



A short
Introduction to Workflows
in a HPC context.

damien.francois@uclouvain.be – Calcul Intensif et Stockage de Masse

Q: What do you do when to want to run computations on a cluster?

A: you write a submission script and submit it to the scheduler (e.g. Slurm)

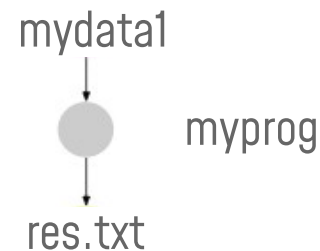
```
#!/bin/bash
# Submission script for demonstrating
# slurm usage.

# Job parameters
#SBATCH --job-name=demo
#SBATCH --output=res.txt
# Needed resources
#SBATCH --ntasks=1
#SBATCH --mem-per-cpu=2000
#SBATCH --time=1:00:00

# Operations
echo "Job start at $(date)"
# Job steps
srun ~/bin/myprog < mydata1

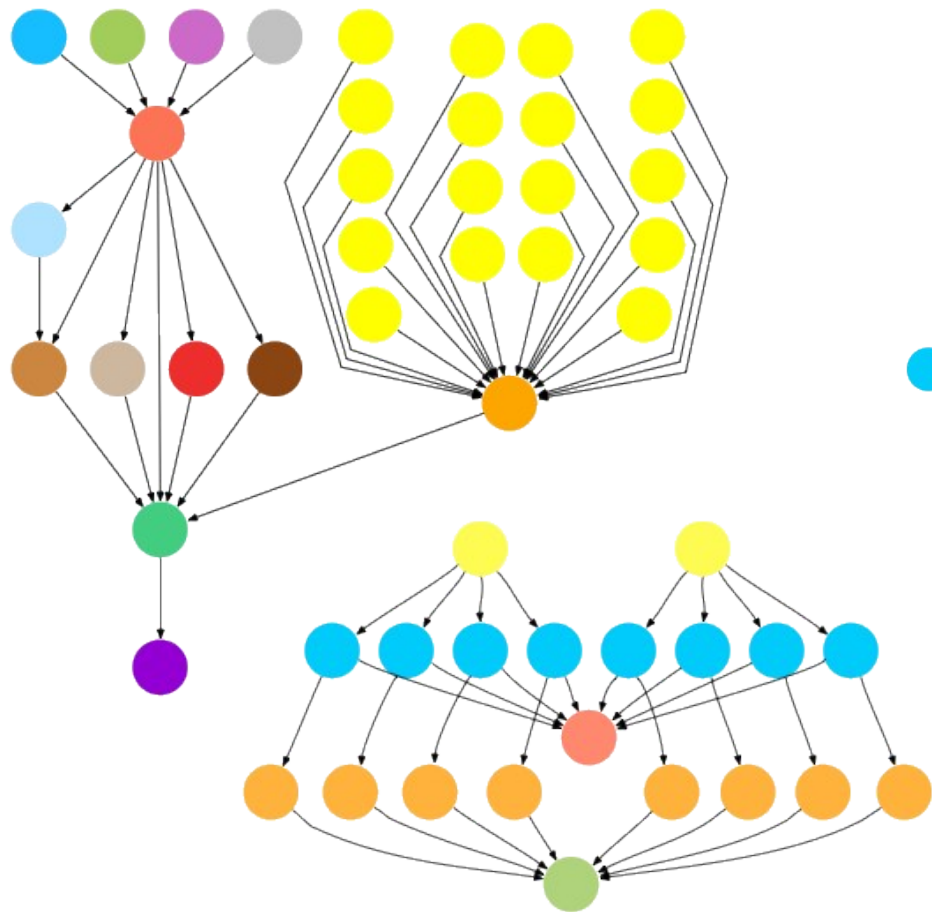
echo "Job end at $(date)"

