

# **Dockstore:**

Enhancing a community platform for sharing cloud-agnostic research tools

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## What is Dockstore?

Dockstore is a free and open source platform for sharing scientific tools and workflows. It is a registry of Docker-based resources described using popular workflow languages CWL, WDL, and Nextflow.

## Portability

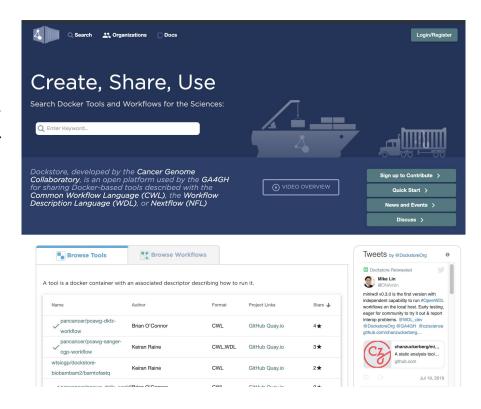
 Run workflows in any environment that supports Docker

## Interoperability

 Standardize computational analysis through GA4GH APIs

## Reproducibility

- o Create, Share, Use
- Containers + Popular descriptor languages



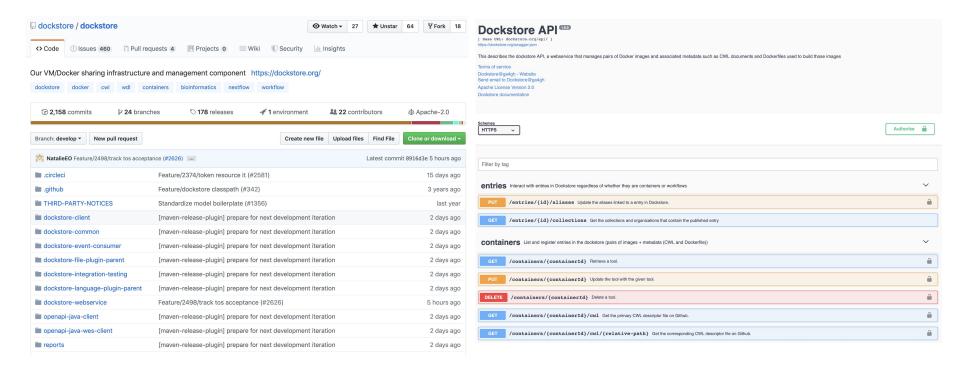
Now on version 1.6.0, first presented version 1.25 at BOSC2017





## What is Dockstore?

## https://dockstore.org/



Github: <a href="https://github.com/dockstore/dockstore">https://github.com/dockstore/dockstore</a>

Swagger: https://dockstore.org/api/static/swagger-ui/index.html#



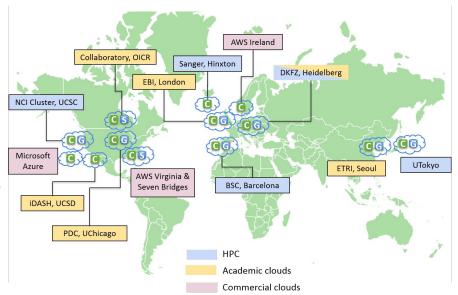


# **Motivations for Dockstore:**

The Pan Cancer Analysis of Whole Genomes (PCAWG)

**Cloud-Based, Distributed Collaboration** 

- International Cancer Genome Consortium (ICGC)
- ~5,800 Whole Genomes
- 8 sites storing and sharing data via GNOS
  - 300TB -> 900TB
- 14 Cloud (and HPC) environments
  - 3 Commercial, 7 OpenStack, 4 HPC
  - ●~630 VMs, ~15K cores, ~60TB of RAM











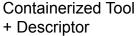


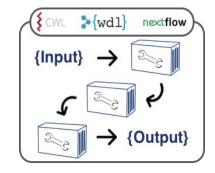
# GA4GH Tool Registry Service (TRS) API

The Global Alliance for Genomics and Health (GA4GH) Tool Registry API standard for listing and describing available tools for exchange, indexing, and searching.

