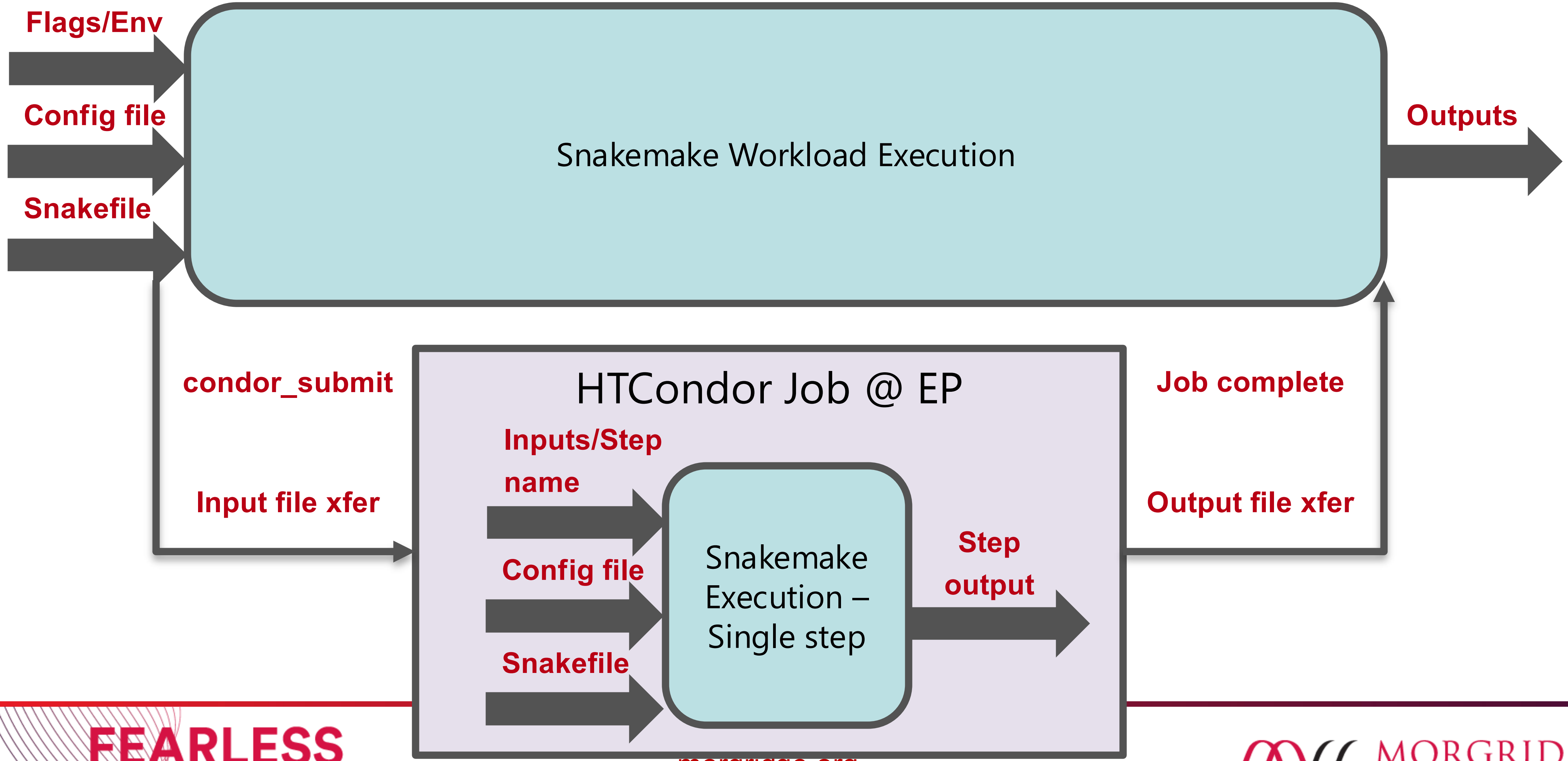
- **Note**: Same issues as any dataflow language. How do you know the "outputs" were completed?!?

A bit on Snakemake



- Snakemake will calculate the missing files and fork/exec itself to execute itself to create the missing data.
  - This "single step" mode is the same as workload mode except it works on a single rule, creating the desired output.
  - Assumptions:
    - At beginning of step execution, the input is at "the right place".
    - At end of execution, the output is at "the right place".
    - **Assumption**: This is all a shared filesystem!
- Via plugin we can replace fork/exec with any arbitrary Python code (such as submitting a HTCondor job).

