snakemake

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Snakemake is a workflow management system to create reproducible and scalable data analyses

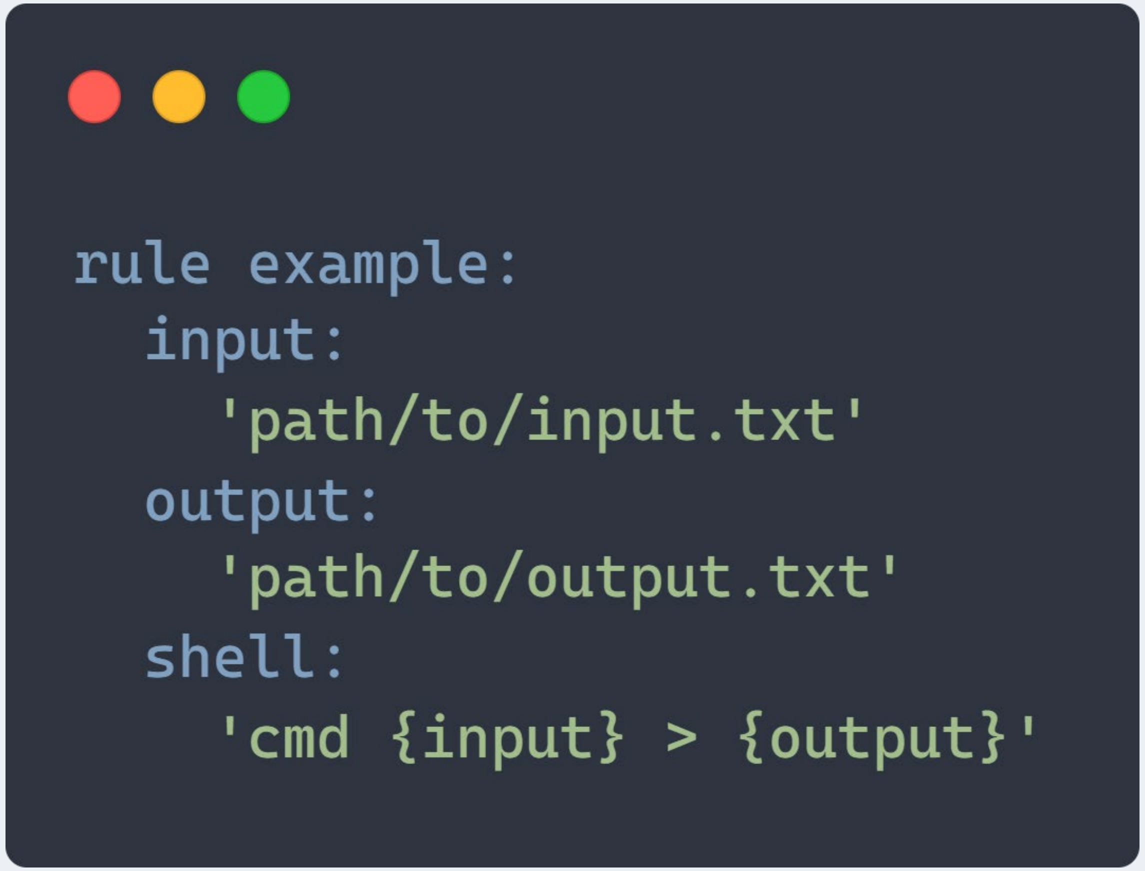
A Snakemake workflow is

- defined in terms of rules that represent the different steps of your data analysis. These rules are described via a human readable, Python based language
- can entail a description of required software with an integration with the Conda package manager and container virtualization
- independent of the available resources and computing platform

Workflow definition

Snakemake Rules

- Rules describe how to get output files from input files
- A shell command or a script to generate the output from the input
- By default, Snakemake will look for rules in a file named Snakefile
- Dependencies between the rules are determined automatically, creating a DAG (directed acyclic graph) of jobs



```
rule example:
  input:
    'path/to/input.txt'
  output:
    'path/to/output.txt'
  shell:
    'cmd {input} > {output}'
```