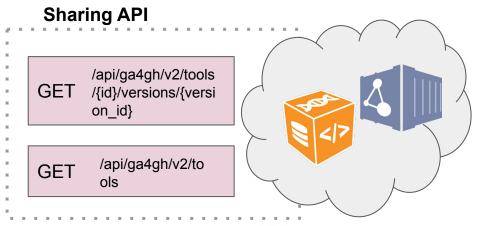
- Stand alone containerized tools
- Workflows with multiple tools wrapped in descriptor languages (Common Workflow Language, Workflow Descriptor Language, Nextflow)







Workflow: Tools + Descriptor



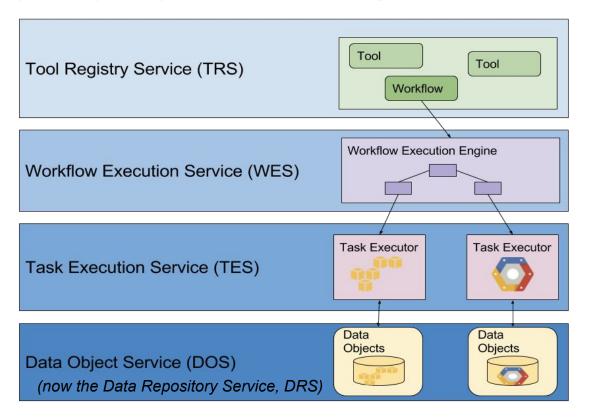
- GitHub page: <a href="https://github.com/ga4gh/tool-registry-service-schemas">https://github.com/ga4gh/tool-registry-service-schemas</a>
- Latest draft release: 1.0.0, working on 2.0.0 now







# **GA4GH Cloud Work Stream APIs**



**Sharing Tools and Workflows** 

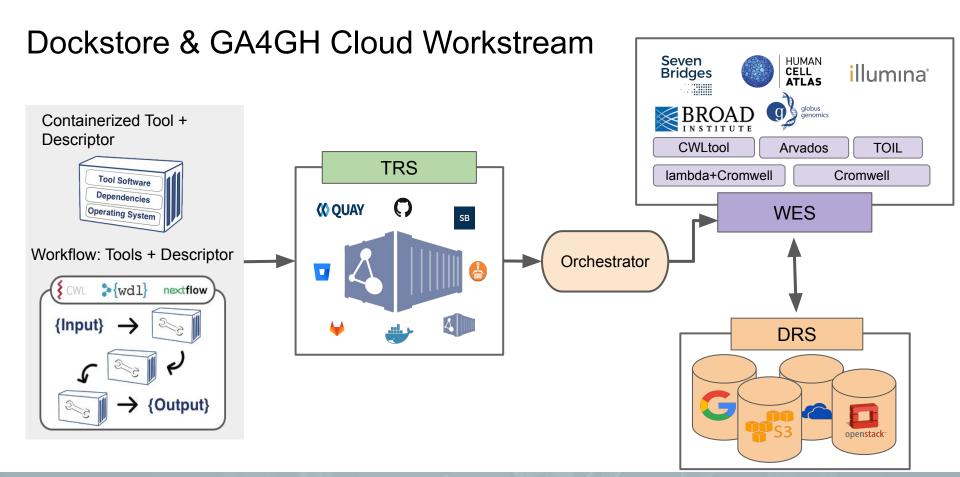
**Executing Workflows** 

**Executing Tasks** 

**Accessing Data** 











# Dockstore, going beyond TRS

- GA4GH TRS API
  - Standardized subset of Dockstore and Biocontainers
  - We provide a <u>validator</u> to help those implementing TRS
- Dockstore API
  - Extends TRS with functionality specific to Dockstore
    - Catalog that brings together multiple external repositories
    - Authenticated access
    - Advanced language support
    - Launch analysis
    - Community and collaboration oriented features
      - Organizations, starring, platform verification

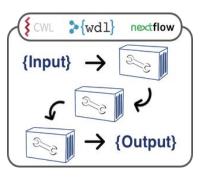


# Containers, Descriptors, and Parameter Files

**Tool**: Container + Descriptor



**Workflow**: Tool(s) + Descriptor



## **Descriptor:**

The workflow language used to describe how to run your tool or workflow/pipeline.