```

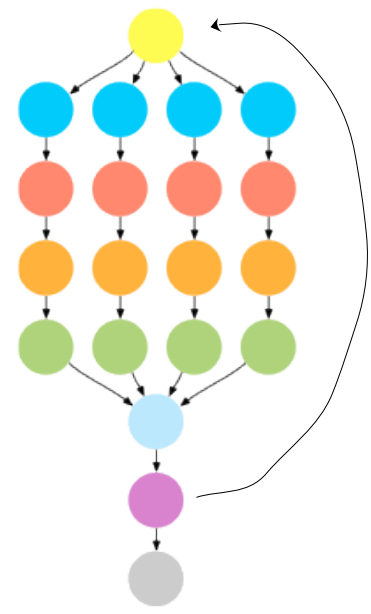
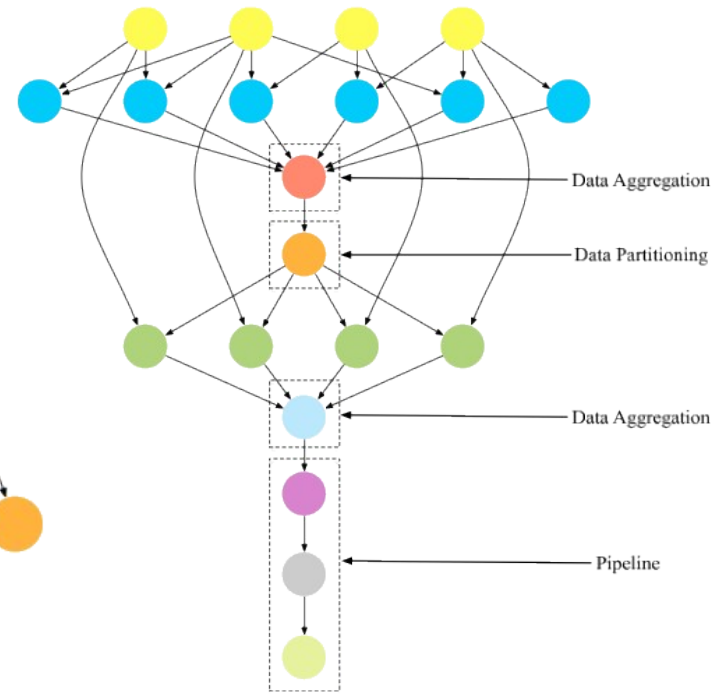


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#S #S #SBATCH --mem-per-cpu=2000
# #SBATCH --time=1:00:00
ec #
# ec # Operations
sr # echo "Job start at $(date)"
sr # Job steps
ec srun ~/bin/myprog < mydata1
~ ec
~ echo "Job end at $(date)"
~
```





Q: What if ...



A: you need to think “workflows”

Workflows

- ♦ exist in business, healthcare, administration, science, etc.

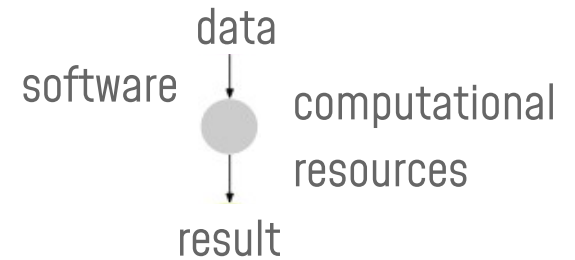
“A workflow is a precise description of a scientific procedure – a multi-step process to coordinate multiple tasks, acting like a sophisticated script”

P. Romano, “Automation of in-silico data analysis processes through workflow management systems,” Brief Bioinform, vol. 9, no. 1, pp. 57–68, Jan. 2008

- ♦ also exist in IT operations, machine learning, Internet of Things, etc.

Workflows

- ◆ a list of tasks or operations (the “work”)
- ◆ a set of dependencies between tasks (the “flow”)
- ◆ but also
 - a set of data sources
 - computational resources
 - scientific software



Workflows by hand...

- ◆ error prone
- ◆ cumbersome
- ◆ complex to share
- ◆ difficult to track provenance



Workflow management systems

can do some (or all) of the following:

- ◆ Compute dependencies and organise work
- ◆ Submit jobs to the scheduler
- ◆ Generate job descriptions [templating, sweeping, etc.]
- ◆ Install scientific software
- ◆ Monitor jobs and recover from failures, fault detection, "smart" reruns
- ◆ Data handling: mapping, referencing, movement, streaming, and staging
- ◆ Log processes and data provenance tracking
- ◆ Enable sharing of data, results, workflows, with security and monitoring of access policies.
- ◆ Provide performance analysis and prediction

An example you already know of..



GNU Make

2.2 A Simple Makefile



Here is a straightforward makefile that describes the way an executable file called `edit` depends on eight object files which, in turn, depend on eight C source and three header files.

In this example, all the C files include `defs.h`, but only those defining editing commands include `command.h`, and only low level files that change the editor buffer include `buffer.h`.