Demo time

binder

https://mybinder.org/v2/gh/olouant/enccb-workflow-snakemake/master

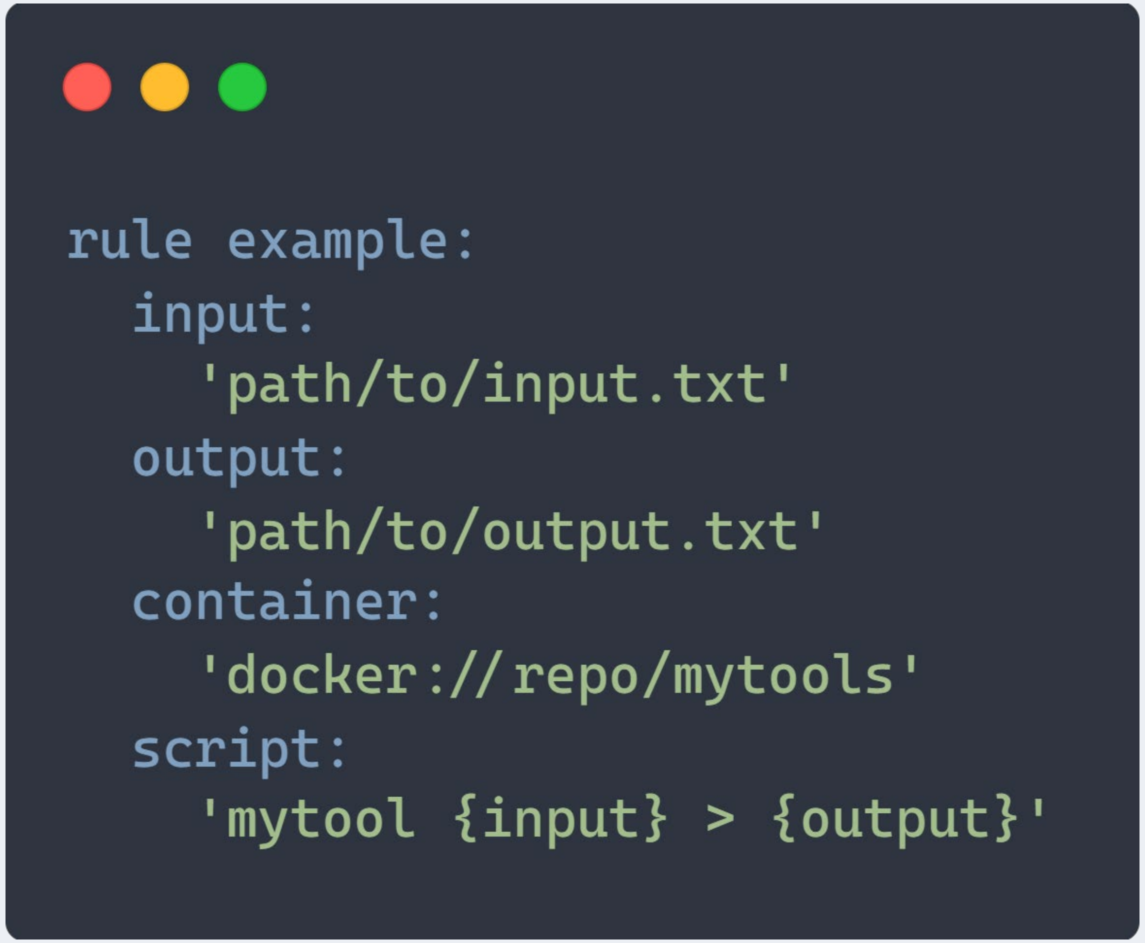
GitHub

https://github.com/olouant/enccb-workflow-snakemake

Reproducibility

Using Containers

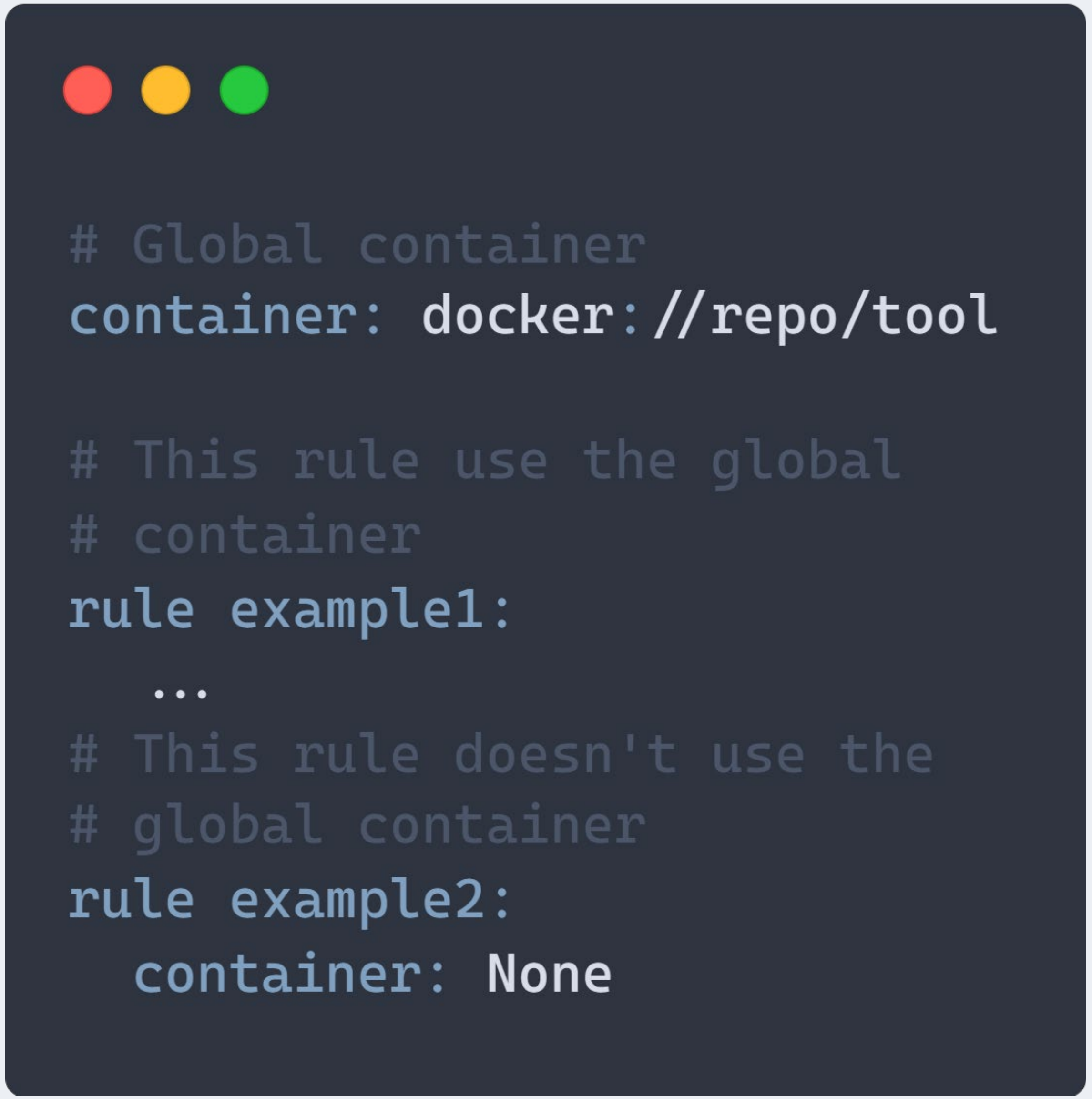
- For each rules in your workflow, you can specify a container to use with the **`container`** directive
- To run the rules that define a container within singularity, use the **`--use-singularity`** option
- You can use URLs starting with **`docker://`** or **`shub://`**



```
rule example:
  input:
    'path/to/input.txt'
  output:
    'path/to/output.txt'
  container:
    'docker://repo/mytools'
  script:
    'mytool {input} > {output}'
```