- Which tools/containers
- What steps and when
- Where I/O parameters
- How to allocate compute requirements
- Can also include metadata information







## Parameter File (wdl, cwl):

- Specifics the actual input/output files and where to find them (local, ftp, http, or cloud)
- JSON, YAML

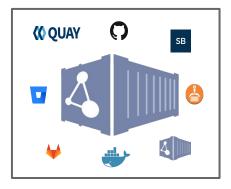
```
"bam input": {
        "class": "File".
        "format": "http://edamontology.org/format
2572",
        "path": "/tmp/NA12878.chrom20.ILLUMINA.bw
a.CEU.low coverage.20121211.bam"
    "bamstats report": {
        "class": "File".
        "path": "/tmp/bamstats_report.zip"
```

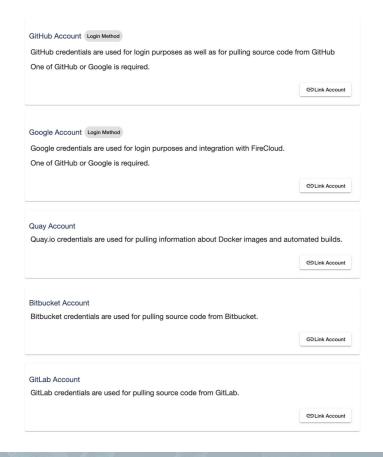




# Dockstore as a Registry

- Searchable and Centralized Catalogue
- Many ways to get your tool or workflow into Dockstore!
  - External Hosting: Github, Bitbucket,
     Quay.io, Docker Hub
  - Direct Hosting (currently just workflows)

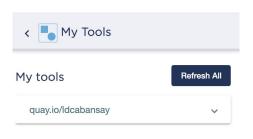




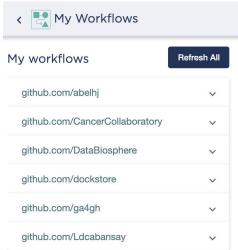




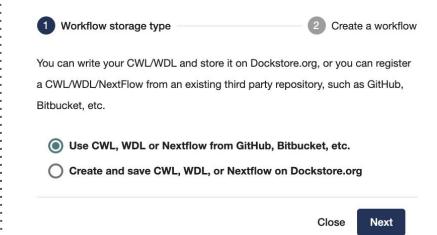
## Ways to Register to Dockstore



Through linked account via supported public APIs



## **Register Workflow**

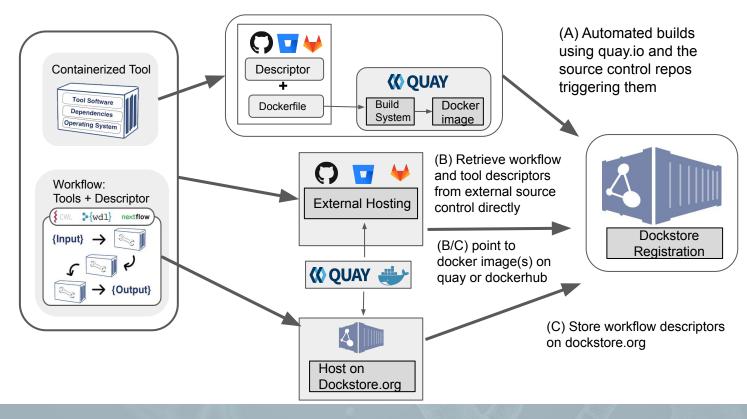


OR through manual registration pointing to external source repo or directly on Dockstore.org





