Tutorial: Design Patterns for Apps and Workflows

Contents

Introduction

This hands-on tutorial presents design patterns for collaborative bioinformatics using precisionFDA Apps and Workflows. There is a considerable range of design patterns for deploying code, marshalling data, and producing results, within precisionFDA's file and transient worker-driven (i.e. batch, non-interactive) application framework. This course will present this framework, including:

- Apps, their input/out specifications for files and other data types, virtual environment specification, and scripting
- Assets (i.e. tar archives) that can be bundled with assets and overlaid onto the worker's root volume
- Incorporation of Docker images into apps from file inputs and from assets
- Workflow creation using the web interface and WDL

Through the development of the tutorial artifacts, precisionFDA's powerful capabilities for secure collaborative development of bioinformatics tools, and sharing of -omics and RWD, are clearly demonstrated, and users will be empowered to develop their own bioinformatics use cases.

Learning Objectives

Through this hands-on tutorial you will:

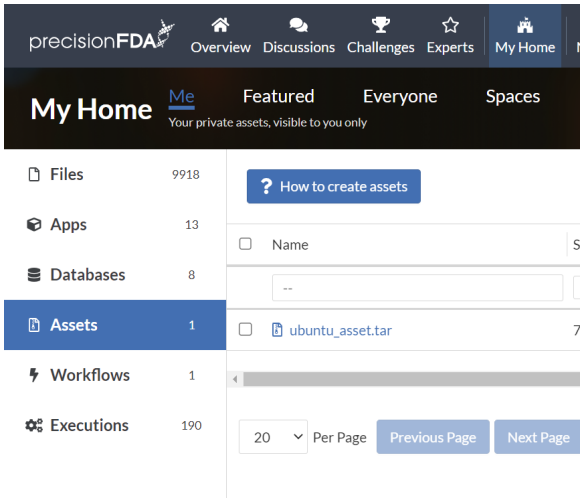
- Install the precisionFDA command line utility and use it upload and download files.
- Explore the multiple types of app inputs and outputs, assets, and their presentation to the app script as shell variables and files.
- Build a bioinformatics app from a biocontainers Docker image.
- Run the latest Ubuntu OS as a Docker image in an app.
- Use the precisionFDA Command Line Interface asset to process an arbitrary number of inputs or produce an arbitrary number of outputs to make up for the lack of an array data type.
- Create a workflow through the web interface.
- Create a workflow through by importing WDL.

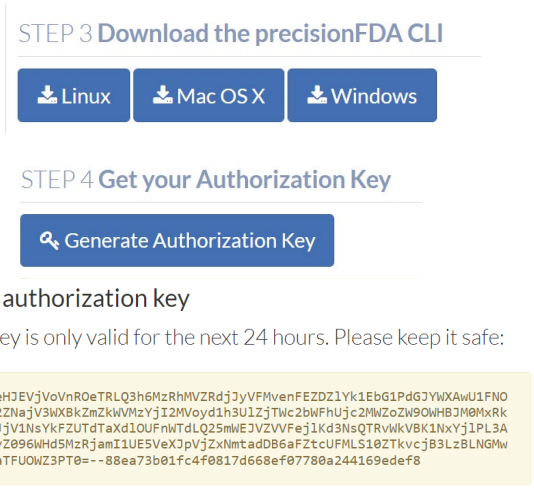
- Access a database cluster from an app.

Download and Install the pfda CLI

The precisionFDA CLI is useful for programmatic uploading and downloading of files from Windows, MacOS, and Linux clients (e.g. your laptop) to and from precisionFDA. Installation and testing for Windows and Linux OS are described below.

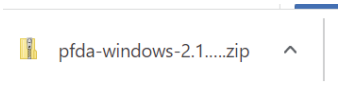
Under My Home Assets, click on the How to create assets button to find links to the precisionFDA CLI, and the button to generate the temporary authorization key that you'll use with the CLI.



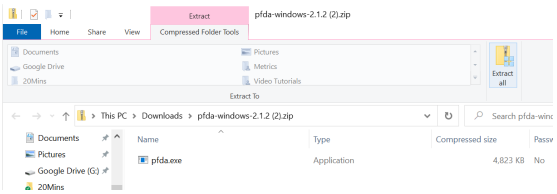


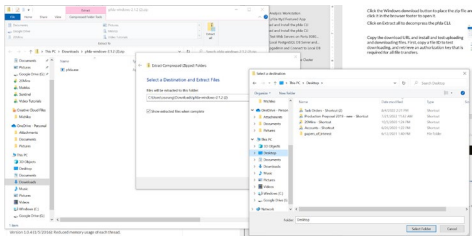
Windows

Click the Windows download button to place the zip file and double click it in the browser footer to open it.