Using Containers

- The **container** directive can be used to define a global container
- When you define a global container, all the jobs will use this container
- You can disable the use of the global container for certain rules by setting value for the **container** directive to **None**



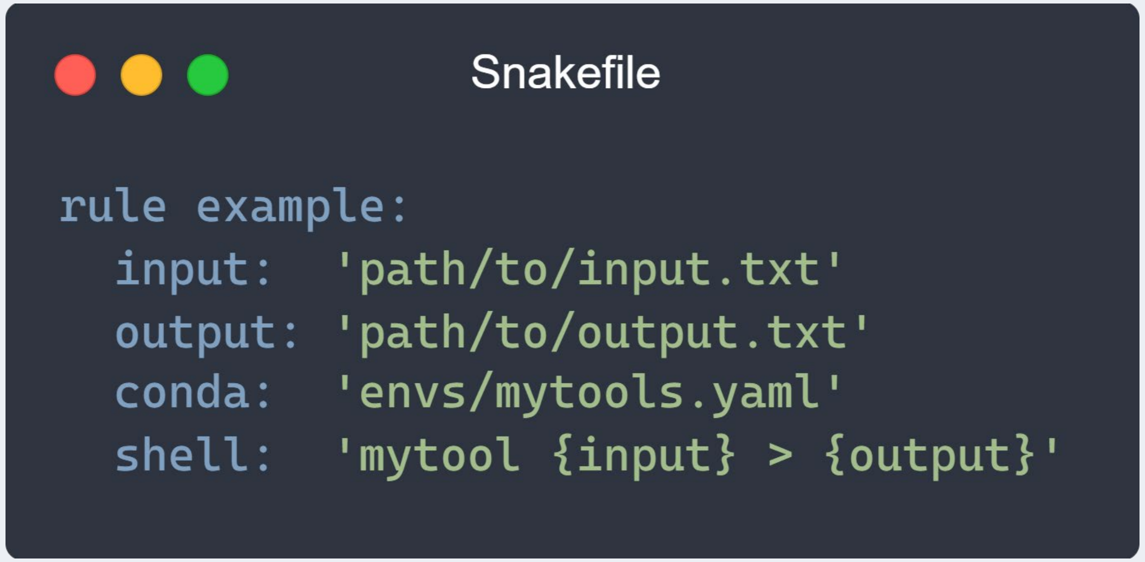
```
# Global container
container: docker://repo/tool

# This rule use the global
# container
rule example1:
  ...
# This rule doesn't use the
# global container
rule example2:
  container: None
```

Define a Conda Environment

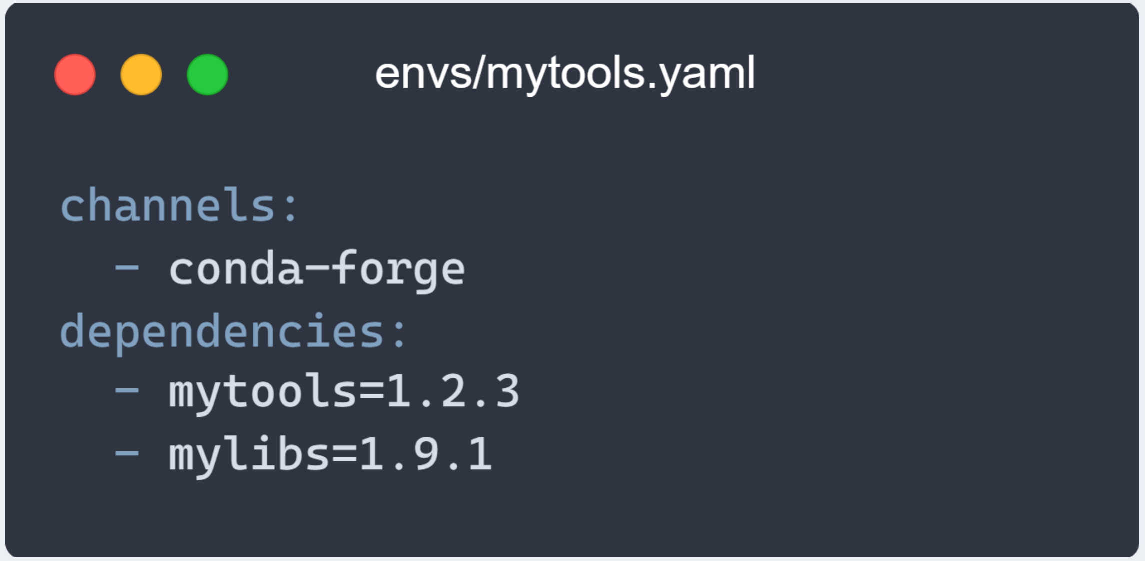
- You can define an isolated software environment per rule using the **conda** directive that takes as argument a YAML file describing the Conda packages to use