## Ways to Register to Dockstore







# Containers and Descriptor Languages

- Containers
  - Docker
- Descriptor Language Support
  - CWL, WDL, and now Nextflow!
    - Syntax Highlighting, Validation
    - Visualization
      - Including additional visualization options from <u>view.commonwl.org</u> and EPAM WDL Viewer
    - Metadata parsing
      - Authorship, contact info, description
      - Markdown syntax (CWL, WDL)
      - I/O Filetypes (CWL)



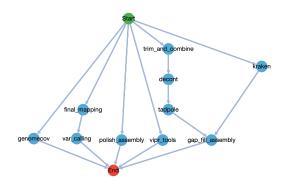


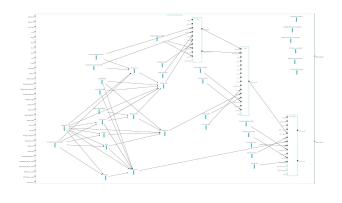






# **Visualizations**





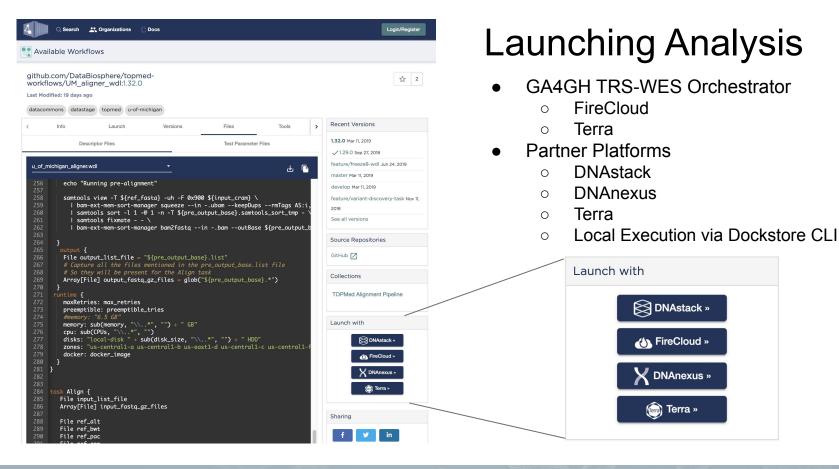
Built-in for CWL, WDL, and Nextflow (pictured)

<u>view.commonwl.org</u> for CWL

**EPAM Pipeline Builder for WDL** 









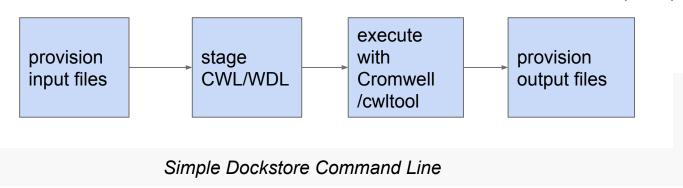


## **Dockstore CLI**

A handy command line resource for developers to play with tools/workflows locally before running them on a cloud

- DRS file provisioning
- WES beta support
- Locally
  - Cromwell
  - Cwltool

Execution with the Dockstore Command Line Interface (CLI)







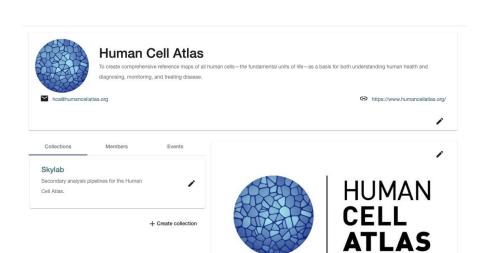
# Organizations and Collections

## Organizations

- A place for groups, labs, consortiums, etc to showcase their projects, collaborate, and group sets of tools/workflows into 'collections'
- Markdown descriptions
- Membership roles

## Collections

- Playlist of workflows or tools highlighted by an Organization
- Markdown descriptions



## ABOUT HUMAN CELL ATLAS

In London on 13 and 14 October, 2016, a collaborative community of world-leading scientists met and discussed how to build a Human Cell Atlas—a collection of maps that will describe and define the cellular basis of health and disease.