```
edit : main.o kbd.o command.o display.o \  
      insert.o search.o files.o utils.o  
      cc -o edit main.o kbd.o command.o display.o \  
          insert.o search.o files.o utils.o  
  
main.o : main.c defs.h  
      cc -c main.c  
kbd.o : kbd.c defs.h command.h  
      cc -c kbd.c  
command.o : command.c defs.h command.h  
      cc -c command.c  
display.o : display.c defs.h buffer.h
```

GNU Make

can do some (or all) of the following:

- ◆ Compute dependencies and organise work 
- ◆ ~~Submit jobs to the scheduler~~
- ◆ ~~Generate job descriptions (templating, sweeping, etc.)~~
- ◆ ~~Install scientific software~~
- ◆ ~~Monitor jobs and recover from failures, fault detection, "smart" reruns~~ 
- ◆ ~~Data handling: mapping, referencing, movement, streaming, and staging~~
- ◆ ~~Log processes and data provenance tracking~~
- ◆ ~~Enable sharing of data, results, workflows, with security and monitoring of access policies.~~
- ◆ ~~Provide performance analysis and prediction~~

Actually, with a little trick...



GNU-Make version **4** was recently released. This new version comes with a number of improvements like **GNU Guile integration**, **Loadable objects** (see <http://plindenbaum.blogspot.fr/2014/08/a-gnu-make-plug-in-for-illumina-fastqs.html>). It also allows to specify the default shell to be invoked (see <http://plindenbaum.blogspot.fr/2014/01/parallelizing-rstats-using-make.html>)


<http://www.gnu.org/software/make/manual/make.html> : The program used as the shell is taken from the variable **SHELL**. If this variable is not set in your makefile, the program `/bin/sh` is used as the shell. The argument(s) passed to the shell are taken from the variable **.SHELLFLAGS**. The default value of **.SHELLFLAGS** is `-c` normally, or `-ec` in POSIX-conforming mode.

So, if you want to parallelize GNU-Make with **SLURM** you can wrap the shell into **srun** using **SHELL** and **.SHELLFLAGS**. Here is an example, creating and concatenating 100 files containing the hostname:

```
ifdef SLURM_JOB_ID
SHELL=srun
.SHELLFLAGS= -N1 -n1 bash -c
endif
```

GNU Make

can do some (or all) of the following:

- 
- ◆ Compute dependencies and organise work
 - ◆ Submit jobs to the scheduler
 - ◆ ~~Generate job descriptions (templating, sweeping, etc.)~~
 - ◆ ~~Install scientific software~~
 - ◆ ~~Monitor jobs and recover from failures, fault detection, "smart" reruns~~
 - ◆ ~~Data handling: mapping, referencing, movement, streaming, and staging~~
 - ◆ ~~Log processes and data provenance tracking~~
 - ◆ ~~Enable sharing of data, results, workflows, with security and monitoring of access policies.~~
 - ◆ ~~Provide performance analysis and prediction~~

Workflow management systems

- ♦ ~~error prone~~ safe
- ♦ ~~cumbersome~~ convenient
- ♦ ~~complex~~ easy to share
- ♦ ~~difficult~~ simple to track provenance



"The main goals of scientific workflows, then, are (i) to save "human cycles" by enabling scientists to focus on domain-specific [science] aspects of their work, rather than dealing with complex data management and software issues; and (ii) to save machine cycles by optimizing workflow execution on available resources."

Workflow management systems

An “incomplete” list ...

The screenshot shows a web browser displaying a GitHub Wiki page. The page title is "Existing Workflow systems" and it was edited by Iwan Aucamp 11 days ago. The page content includes a permalink, citation information, and a section titled "Computational Data Analysis Workflow Systems". Within this section, the text "An incomplete list" is circled in orange. Below this, there is a list of two items: "1. Arvados - CWL-based distributed computing platform for data analysis on massive data sets." and "2. Apache Taverna". A right-hand sidebar shows a list of pages, including "Home", "2021 CWL Mini Conference", "2022 CWL Conference", "Arvados", "Common Workflow Language != Kile TexStudio 'completion word list'", "Conference Video Guidelines", "CWL Implementations", and "CWL v1.2.1 'Barn Raising'".

Existing Workflow systems

Iwan Aucamp edited this page 11 days ago · 308 revisions

Permalink: <https://s.apache.org/existing-workflow-systems>

Cite as (update dates):

Peter Amstutz, Maxim Mikheev, Michael R. Crusoe, Nebojša Tijanić, Samuel Lampa, et al. (2021): **Existing Workflow systems**. *Common Workflow Language wiki*, GitHub. <https://s.apache.org/existing-workflow-systems> updated 2021-12-14, accessed 2021-12-1.

Computational Data Analysis Workflow Systems

An incomplete list

See also: <https://github.com/pditommaso/awesome-pipeline>

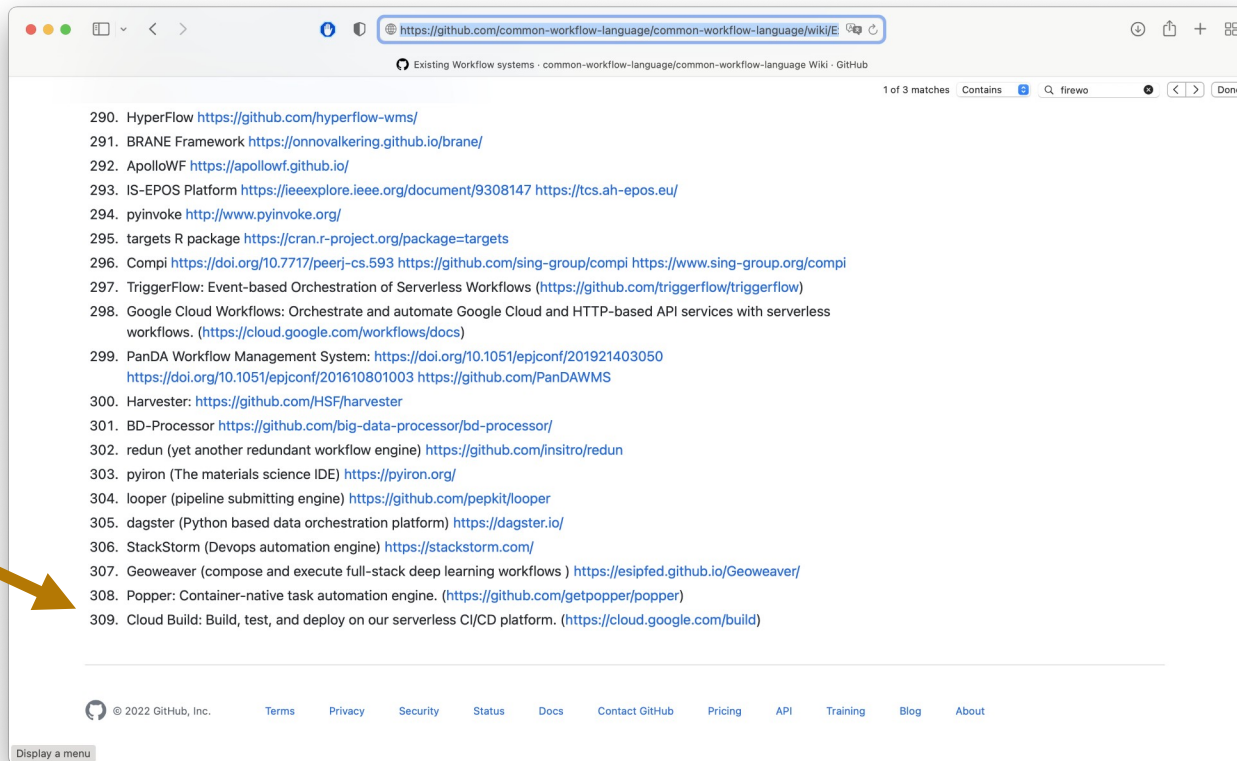
1. Arvados - CWL-based distributed computing platform for data analysis on massive data sets. <https://arvados.org/>
<https://github.com/arvados/arvados>
2. Apache Taverna <http://www.taverna.org.uk/> <https://taverna.incubator.apache.org/>

Pages (24)

- Home
- 2021 CWL Mini Conference
- 2022 CWL Conference
- Arvados
- Common Workflow Language != Kile TexStudio "completion word list"
- Conference Video Guidelines
- CWL Implementations
- CWL v1.2.1 "Barn Raising"

Workflow management systems

... of 309 entries (!?)



<https://github.com/common-workflow-language/common-workflow-language/wiki/Existing-Workflow-systems>

Why so many?

2009 - Curcin - Scientific workflow system...
Page 2 of 10

Scientific workflow systems - can one size fit all?

V. Curcin, M. Ghanem
Department of Computing
Imperial College London
180 Queen's Gate, London SW7 2AZ
Email: vc100@doc.ic.ac.uk, mmg@doc.ic.ac.uk

Abstract—The past decade has witnessed a growing trend in designing and using workflow systems with a focus on supporting the scientific research process in bioinformatics and other areas of life sciences. The aim of these systems is mainly to simplify access, control and orchestration of remote distributed scientific data sets using remote computational resources, such as EBI web services. In this paper we present the state of the art in the field by reviewing six such systems: Discovery Net, Taverna, Triana, Kepler, Yawl and BPEL.

We provide a high-level framework for comparing the systems based on their control flow and data flow properties with a view of both informing future research in the area by academic researchers and facilitating the selection of the most appropriate system for a specific application task by practitioners.

I. INTRODUCTION