- To use the Conda integration add the **--use-conda** option when launching Snakemake



Snakefile

```
rule example:
  input:   'path/to/input.txt'
  output:  'path/to/output.txt'
  conda:   'envs/mytools.yaml'
  shell:   'mytool {input} > {output}'
```

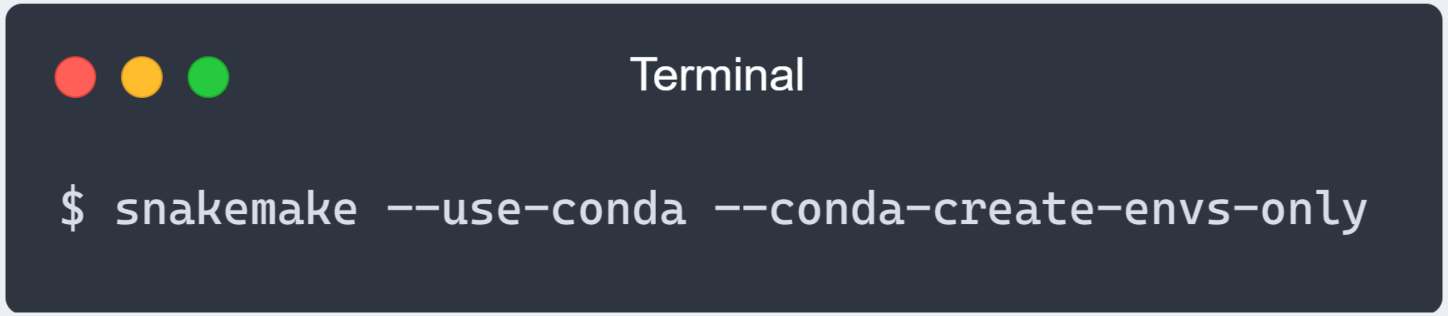


envs/mytools.yaml

```
channels:
  - conda-forge
dependencies:
  - mytools=1.2.3
  - mylibs=1.9.1
```

Create the Environment Before Running the Workflow

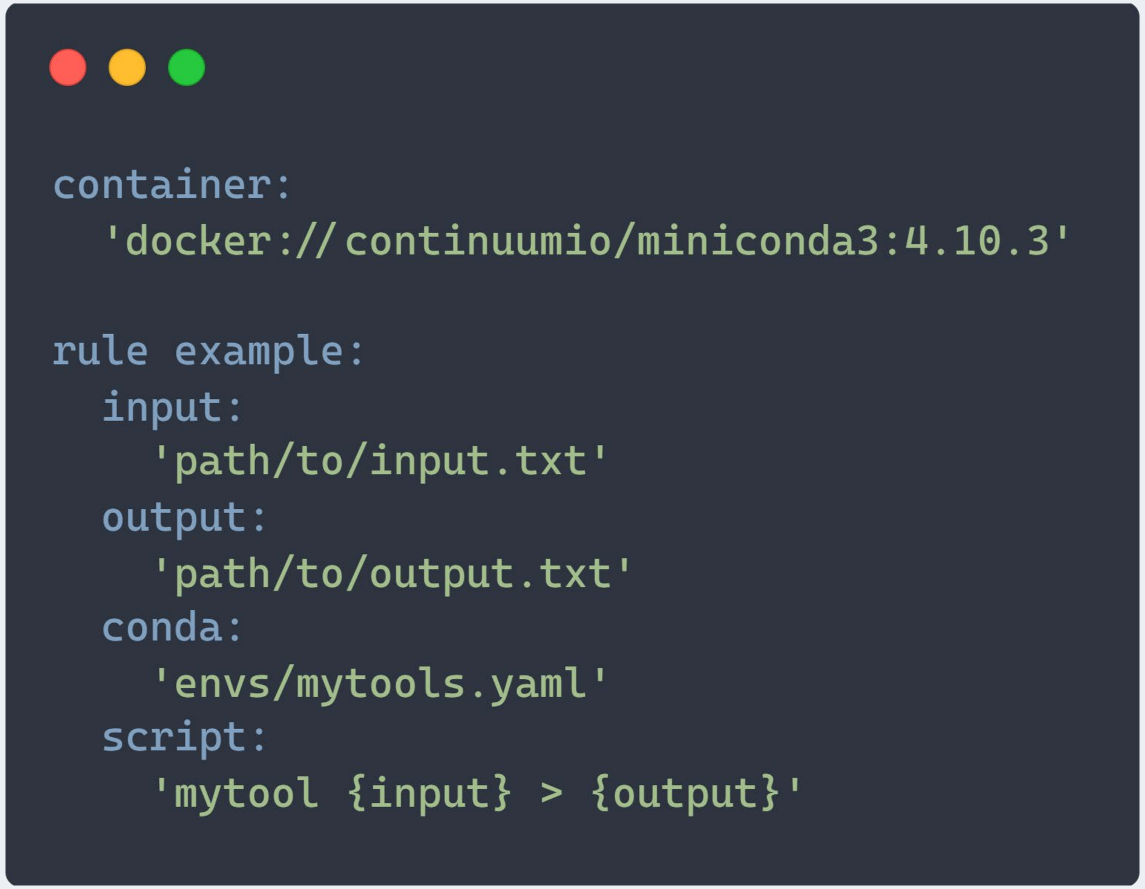
- In some cases, when running in a HPC environment the compute nodes do not have internet access and the creation of the Conda environment will fail
- Solution is to create the Conda environment on the login node but not run the full workflow



```
$ snakemake --use-conda --conda-create-envs-only
```