The HTCondor Executor



Invoking at a technical level

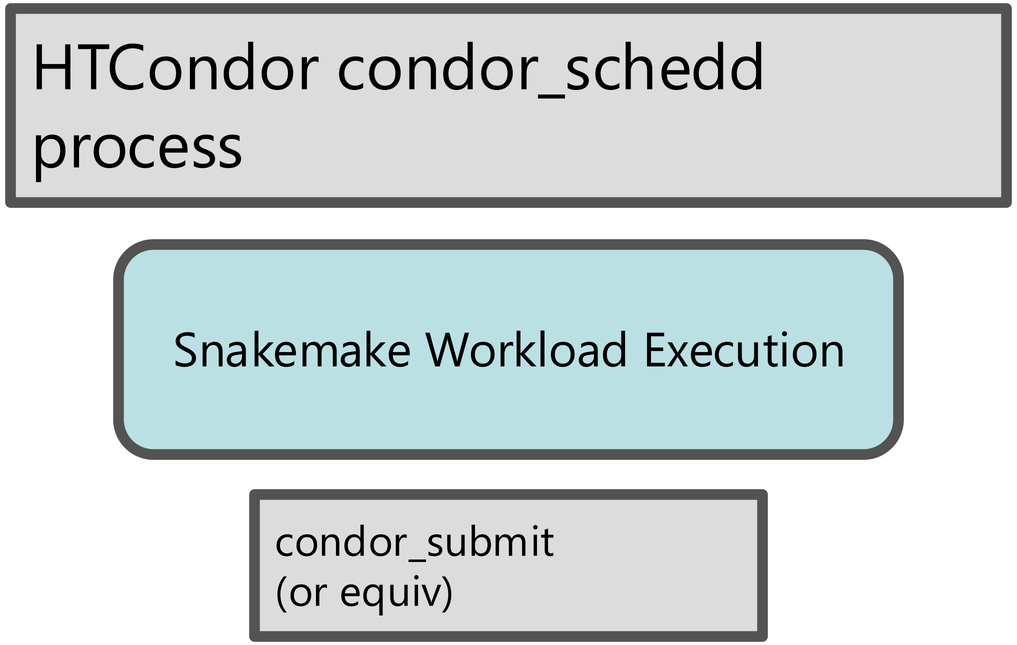
- At the core, it’s as simple as adding the following arguments:

```
snakemake --executor htcondor --shared-fs-usage none
```

- That is:
  - ‘**--executor htcondor**’: When executing a rule, use the HTCondor executor plugin instead of fork/exec.
  - ‘**--shared-fs-usage none**’: Request HTCondor executor to handle all input/output file movement.
- Additionally, the following are supported as user-defined resources in the configuration YAML:
  - request_{gpus,memory,disk}
  - requirements, rank, max_retries, retry_until
  - environment, job_wrapper

Next steps – “The True Believer” (full integration)

- In the prior slide, the “parent” snakemake process was running throughout the workload’s lifetime.
  - Something must monitor for completion, submit next steps, etc.
  - Equivalent: **condor_dagman** process.
- **Downside**: *Has anyone here actually executed* ***condor_dagman*** *directly*?
  - In fact: Snakemake will be killed if you close the terminal.
- Instead, we need the equivalent of **condor_submit_dag**:
  - Have the AP run the snakemake workflow instead of terminal.
  - Work-in-progress: submit the snakemake executable as a “scheduler universe” job running underneath the condor_schedd process in the AP.



Get it for yourself!

Check out the HTCondor-maintained Snakemake executor from https://github.com/htcondor/snakemake-executor-plugin-htcondor.

Check out the externally-maintained wf2wf package: https://github.com/csail/wf2wf

Parting Thoughts

- It’s Good to have engaged users enthusiastic about their favorite workload engine.
  - However, it’s tough to pick winners: not all will have the same lifetime at your site, not all are created equal
- There are three basic approaches to facilitating users:
  - “All in one”, embedding the engine inside a single job.
  - “Translation”, providing tools to (automatically) migrate users to HTCondor-native workloads.
  - “Integration”, providing plugins for the engine to HTCondor.
- Don’t assume “integration” is the best option: may be overkill for your local needs!
  - Also, by far, the most <u>expensive</u> option.
- For the Snakemake engine, at CHTC, we’ve seen all three in action!
  - Hopefully our Snakemake experience specifically …
  - … and workflow integration generically …
  - **Will benefit your site well!**
- **What’s the <u>Next Best Workload Engine</u> on your radar?**

Questions?

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