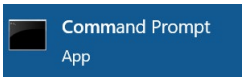


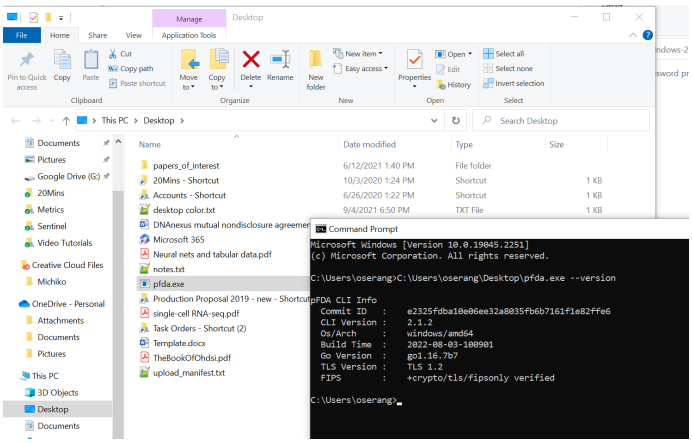
Click on Extract all to decompress the pfda CLI and browse to select the Desktop as the destination for the pfda.exe file.



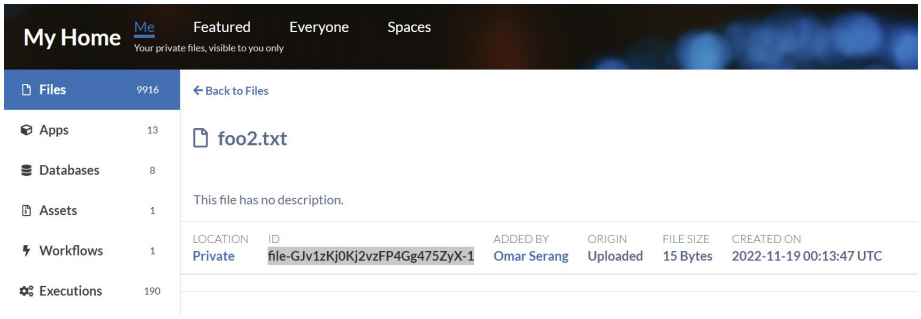


Using the Windows start menu, bring up a Command Prompt window with the pfda.exe file visible in a file explorer side-by-side. Drag *pfda.exe* onto the Command Prompt window to expand the full path the executable and add –*version* and hit return.

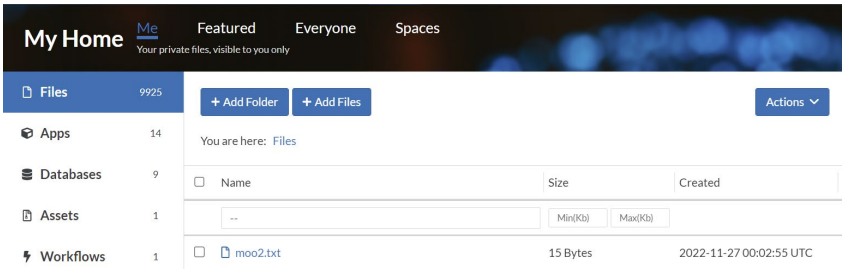




First, copy a file ID to test downloading, and retrieve an authorization key that is required for all file transfers.

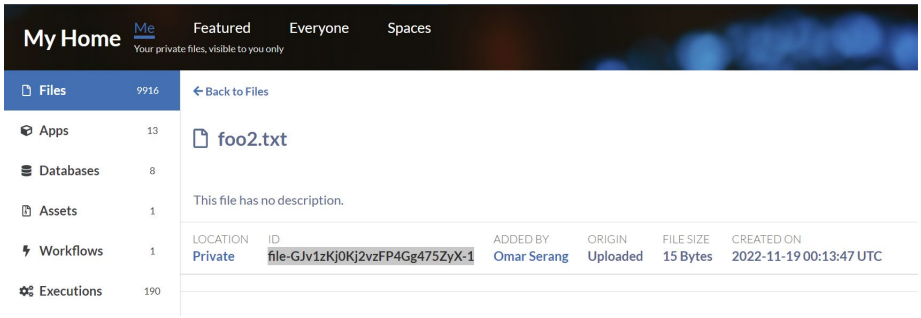



```
:: Provide the auth key
:: Download the selected file
C:\Users\oserang\Desktop\pfda.exe download -key <key> -file-id file-
GJv1zKj0Kj2vzFP4Gg475ZyX-1

:: Copy it to a new file and upload it
copy foo2.txt moo2.txt
C:\Users\oserang\Desktop\pfda.exe upload-file -file moo2.txt

dir *.txt
11/26/2022  04:26 PM                15 foo2.txt
11/26/2022  04:26 PM                15 moo2.txt
```