Combining Conda and Container

- Snakemake allows you to combine the definition of a Conda environment with running jobs in containers
- In that case you need to invoke Snakemake with both the **`--use-conda`** and **`--use-singularity`** options

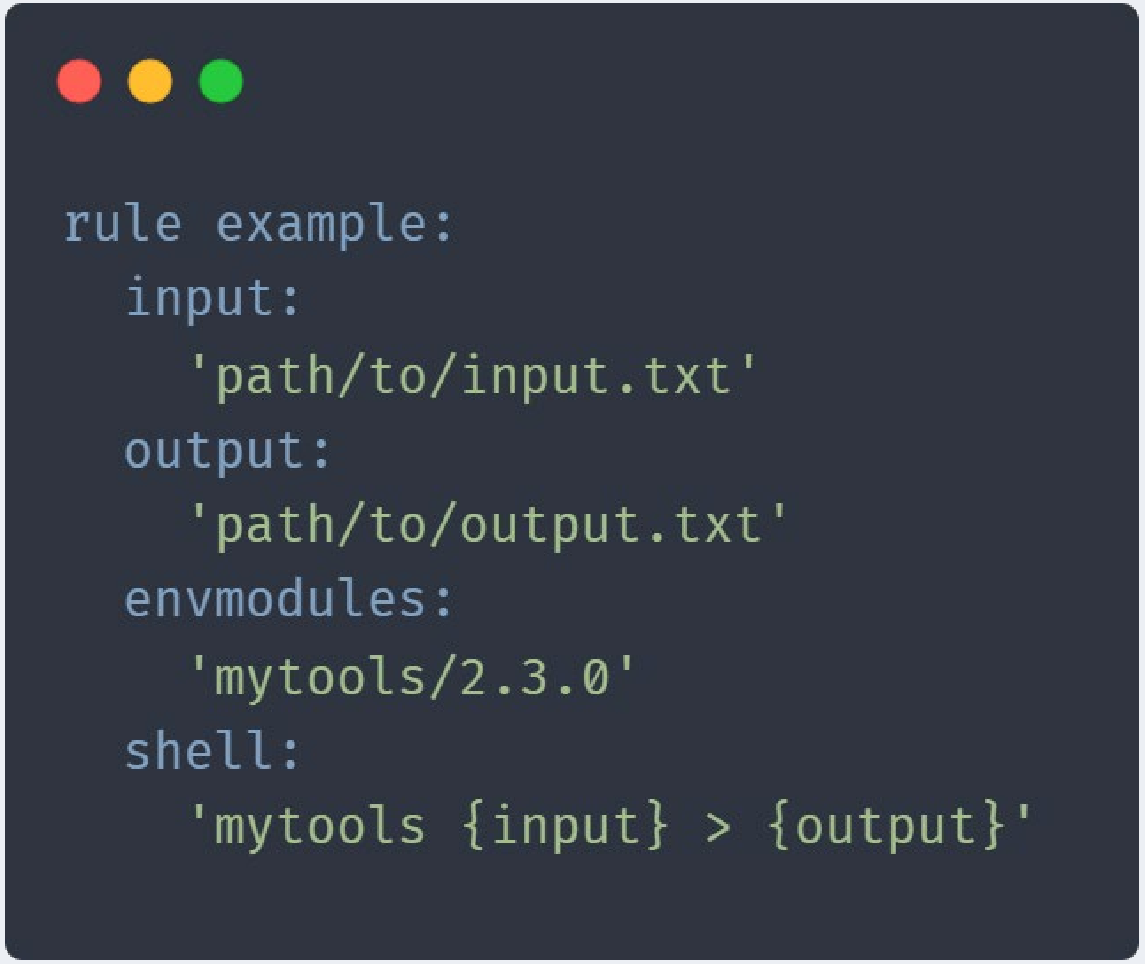


```
container:
  'docker://continuumio/miniconda3:4.10.3'

rule example:
  input:
    'path/to/input.txt'
  output:
    'path/to/output.txt'
  conda:
    'envs/mytools.yaml'
  script:
    'mytool {input} > {output}'
```

Using Environment Modules

- Snakemake allows to define environment modules per rule using the **`envsmodules`** directive to provide a list of modules that should be loaded in the environment
- To use environment modules, add the **`--use-envmodules`** option when launching Snakemake



