Introduction to Workflow Description Language (WDL)



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Reproducing, validating, and extending analyses is essential to science

But reproducing a computational analysis is hard!

- How do I install the software and its dependencies?
- Am I using all the same versions of the software?
- Why is this script in Python and that script in R?
- Can I know that this runs exactly the same on my computer vs my colleague's?



Workflow languages were designed to help

Consistency / Reproducibility

- Across batches
- Across users
- Across platforms

Ease of use:

- Reduces user error
- Helps you scale up to easily process thousands of samples



Workflows are a community resource

There are thousands of workflows published in the community repository, <u>Dockstore.org!</u>

Sharing your workflows with the community:

- Centralizes knowledge
- Builds community resources
- Helps you get feedback
- Makes your scientific method citable
- Gives you metrics to include in proposals





A draft human pangenome reference

Wen-Wei Liao, Mobin Asri, Jana Ebler, Daniel Doerr, Marina Haukness, Glenn Hickey, Shuangjia Lu, Julian K. Lucas, Jean Monlong, Haley J. Abel, Silvia Buonaiuto, Xian H. Chang, Haoyu Cheng, Justin

Chu, Vincenz

Garg, Cristia Phased assembly pipeline

+ Show a

We describe the main automated and manual steps taken before, during and after assembly. A

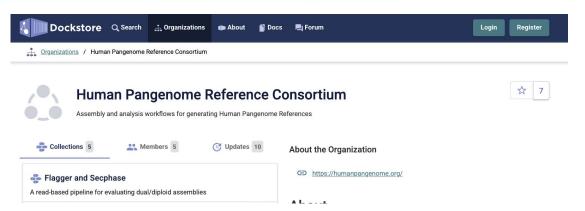
Nature 617,

combined set of workflow description language (WDL) formatted assembly workflows is

286k Acces

available from **Dockstore** that captures each of the steps for filtering adapter-contained reads and running Hifiasm

(https://dockstore.org/organizations/HumanPangenome/collections/Hifiasm). All





Which workflow language should I use?

Workflow Description Language (WDL), Common Workflow Language (CWL), Nextflow, Snakemake...they are all helpful!

What workflows are available already that are similar to my analysis?

- Check out <u>Dockstore.org</u> for workflows shared by the community.

What language are my colleagues using?

You have community to learn from!



Workflow Description Language (WDL)



- A language to describe the steps of an analysis
- Created to be human readable and easy to write
- Bioinformatics / genomics focus due to it being developed by the Broad Institute (but can be used for any data science)
- Open source, community-developed (by OpenWDL)



What WDL is NOT



- Not a programming language
- Not a tool that does analysis
- Not a GUI or platform
- Not just for Broad pipelines
- Not an alternative to containers or scripting languages





Container



Descriptor file (.wdl)



Parameter file



Cromwell







Descriptor file (.wdl)



Parameter file



Cromwell



Intro to containers



- Packaged up tools and all of its dependencies
- Makes software portable from one computing environment to another.

- Docker is commonly used by cloud platforms
- Singularity is common for HPCs because it doesn't require root permissions

Check out <u>BioContainers.pro</u> from the BioConda community. They also automate releasing Singularity containers for reuse by the community in workflows.





Container



Descriptor file (.wdl)



Parameter file



Cromwell



Intro to workflow descriptor files



This file describes your software commands as "tasks", specifying inputs, outputs, and the environment (container).

Tasks are organized together to create workflows.

```
task task A {
    File ref
    File in
    String id
  command {
   do stuff -R ${ref} -I ${in} -O ${id}.ext
  runtime {
   docker: "my project/do stuff:1.2.0"
  output {
   File out= "${id}.ext"
```



Review: Workflow Description Language (WDL)

```
version 1.0
                                                                 version 1.0
                                                                 workflow MyWorkflowName {
workflow MyWorkflowName {
                                                                     input {
                                                                      File my ref
                                                                      File my input
                                                                      String name
task task A {
                                                                     call task A {
                                                                      input:
                                                                        ref = my ref
                                                                        in = my input
                                                                        id = name
task task B {
                                                                     call task B
                                                                      input:
                                                                        in = task A.out name A
                                                                     output {
                                                                      out A = task A.out name A
                                                                      out B = task B.out name B
                                                                 task task A
```

Review: Workflow Description Language (WDL)

```
task task A {
version 1.0
workflow MyWorkflowName {
                                                                  input {
                                                                   File ref
                                                                   File in
                                                                   String id
task task A {
                                                                 do stuff -R ~{ref} -I ~{in} -O
                                                                 ~{id}.ext
task task B {
                                                                   docker: 'my_project/do_stuff:1.2.0'
                                                                   File out name A = "~{id}.ext"
                                                              task task B {
```

Review: Workflow Description Language (WDL)