```
graph LR; WS[Web source] --> S[Staging]; WS --> I[Integration]; NCB[NCBI/EMBL] --> P[Pre-processing (data-parallel)]; S --> I; I --> TS[Training set]; P --> TS; TS --> M[Modelling]; M --> T[Test set]; T --> V[Validation]; V --> ST[Storage]
```

Fig. 1. Workflow example

workflows system (scientific or non-scientific) can be relied on to cover the scope of requirements from different domains.

This paper approaches the problem by analysing leading scientific and non-scientific workflow systems, exposing their handling of control and data constructs, with the view of informing future research and also facilitating the selection of the most appropriate system for a specific application task.

As a start, Discovery Net [1] system will be presented to illustrate the architectural and implementation complexity associated with a full workflow system. Then, three other main scientific workflow systems, Taverna [2], Triana [3] and Kepler [4], will be described, followed by two workflow languages aiming to be a generic solution across both business and scientific domains. First of those, YAWL [5] is a theoretical workflow system based on the Petri Net paradigm that has been designed to satisfy the full set of workflow patterns, under the assumption that this will satisfy the needs of both communities. Second, BPEL [6] is the accepted standard for business process orchestration, with several attempts being made to adapt it for use in scientific settings, most notably by the OMII initiative [7].

Informally, a workflow, Figure 1, is an abstract description

Why so many?

2009 - Curcin - Scientific workflow system...
Page 2 of 10

Scientific workflow systems - can one size fit all?

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We provide a high-level framework for comparing the systems based on their control flow and data flow properties with a view of both informing future research in the area by academic researchers and facilitating the selection of the most appropriate system for a specific application task by practitioners.

I. INTRODUCTION

Fig. 1. Workflow example

Informally, a workflow, Figure 1, is an abstract description of a workflow system (scientific or non-scientific) capable of covering the scope of requirements from different scientific and non-scientific workflow systems, handling of control and data constructs, with informing future research and also facilitating of the most appropriate system for a specific application.

As a start, Discovery Net [1] system will illustrate the architectural and implementation associated with a full workflow system. Then, the scientific workflow systems, Taverna [2], Triana [4], will be described, followed by two workflow systems aiming to be a generic solution across both scientific domains. First of those, YAWL [5] is a workflow system based on the Petri Net paradigm under the assumption that this will satisfy the communities. Second, BPEL [6] is the accepted business process orchestration, with several adaptations made to adapt it for use in scientific settings, by the OMII initiative [7].

en.wikipedia.org/wiki/...

Betteridge's law of headlines - Wikipedia

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Article | Talk | Read | Edit | View history | Search Wikipedia

WIKIPEDIA
The Free Encyclopedia

Betteridge's law of headlines

From Wikipedia, the free encyclopedia

Betteridge's law of headlines is an **adage** that states: "Any headline that ends in a question mark can be answered by the word *no*." It is named after Ian Betteridge, a British technology journalist who wrote about it in 2009, although the principle is much older.^{[1][2]} It is based on the assumption that if the publishers were confident that the answer was *yes*, they would have presented it as an assertion; by presenting it as a question, they are not accountable for whether it is correct or not. The adage does not apply to questions that are more open-ended than strict **yes-no questions**.^[3]

Contribute | Help | Learn to edit | Community portal

Curcin, Vasa & Ghanem, Moustafa. (2009). Scientific workflow systems - Can one size fit all?. Cairo Int Biomed Eng Conf. 2008. 1 - 9. 10.1109/CIBEC.2008.4786077.

In this session

we will give you an overview of tools

- ◆ Relevant to the HPC environments (not cloud, K8s, Hadoop, etc.)
- ◆ Standalone (not language-specific libraries)
- ◆ With a simple DSL (no XML or other convoluted language)
- ◆ General purpose (not reserved to 'omics' for instance)
- ◆ Mature, active community, easy to install

Simple types of workflows

wide

workflows



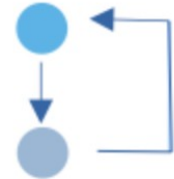
deep

workflows



cyclic

workflows





atools

The screenshot shows a web browser displaying the atools documentation. The page title is "atools (Job array tools) documentation". The main heading is "Welcome to the atools (Job Array Tools) documentation". The text explains that atools is designed for job arrays and lists typical scenarios like performing the same computation on many input files or running algorithms with different parameter sets. It also mentions supported queue systems like PBS torque, Moab, and Slurm.