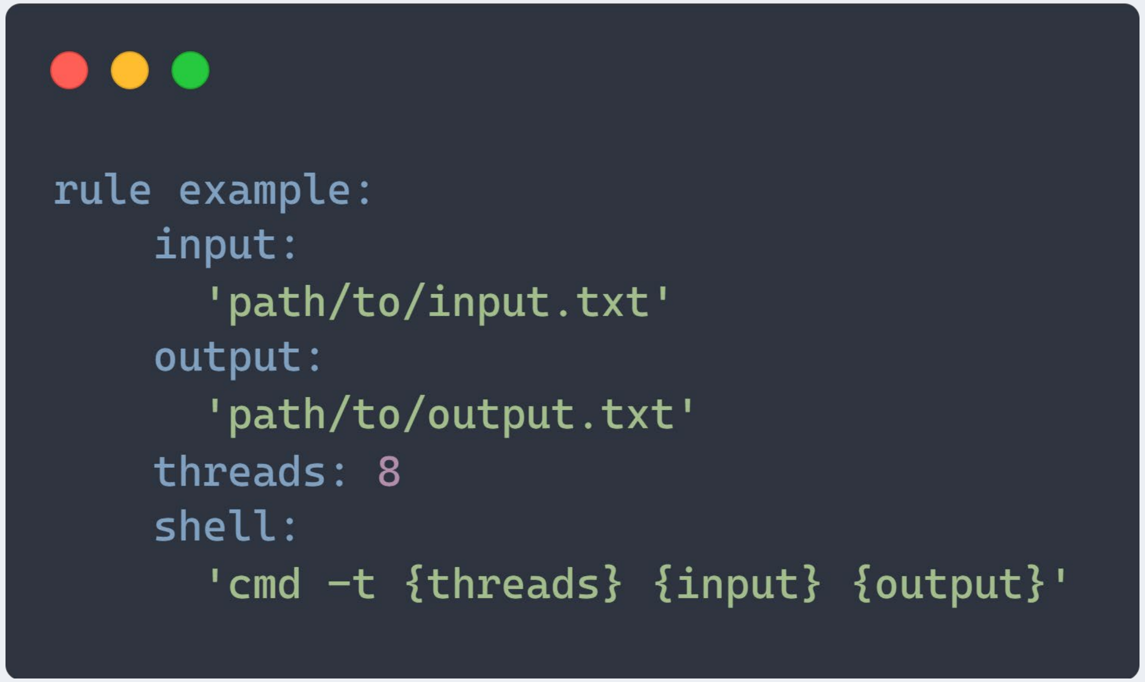
```
rule example:
  input:
    'path/to/input.txt'
  output:
    'path/to/output.txt'
  envmodules:
    'mytools/2.3.0'
  shell:
    'mytools {input} > {output}'
```

Scalability

Setting the Number of Threads

- You can specify the number of threads to use for a specific rule with the **`threads`** directive

- Snakemake will set common environment variables to the value given of the **`threads`** directive:
  - `OMP_NUM_THREADS`
  - `OPENBLAS_NUM_THREADS`
  - `MKL_NUM_THREADS`



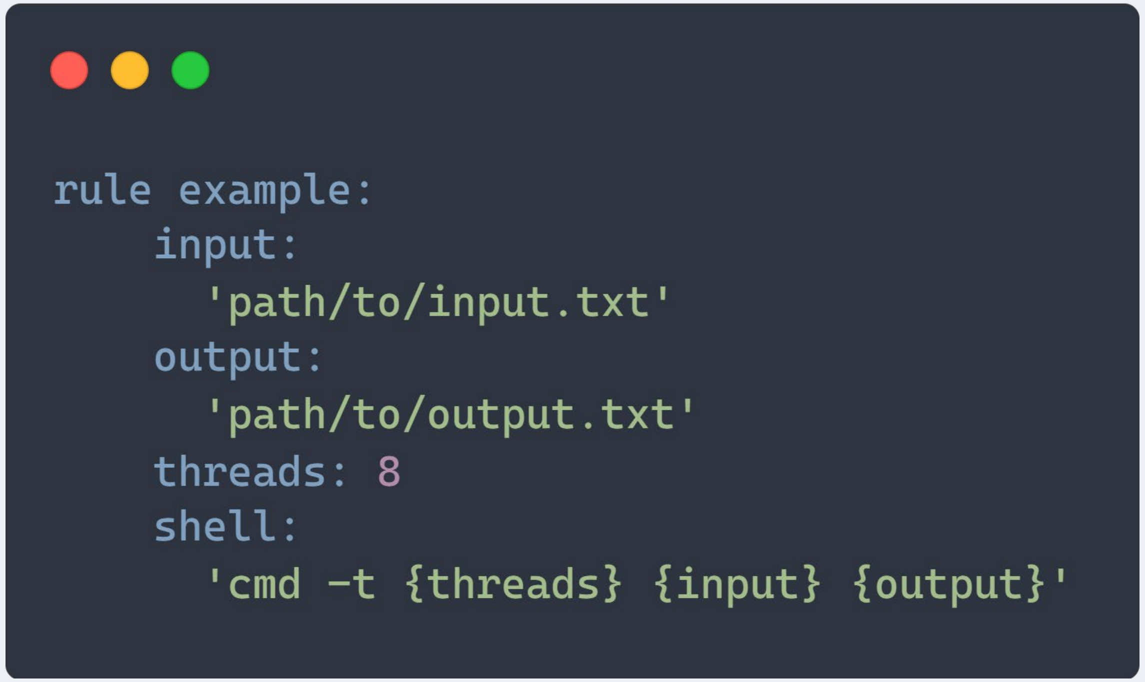
```
rule example:
    input:
      'path/to/input.txt'
    output:
      'path/to/output.txt'
    threads: 8
    shell:
      'cmd -t {threads} {input} {output}'
```

Setting the Number of Threads

- Specified threads must be seen as a maximum
- When Snakemake is executed with fewer cores, the number of threads will be adjusted:

```
threads = min(threads, cores)
```

with `cores`, the number of cores specified at the command line (`--cores` option)