Cells are the most fundamental unit of life, yet we know surprisingly little about them. They vary enormously within the body, and express different sets of genes. Without maps of different cell types and where they are located in the body, we cannot describe all their functions and understand the biological networks that direct their activities.

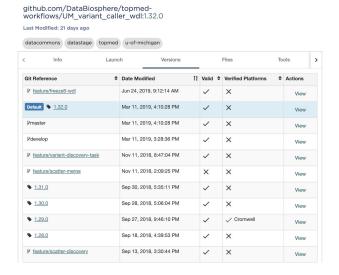
A complete Human Cell Atlas would give us a unique ID card for each cell type, a three-dimensional map of how cell types work together to form tissues, knowledge of how all body systems are connected, and insights into how changes in the map underlie health and disease. It would allow us to identify which genes associated with disease are active in our bodies and where, and analyze the regulatory mechanisms that govern the production of different cell types.

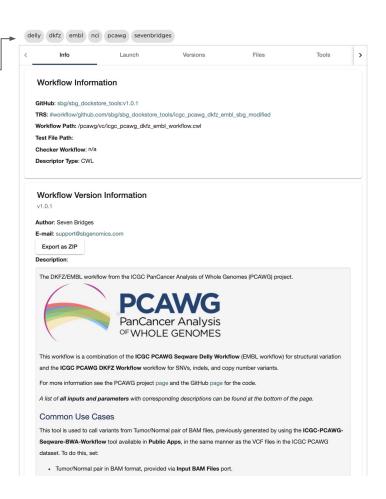




# Usability Improvements

- Improved Published Tool/Workflow Interface
  - Labels improve searchability
  - Metadata and markdown display
    - Authorship, contact info, descriptions
    - Readme like descriptions (CWL, WDL)
  - Versioning: display all tags/versions, set defaults, check validity, verify compatible platforms
  - Link to checker workflow



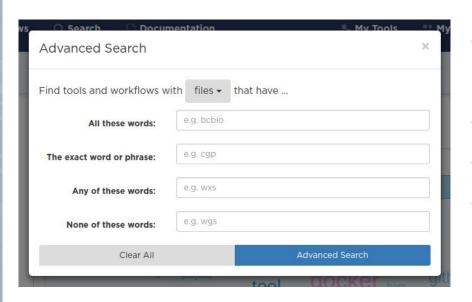


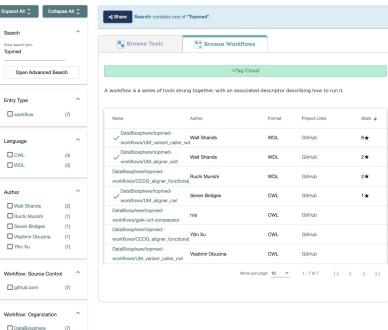


# **Usability Improvements**

## Search Interface

- Search name, author, organization, descriptor, etc
- Filter results using facets
  - Descriptor Language
  - Labels







# SANTA CHIPORNA GENOMICS

# **Usability Improvements**

- Lots of new documentation and tutorials!
- Example Topics:
  - Getting Started With...(Docker, Nextflow, CWL, WDL)
  - Launching Tools and Workflows
  - Writing checker workflows
  - Developing File Provisioning Plugins
  - Creating Organizations
  - And many more!

https://docs.dockstore.org/

## **Developer Tutorial**

Go through the process of creating a tool and registering it on Dockstore.

## **End User Tutorials**

Learn how to use Dockstore from the perspective of a user who runs tools and workflows.