```
alpha,beta
0.5,-1.3
0.5,-1.5
0.5,-1.9
0.6,-1.3
...
```

```
#!/bin/bash
...
alog --state start
source <(aenv --data data.csv)
Rscript bootstrap.R $alpha $beta
alog --state end --exit $?
```

```
1 started by r1i1n3 at 2016-09-02 11:47:45
2 started by r1i1n3 at 2016-09-02 11:47:45
3 started by r1i1n3 at 2016-09-02 11:47:46
2 failed by r1i1n3 at 2016-09-02 11:47:46: 1
3 completed by r1i1n3 at 2016-09-02 11:47:47
```

```
$ arange --data data.csv --log bootstrap.pbs.log10493`
```

<https://atools.readthedocs.io/en/latest/>

SlurmDagman

The screenshot shows the GitHub repository page for `SlurmDagman` by `AndresTanasijczuk`. The repository is public and has 13 commits, 3 branches, and 4 tags. The `Code` tab is selected, showing a file tree with `bin`, `etc`, `lib/SlurmDagman`, `LICENSE`, `README.md`, and `setup.py`. The `README.md` file is open, displaying the project name `SlurmDagman` and a description: "This application allows to run (the jobs in) a DAG with `Slurm` workload manager." The `Installation and configuration` section is partially visible, mentioning installation via `pip`. The right sidebar shows the `About` section with the description "Run the jobs in a DAG with Slurm.", the license `GPL-3.0 license`, and activity statistics: 0 stars, 1 watching, and 1 fork.

DAG file syntax

The syntax of the DAG file is similar to the one used in [HTCondor DAGMan](#). The following four constructs are recognized by SlurmDagman in a DAG file:

```
JOB dag-node slurm-submission-file
VARS dag-node var-name=var-value [...]
RETRY dag-node max-retries
PARENT parent-dag-node[,...] CHILD child-dag-node[,...]
```

<https://github.com/AndresTanasijczuk/SlurmDagman>

Makeflow



The screenshot shows a web browser window displaying the 'Makeflow - CCTools Documentation' page. The page title is 'CCTools Documentation' and the breadcrumb is 'Software » / Makeflow'. The main content area features the 'Makeflow' logo in a large, bold, black serif font, followed by a diagram of a workflow graph with blue and green nodes and arrows. Below the logo is the section 'Makeflow User's Manual' with a sub-section 'Overview'. The text in the overview describes Makeflow as a workflow engine for large-scale distributed computing, mentioning its fault-tolerance and ability to run on various computing environments like local laptops, university facilities, and commercial cloud systems.

```
capitol.anim.gif: capitol.jpg capitol.90.jpg capitol.180.jpg capitol.270.jpg capitol.360.  
LOCAL $(CONVERT) -delay 10 -loop 0 capitol.jpg capitol.90.jpg capitol.180.jpg capitol.  
  