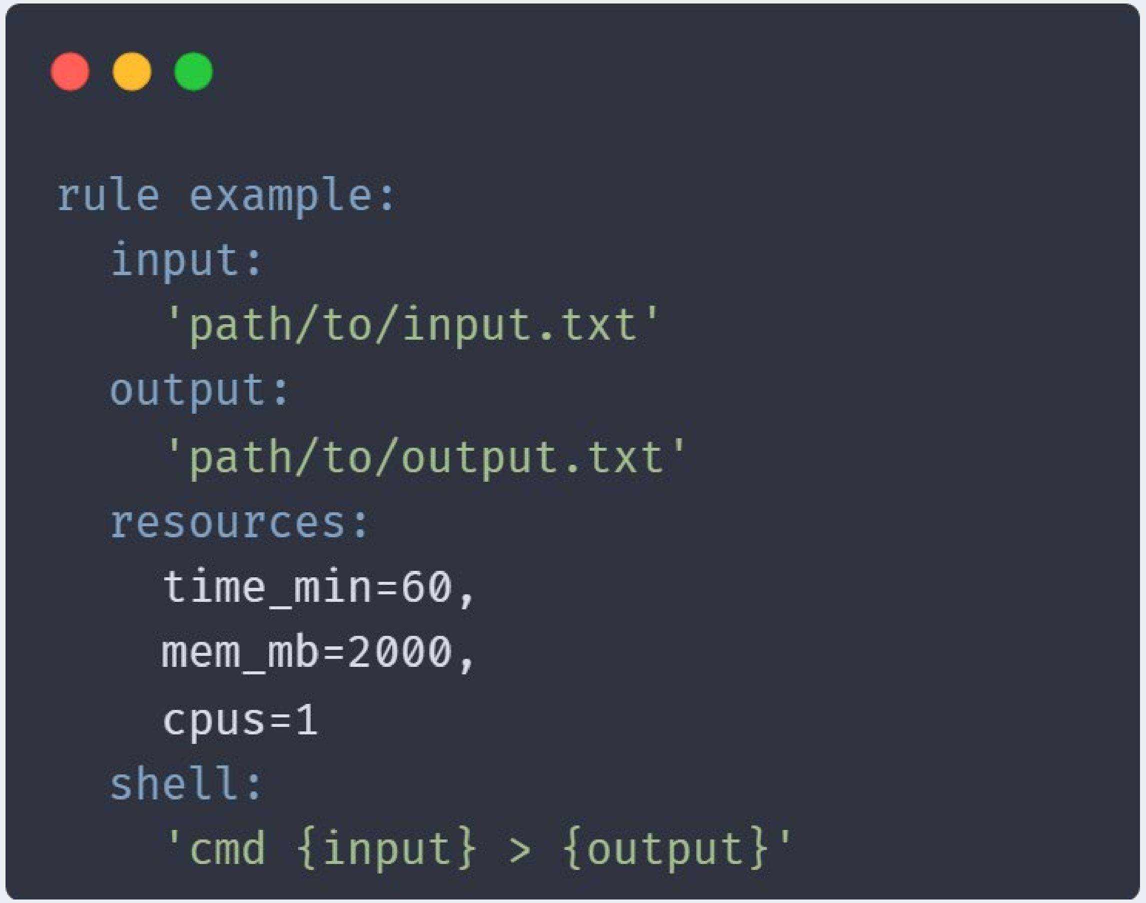


```
rule example:
    input:
      'path/to/input.txt'
    output:
      'path/to/output.txt'
    threads: 8
    shell:
      'cmd -t {threads} {input} {output}'
```

Managing Resources

- Running on in a cluster environment may require resources definition that are defined using the **`resources`** directive

- There are 3 standard resources used by Snakemake:
  - **`mem_mb`**: memory usage
  - **`disk_mb`**: disk usage
  - **`tmpdir`**: temporary directory



```
rule example:
  input:
    'path/to/input.txt'
  output:
    'path/to/output.txt'
  resources:
    time_min=60,
    mem_mb=2000,
    cpus=1
  shell:
    'cmd {input} > {output}'
```

- Resources that shall constrain the scheduling are specified using the **`--resources`** command line option

Snakemake Scheduling

- Available jobs are scheduled to maximize parallelization while satisfying resource constraints

```
rule sort:
  input:
    'path/to/input.txt'
  output:
    'input.sorted.txt'
  threads: 4
  resources:
    mem_mb=100
  shell:
    'sort --parallel {threads} {input} > {output}'
```

```
$ snakemake --cores 2


$ snakemake --cores 8


$ snakemake --cores 8 --resources mem_mb=100
```

1 **sort** job using 2 threads

2 **sort** job using 4 threads each

1 **sort** job using 4 threads

Managing Resources and Cluster Execution

- Resources for rules that do not define explicitly resources can be provided through the command line option `--default-resources`

```
$ snakemake --default-resources time_min=600 mem_mb=2000 cpus=1 ...
```

- Resources defined within the rules can be overwitted using the command line option `--set-resources`

Running on an HPC cluster

- Snakemake can compile jobs into scripts that will run on the compute node of and HPC cluster
- The jobs are submitted to the cluster via a submission command that is provided by passing the `--cluster` option to the command line
- The maximum number of jobs to be submitted at once is set using the `--jobs` option

Slurm

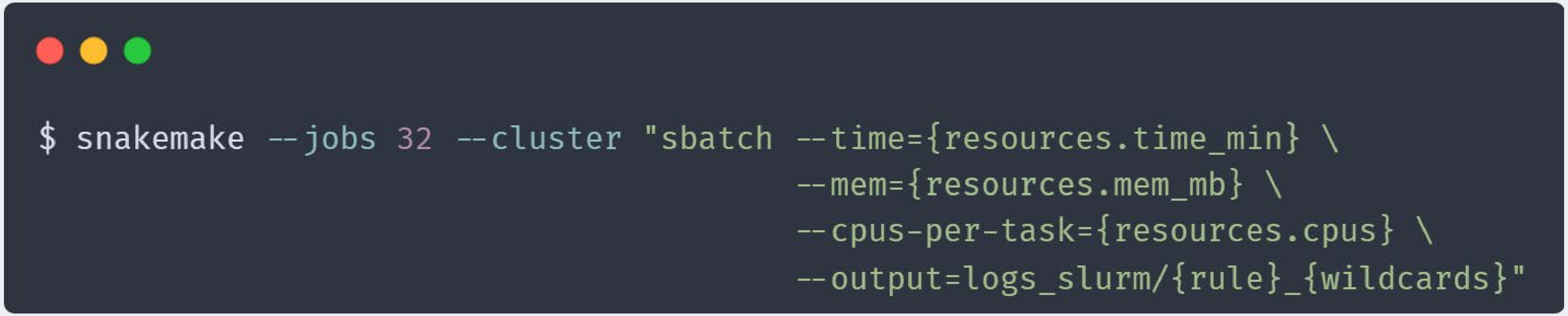
```
$ snakemake --jobs 32 --cluster "sbatch"
```