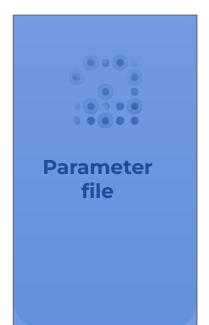
```
version 1.0
                                                                version 1.0
                                                                import /path/to/wdl/with/new wf.wdl as
workflow MyWorkflowName {
                                                                new wf
                                                                work
                                                                    input {
                                                                     File my ref
                                                                     File my input
                                                                     String name
task task A {
                                                                    call task A {
                                                                    call task B {
task task B {
                                                                    call new wf.task C {
                                                                     out A = task A.out name A
                                                                     out B = task B.out name B
                                                                     out C = task C.out name C
```



Container



Descriptor file (.wdl)







Workflow Inputs

Example Workflow

```
version1.0
workflow wf {
  input {
    Int int val
    Int int val2 = 10
    Array[Int] my ints
    File ref file
  String not an input = "hello"
  call t1 {
    input: x = int val
  call t2 {
    input: x = int val, t=t1.count
```

Example JSON Input

```
{
   "wf.int_val": 3,
   "wf.my_ints": [5,6,7,8],
   "wf.ref_file": "/path/to/file.txt"
}
```

- 1. Identify all workflow inputs.
- 2. For each input, determine the input type (str, int, etc).
- 3. Create a JSON file with key/value pairs for each workflow input.
 - a. Key format : <workflow name>.<input name>
- 4. Set the value of each key/value pair to the value of the workflow input.



Parameter file (json format)

Specifies inputs, outputs, and computing resources that are specific to your analysis. This is where you can specify cloud vs local environment logic.

```
hello.json
              KEY
                                                     VALUE
 "hello_world.hello.myName": "/<usr>/bcc2020/wdl-training/exercise1/name.txt"
     workflow
                 task
                      parameter
                                        value can be path, string, int, array, etc
                 name
                        name
      name
```



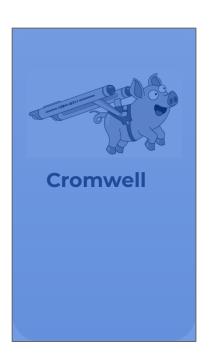
Container



Descriptor file (.wdl)

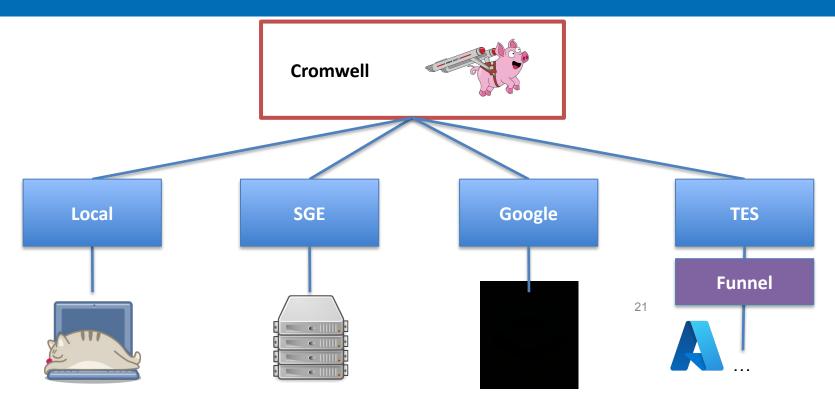


Parameter file





What is Cromwell



https://github.com/broadinstitute/cromwell

Two main ways to run Cromwell

One-off

Simple self-contained command

```
cromwell run \
  hello.wdl \
  --inputs hello_inputs.json
```

 Appropriate for independent analysts

Server mode

- API endpoints
- More scalable
- Some devops needs
- Appropriate for production environments
- Call-caching! (aka ka-ching")







Steps to running a WDL in standalone mode

Validate syntax

womtool validate hello.wdl

Generate inputs JSON

womtool inputs hello.wdl > hello_inputs.json

• Run

cromwell run hello.wdl --inputs hello_inputs.json





Resources for getting started

Resource	Link
OpenWDL GitHub	https://github.com/openwdl/wdl
WDL 1.0 Spec	https://github.com/openwdl/wdl/blob/main/versions/1.0/SPEC.md
WDL 1.0 Docs (wdl-docs)	https://wdl-docs.readthedocs.io/en/stable/
WDL Cookbook	https://wdl-docs.readthedocs.io/en/stable/WDL/chain_tasks_together/
Learn-WDL Videos	https://github.com/openwdl/learn-wdl
WARP WDL Best Practices	https://broadinstitute.github.io/warp/docs/Best_practices/GC_cost_optimization
OpenWDL Slack	https://openwdl.slack.com/
Examples in WARP (WDL Analysis Research Pipelines; Terra-optimized)	https://broadinstitute.github.io/warp/
Theiagen Genomics WDL Workshop	https://github.com/theiagen/wm_training_202205
Task examples in BioWDL	https://biowdl.github.io/

Questions?