capitol.90.jpg: capitol.jpg  
$(CONVERT) -swirl 90 capitol.jpg capitol.90.jpg  
  
capitol.180.jpg: capitol.jpg  
$(CONVERT) -swirl 180 capitol.jpg capitol.180.jpg  
  
capitol.270.jpg: capitol.jpg  
$(CONVERT) -swirl 270 capitol.jpg capitol.270.jpg  
  
capitol.360.jpg: capitol.jpg  
$(CONVERT) -swirl 360 capitol.jpg capitol.360.jpg  
  
capitol.jpg:  
LOCAL $(CURL) -o capitol.jpg $(URL)
```

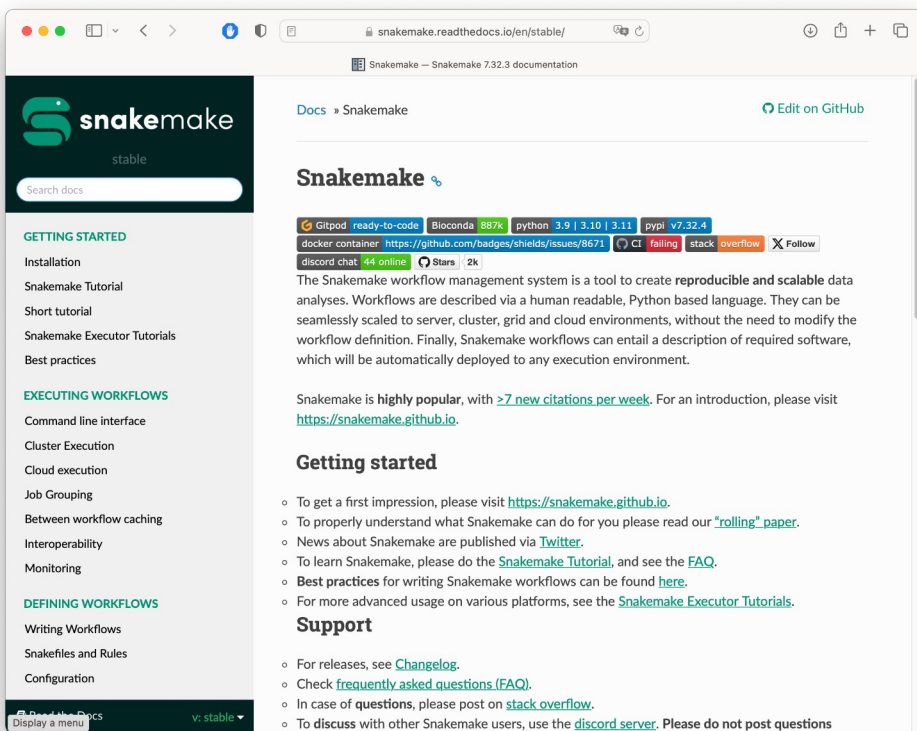
Use the `-T slurm` option to submit jobs to the **SLURM** batch system.

This will add the values for cores and memory. These values will be added onto `sbatch` in this format:

```
-N 1 -n 1 -c ${CORES} --mem=${MEMORY}M --time=${WALL_TIME_in_minutes}
```

<https://cctools.readthedocs.io/en/latest/makeflow/>

Snakemake



The screenshot shows the Snakemake documentation website. The header includes the Snakemake logo and the word 'stable'. A search bar is present. The left sidebar contains navigation links for 'GETTING STARTED', 'EXECUTING WORKFLOWS', and 'DEFINING WORKFLOWS'. The main content area is titled 'Snakemake' and includes a 'Getting started' section with a list of links and a 'Support' section with a list of links. The page also features a 'Docs' breadcrumb and an 'Edit on GitHub' link.

Docs » Snakemake [Edit on GitHub](#)

Snakemake

The Snakemake workflow management system is a tool to create **reproducible** and **scalable** data analyses. Workflows are described via a human readable, Python based language. They can be seamlessly scaled to server, cluster, grid and cloud environments, without the need to modify the workflow definition. Finally, Snakemake workflows can entail a description of required software, which will be automatically deployed to any execution environment.

Snakemake is **highly popular**, with **>7 new citations per week**. For an introduction, please visit <https://snakemake.github.io>.

Getting started

- To get a first impression, please visit <https://snakemake.github.io>.
- To properly understand what Snakemake can do for you please read our "[rolling paper](#)".
- News about Snakemake are published via [Twitter](#).
- To learn Snakemake, please do the [Snakemake Tutorial](#), and see the [FAQ](#).
- **Best practices** for writing Snakemake workflows can be found [here](#).
- For more advanced usage on various platforms, see the [Snakemake Executor Tutorials](#).

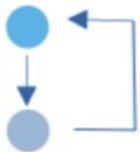
Support

- For releases, see [Changelog](#).
- Check [frequently asked questions \(FAQ\)](#).
- In case of **questions**, please post on [stack overflow](#).
- To discuss with other Snakemake users, use the [discord server](#). **Please do not post questions**

```
rule NAME:
  input: "path/to/inputfile", "path/to/other/inputfile"
  output: "path/to/outputfile", "path/to/another/outputfile"
  shell: "somecommand {input} {output}"
```