PBS

```
$ snakemake --jobs 32 --cluster "qsub"
```

Managing Resources and Cluster Execution

- The submit command can be decorated to make it aware of certain job properties: (name, rule name, input, output, params, wildcards, log, threads...)



```
$ snakemake --jobs 32 --cluster "sbatch --time={resources.time_min} \
                                       --mem={resources.mem_mb} \
                                       --cpus-per-task={resources.cpus} \
                                       --output=logs_slurm/{rule}_{wildcards}"
```

Cluster Execution: be nice to the scheduler...

... and your fellow users

- If too many requests are made at once to the job scheduler, the performance will suffer for all users

- If the rules in your Snakemake jobs take minutes to complete, it's overkill to check their status every second. In that case, it may be desirable to set the following option:

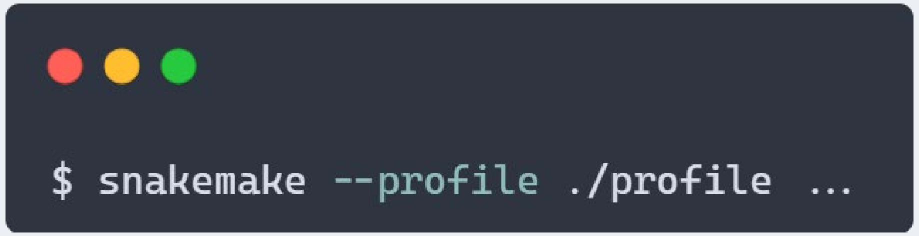
  - `--max-jobs-per-second`
  - `--max-status-checks-per-second`

Using a Configuration File

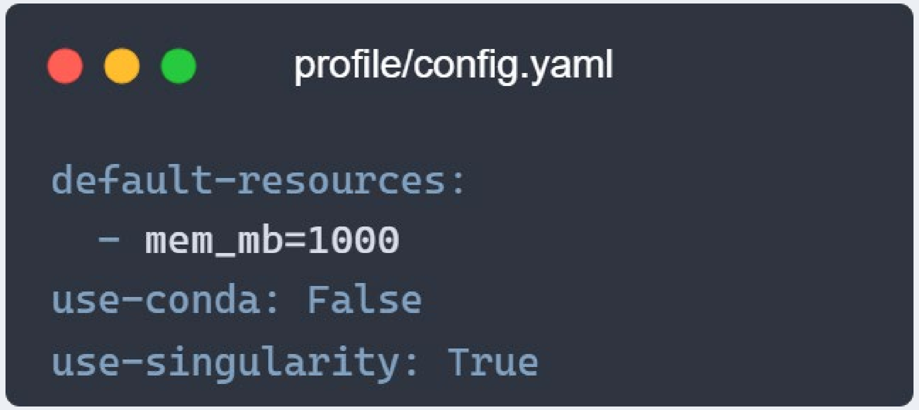
- When running workflows on a regular basis, it might be tedious to provide all the required flags every time
- It is possible to specify a configuration profile to specify the default options using the `--profile profile_name` command line option
- Snakemake will search for a folder named `profile_name` in the user and global configuration directories (`~/.config/snakemake`). You can also provide an absolute or relative path to a directory
- In the folder, Snakemake expect to find a file named `config.yaml`

Using a Configuration File

- The profile can be used to set a default for each option of the Snakemake command line
- In a profile, command-line option `--someoption` becomes `someoption`



```
$ snakemake --profile ./profile ...
```



profile/config.yaml

```yaml
default-resources:
  - mem_mb=1000
use-conda: False
use-singularity: True
```

See also: https://github.com/snakemake-profiles/doc

Using a Custom Job Script

- You can provide a custom job script for submission to a cluster using the `--jobscript` command line option or use a profile
- This allows you to perform additional operations in your job script
- For example, it can be used to add additionnal binding when using singularity

profile/config.yaml

```
cluster:
  mkdir -p logs/{rule} &&
  sbatch
    --cpus-per-task={threads}
    --job-name={rule}-{wildcards}
    --output=logs/{rule}/{rule}-{wildcards}-%j.out
jobs: 10
jobscript: job_script.sh
use-conda: False
use-singularity: True
```

profile/job_script.sh

```
#!/bin/bash
# properties = {properties}

export SINGULARITY_BIND=$SINGULARITY_BIND,$TMPDIR

{exec_job}
```

Wrapping up

- Snakemake is a workflow manager offering a simple Python-like syntax with high readability and flexibility
- Snakemake allows for easy mixing of shell commands and high-level language scripts (Python, Julia, R, Rust)
- Reproducibility and dependencies management of the workflow can be achieved through the integration with the Conda package manager and containers
- Snakemake provide mechanisms to manage resources and cluster execution

Get More Information About Snakemake

- Website: https://snakemake.github.io/
- Documentation: https://snakemake.readthedocs.io/en/stable/

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