## Advanced Tutorials

A collection of articles and tutorials regarding advanced Dockstore topics

Documentation / Advanced Developer / Organizations and Collections

## Organizations and Collections

## Organizations

Organizations are landing pages for collaborations, institutions, consortiums, companies, etc. that allow users to showcase tools and workflows. This is achieved through the creation of collections, which are groupings of related tools and workflows in any way; the tools and workflows in any way; the tools and workflows in any way; the tools and workflows just have to be published. Collections can be thought of as a playlist on a music streaming service where tools and workflows are analogous to individual songs. They can be shared publicly, and the user does not need to

### Creating an organization

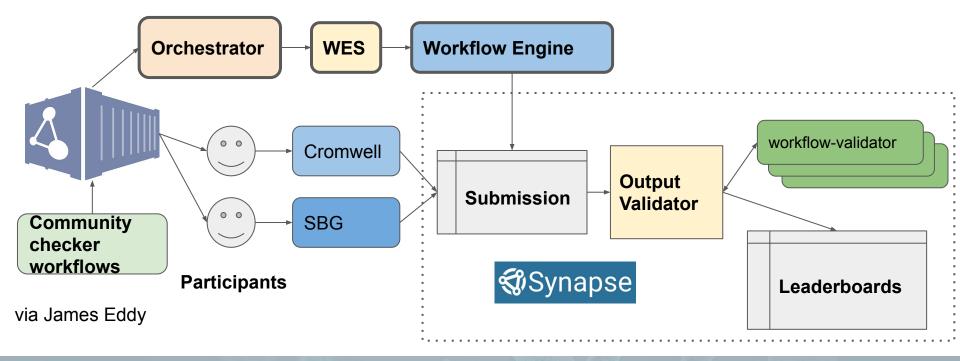
To create an organization request, go to the organizations page and select <a href="Create Organization Request">Create Organization Request</a>. Any user can request to create an organization by filling out the following form. For now, the request must be approved by a Dockstore curator in order to be public. Until it is approved, you are still able to edit it, add collections, add members, etc.

Create Organization Request
Fill out the form to send an organization request to a Dockstore curator to
approve. Once approved, the organization will be publicly visible.
Name *
OICR
The name of the organization Display Name *
Ontario Institute for Cancer Research
The display name of the organization Topic *
OICR is a collaborative, not-for-profit research institute accelerating the development of
A short description of the organization Organization website
https://oicr.on.ca/
Link to organization website Location



# Highlighted Community Content

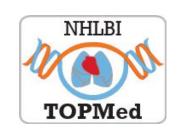
GA4GH-DREAM Workflow Testbed (2018)







# Collaborations - The Commons Alliance and Other Projects





NHLBI Data STAGE





NHGRI AnVIL









**And Many Others** 

Dockstore will serve as an official workflow provider for the Commons Alliance, a common infrastructure collaboration to facilitate combining **Data + Cloud Compute** 





# Next Release - 1.7.0 (Late August/September)

- Prototype for services/apps
  - Dockerized genome browsers, jupyter notebooks, and reference data providers
  - Playground for Github Apps and automatic update syncing
- Immutable workflow versions
  - DOI issuing via linked Zenodo credentials
- Language support updates
  - WDL draft-3 to 1.0
  - cwltool update (possibly CWL 1.1 support)
- Display of logs from when we test and verify workflows
- Improved security of your data and logging, monitoring of the site
- Summary of changes at <a href="https://docs.dockstore.org/changelog/">https://docs.dockstore.org/changelog/</a>

## Future Work

- Signing of Entries on Dockstore
  - Verify ownership and integrity of Docker images
- Alternative Containerization Support
  - Singularity and/or uDocker support
- Additional Workflow Languages
- Services/"Apps"
- Testbed Expansion
  - Automated testing for workflows across cloud platforms
- Open to collaborations with partners for any of these kind of projects!



# The Dockstore Team



Lincoln Stein

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Andrew Duncan

Gary Luu



Brian O'Connor

Benedict Paten

Cricket Sloan

**Charles Overbeck** 

Walt Shands

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Louise Cabansay

Natalie Alvarez

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Melaina Galaspie

Shreya Radesh

**Emily Soth** 

# Acknowledgements



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## Funded by:







# Extra Slides

Handy stuff in case of questions





# Language Support

## More info:

https://docs.dockstore.org/docs/user-t utorials/language-support/

Tool registration  Yes  Workflow registration  Yes  Yes  Yes  Yes  Yes  Yes  And  Yes  Yes  Yes  Yes  Yes  Yes  Yes  Ye	Feature	CWL	WDL	Nextflow		
Workflow registration Yes Yes Yes Yes Yes Yes Add Vorkflows Yes (cwl version=>1.0) [0] Yes (wdl version<=draft-2) [1] Limited support Yes (cwl version=>1.0) Yes (wdl version<=draft-2) Yes  Launch-with Platforms Not yet! FireCloud (workflows only) [2] DNAstack (workflows only) [3] DNAnexus (workflows only) Terra (workflo	Dockstore site					
Hosted Workflows  Yes  Yes  Yes  Yes  Yes  Yes  Yes  AGD Display  Yes (cwl version=>1.0) [0]  Yes (wdl version<=draft-2) [1]  Limited support  Yes  Yes  Yes  Yes  Yes  Yes  Yes  Ye	Tool registration	Yes	Yes	No		
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Tool Tab Display  Yes (cwl version=>1.0)  Yes (wdl version<=draft-2)  Launch-with Platforms  Not yet!  FireCloud (workflows only) <sup>[2]</sup> DNAstack (workflows only)  Terra (workflows only)  Metadata Display  Yes  Yes  Yes (wdl version<=draft-2)  Yes  Pockstore CLI  Local workflow engines  Cwltool, Cromwell  Cromwell [4]  Nextflow  File Provisioning In  Local File System HTTP HTTP FTP S3 via plugins Data Object Service  Plugins Support  S3  S3  S3  Plugins System HTTP Data Object Service  File Provisioning Out  Local File System HTTP HTTP S3 via plugins Data Object Service  Data Object Service  Local File System  Local File System  No  S3  S3  No  Local File System  S3  Local File System  S3  Local File System  S3  Local File System	Hosted Workflows	Yes	Yes	Yes		
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DNAstack (workflows only) DNAnexus (workflows only) Terra (workflows only) Terra (workflows only)  Metadata Display Yes Yes (wdl version<=draft-2) Yes  Dockstore CLI  Local workflow engines  Cwltool, Cromwell Cromwell [4] Nextflow  File Provisioning In Local File System HTTP HTTP FTP S3 via plugins Data Object Service Plugins Support  S3 S3 S3 S3 S3 S3 Md icgc-get Data Object Service Data Object Service  File Provisioning Out Local File System HTTP FTP S3 via plugins Local File System Local File System No Local File System HTTP FTP S3 via plugins Local File System HTTP FTP S3 via plugins Local File System HTTP FTP S3 via plugins Local File System Local File System Local File System S3 Local File System S3 S3 S3 S3 S3 S3 S4 S5 S5 S5 S6 S6 S7 S7 S7 S7 S8	Tool Tab Display	Yes (cwl version=>1.0)	Yes (wdl version<=draft-2)	Yes		
Dockstore CLI  Local workflow engines	Launch-with Platforms	Not yet!	DNAstack (workflows only) <sup>[3]</sup> DNAnexus (workflows only)	Not yet!		
Local workflow engines  cwltool, Cromwell  Cromwell [4]  Nextflow  File Provisioning In  Local File System HTTP HTTP FTP S3 via plugins Data Object Service  Plugins Support  s3 s3cmd icgc-get Data Object Service  Data Object Service  File Provisioning Out  Local File System HTTP  BTP S3 via plugins Data Object Service  Data Object Service  Data Object Service  Local File System HTTP FTP S3 via plugins  Local File System HTTP FTP S3 via plugins	Metadata Display	Yes	Yes (wdl version<=draft-2)	Yes		
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HTTP S3 via plugins S3	Plugins Support	s3cmd icgc-get	s3cmd icgc-get	No		
Notifications Yes Yes No	File Provisioning Out	HTTP FTP	Local File System	-		
	Notifications	Yes	Yes	No		