```
rule complex_conversion:
  input:
    "{dataset}/inputfile"
  output:
    "{dataset}/file.{group}.txt"
  shell:
    "somecommand --group {wildcards.group} < {input} > {output}"
```

<https://snakemake.readthedocs.io/en/stable/>



Cycl

cylc.github.io

Cycl | The Cycl Workflow Engine Production workflow orchestration for cycling systems

Cycl is a **general purpose workflow engine** that also orchestrates **cycling systems** very efficiently. It is used in production weather, climate, and environmental forecasting on HPC, but is not specialized to those domains.

Cycl is an active Open Source project on [GitHub](#). See [Cycl Publications and Reports](#) below.

Latest (Python 3)	Legacy (Python 2)
 cylc-flow-8.2.1	 cylc-7.9.8
Released: 14/08/2023	Released: 13/06/2023

Next Release: cylc-8.3.0 (8%)

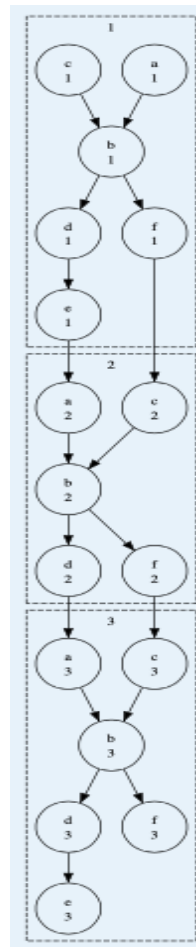
0% 100%

Cycl Does Cycling Properly

Cycl unwinds the cycle loop to get a dependency graph with no barrier between cycles. This allows interleaved cycles for:

- Fast catch-up from delays
- Sustained high throughput off the clock
- Seamless transitions between fast catch-up and clock-limited real-time scheduling

Why Use Cycl?



```
[scheduler]
    allow implicit tasks = True
[scheduling]
    cycling mode = integer
    initial cycle point = 1
[[graph]]
    P1 = """
        a & c => b => d & f
        f[-P1] => c # (1)
    """
    P2 = """
        d => e
        d[-P1] => a # (2)
    """
    2/P2 = """
        e[-P1] => a # (3)
    """
```

Micro-scheduling systems

to organise a large number of tasks in a small number of jobs
a selection

HyperQueue

<https://github.com/It4innovations/hyperqueue>

The logo for the Flux scheduler, featuring the word "flux" in a blue, italicized serif font. To the left of the text is a circular icon composed of several concentric, slightly offset rings, resembling a target or a stylized globe.

<https://hpc-tutorials.llnl.gov/flux/>

Full-featured systems

that offer a web interface, data management, etc.
a selection

Name	Website	Domain
Fireworks	https://materialsproject.github.io/fireworks/	Material science
Nextflow	https://nextflow.io	Bioinformatics
Merlin	https://merlin.readthedocs.io/	Machine learning
DAGMan	https://htcondor.readthedocs.io/	Particle physics
Pegasus	https://pegasus.isi.edu/	Agnostic

Further reading

Deelman, Ewa & Gannon, Dennis & Shields, Matthew & Taylor, Ian. (2009). **Workflows and e-Science: An overview of workflow system features and capabilities.** *Future Generation Computer Systems*. 25. 524-540. 10.1016/j.future.2008.06.012.

Liu, Ji & Pacitti, Esther & Valduriez, Patrick & Mattoso, Marta. (2015). **A Survey of Data-Intensive Scientific Workflow Management.** *Journal of Grid Computing*. 13. 10.1007/s10723-015-9329-8.

Badia, Rosa M. & Ayguade, E. & Labarta, Jesús. (2017). **Workflows for science: a challenge when facing the convergence of HPC and Big Data.** *Supercomputing Frontiers and Innovations*. 4. 27-47. 10.14529/jsfi170102.

Ferreira da Silva, Rafael & Figueira, Rosa & Pietri, Ilia & Jiang, Ming & Sakellariou, Rizos & Deelman, Ewa. (2017). **A characterization of workflow management systems for extreme-scale applications.** *Future Generation Computer Systems*. 75. 10.1016/j.future.2017.02.026.

Deelman, Ewa & Peterka, Tom & Altintas, Ilkay & Carothers, Christopher & Dam, Kerstin & Moreland, Kenneth & Parashar, Manish & Ramakrishnan, Lavanya & Taufer, Michela & Vetter, Jeffrey. (2017). **The future of scientific workflows.** *The International Journal of High Performance Computing Applications*. 32. 109434201770489. 10.1177/1094342017704893.