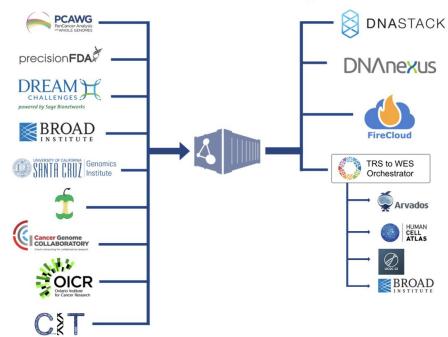




# Dockstore Ecosystem

Dockstore is thankful to its many contributors, users, and partners. This community has pulled together a library of over 450 tools and workflows. In the diagram to the right we've highlighted a few select contributors to give a sense of what has been occuring in this space.

## Select Contributors and Integrations







## Importing from Dockstore

github.com/DataBiosphere/topmed-workflows/UM\_variant\_caller\_wdl

Please note: Dockstore cannot guarantee that the WDL and Docker image referenced by this Workflow will not change. We advise you to review the WDL before future runs.

```
import "https://raw.githubusercontent.com/DataBiosphere/topmed-workflows"
    ## This is the U of Michigan variant caller workflow WDL for the workflo
    ## https://github.com/statgen/topmed_freeze3_calling
     ##
    ## It uses a Docker image built with software tools that can reproduce
    ## variant calls compatible to TopMed Freeze 3a
    ## NOTE: This workflow assumes that input CRAM files have been built wit
    ## human reference genome. In particular for the TopMed CRAM files the
11
    ## reference genome files to use are located here:
    ## ftp://share.sph.umich.edu/gotcloud/ref/hs38DH-db142-v1.tgz
13
14
     ##
15
16
    workflow TopMedVariantCaller {
17
18
      Boolean? calculate_DNA_contamination
      Boolean calculate_contamination = select_first([calculate_DNA_contamin
19
20
      Boolean? dynamically_calculate_file_size
21
      Boolean dynamically_calculate_disk_requirement = select_first([dynamic
```

## **Destination Workspace**

Select a workspace Or create a new workspace





# Running Dockstore Tools - Launch With FireCloud

**FireCloud** 

Workspaces

Data Library

Method Repository



## Importing github.com/DataBiosphere/topmed-workflows/Functional\_Equivalence:1.30.0 from Dockstore

A Please note: Dockstore cannot guarantee that the WDL and Docker image referenced by this Workflow will not change. We advise you to review the WDL before future runs.

Functional_Equivalence	
Pestination Workspace	
Select a workspace	*

		Copyright Broad Institute, 2017
2		
		This WDL pipeline implements CCDG Pipeline standards to process
		high-throughput sequencing data for downstream processing.
5		
		Requirements/expectations :
		- Human whole-genome pair-end sequencing data in unmapped BAM (uBAM) format
		- One or more read groups, one per uBAM file, all belonging to a single sample (SM)
		- Input uBAM files must additionally comply with the following requirements: filenames all have the same surfix (we use ".ummapoed.bam")
		literames at nave the same surix (we use "Jumapped.dam") files must pass validation by ValidatesamFile
		lites must pass vatitation by vatitatesaminite - reads mare provided in query-sorted order
		lads are provided an industry softed order
		act reads must have all No tay
15		
		Runtime parameters are optimized for Broad's Google Cloud Platform implementation.
		For program versions, see docker containers.
18		
		LICENSING:
		This script is released under the WDL source code license (BSD-3) (see LICENSE in
		https://github.com/broadinstitute/wdl). Note however that the programs it calls may
		be subject to different licenses. Users are responsible for checking that they are
		authorized to run all programs before running this script. Please see the docker
		page at https://hub.docker.com/r/broadinstitute/genomes-in-the-cloud/ for detailed
25	##	licensing information pertaining to the included programs.
26		
27	#	WORKFLOW DEFINITION
28	WO	rkflow PairedEndSingleSampleWorkflow {
29		
30		File wgs_evaluation_interval_list
31		File wgs_coverage_interval_list
32		
33		String sample_name
34		String base_file_name
35	Į.	Array[File] flowcell_unmapped_bams
200		



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