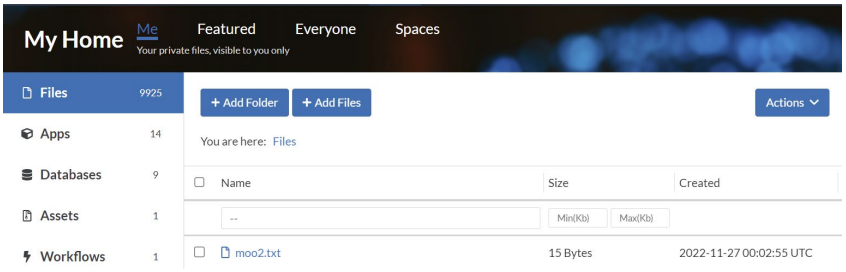


Linux

Copy the download URL and install and test uploading and downloading files. First, copy a file ID to test downloading, and retrieve an authorization key that is required for all file transfers.




```
-- Install pfda CLI
wget https://pfda-production-static-files.s3.amazonaws.com/cli/pfda-
linux-2.2.tar.gz
tar xf pfda-linux-2.2.tar.gz
mv pfda /usr/bin/
pfda --version

-- Provide the auth key
key="…."

-- Download the selected file
pfda download -key $key -file-id file-GJv1zKj0Kj2vzFP4Gg475ZyX-1

-- Copy it to a new file and upload it
cp foo2.txt moo2.txt
pfda upload-file -key $key -file moo2.txt

ls *.txt
foo2.txt  moo2.txt
```



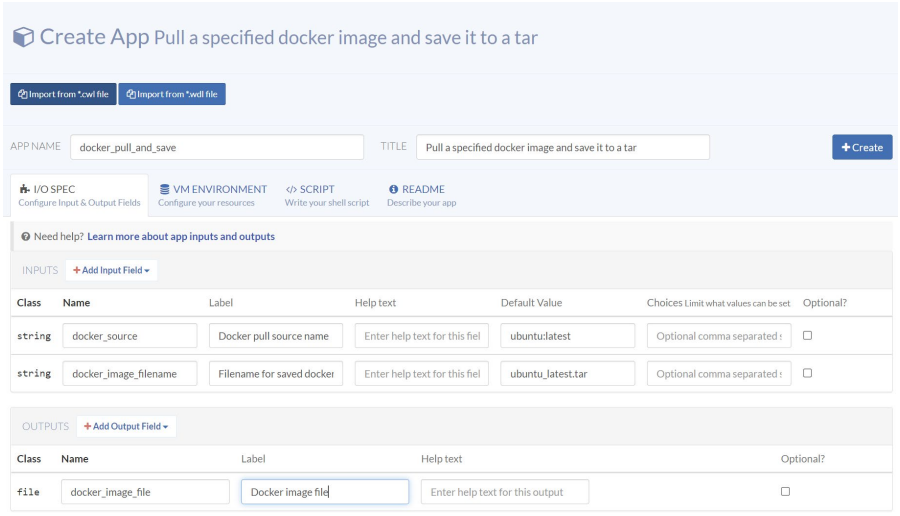
First App: *docker_pull_and_save*

The first app demonstrates the use of string input variables, allowing the app to access the internet, how to use the emit shell function to output a named file. This app pulls a docker image and saves it to a .tar file suitable for use in precisionFDA apps. We'll create three image files in our Files:

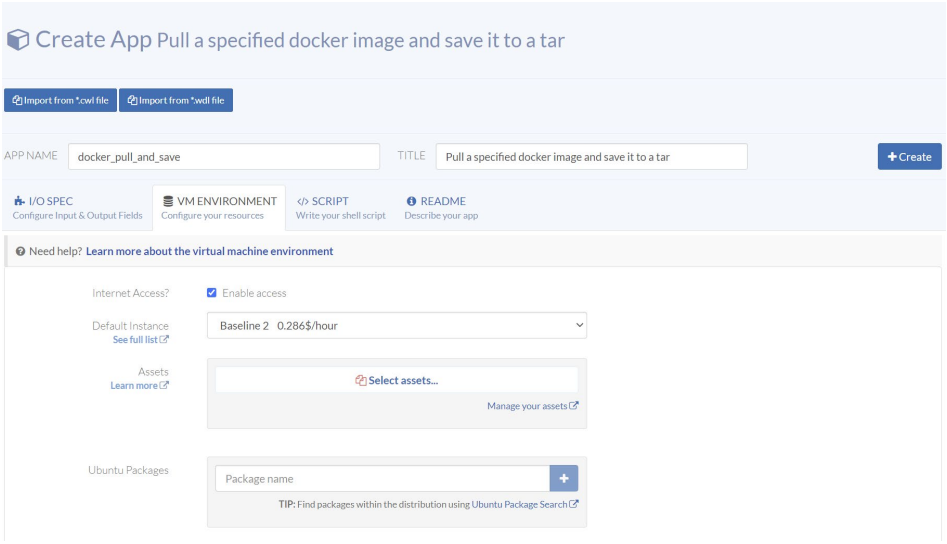
	docker_source	docker_image_filename
1	ubuntu:latest	ubuntu_latest.tar
2	biocontainers/samtools:v1.9-4-deb_cv1	samtools_biocontainers.tar
3	postgres:13.4-buster	postgres_13.4-buster.tar

Create the docker_pull_and_save App

From My Home / Apps, click on Create App to create the *docker_pull_and_save* app. In the I/O Spec tab, add the input and output fields.



Select the VM Environment tab, enable internet access, and select Baseline 2 as the default instance type.

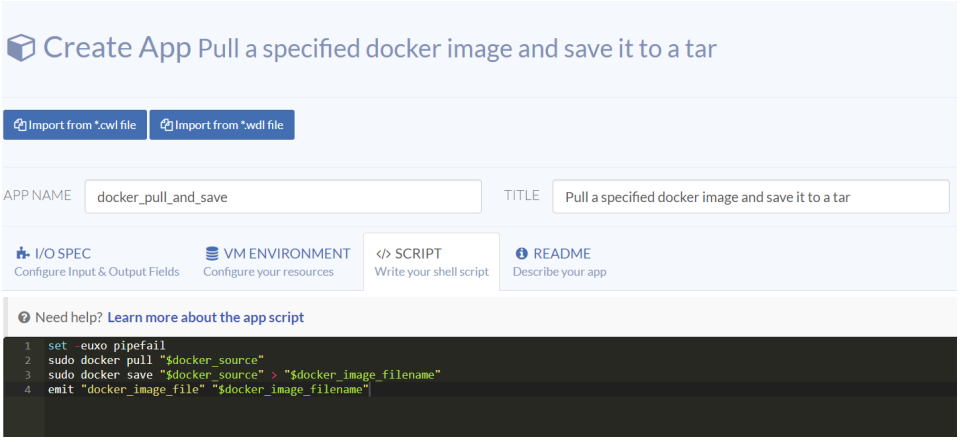


Select the Script tab and enter the following shell script:

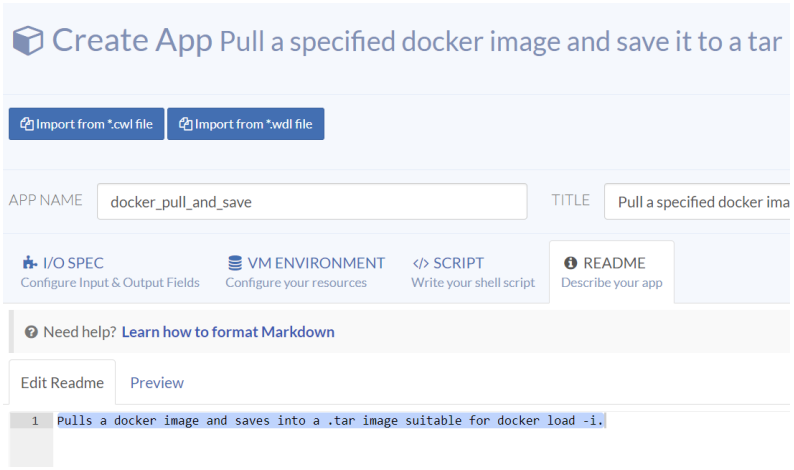
```
set -euxo pipefail
sudo docker pull "$docker_source"
sudo docker save "$docker_source" > "$docker_image_filename"
```

```
emit "docker_image_file" "$docker_image_filename"
```

The set -euxo pipefail set is advisable at the start of all your app scripts. The docker source string is resolved and used to pull the image and to save it to the docker image filename. Lastly the resulting image is saved as a precisionFDA file with the specified image filename.

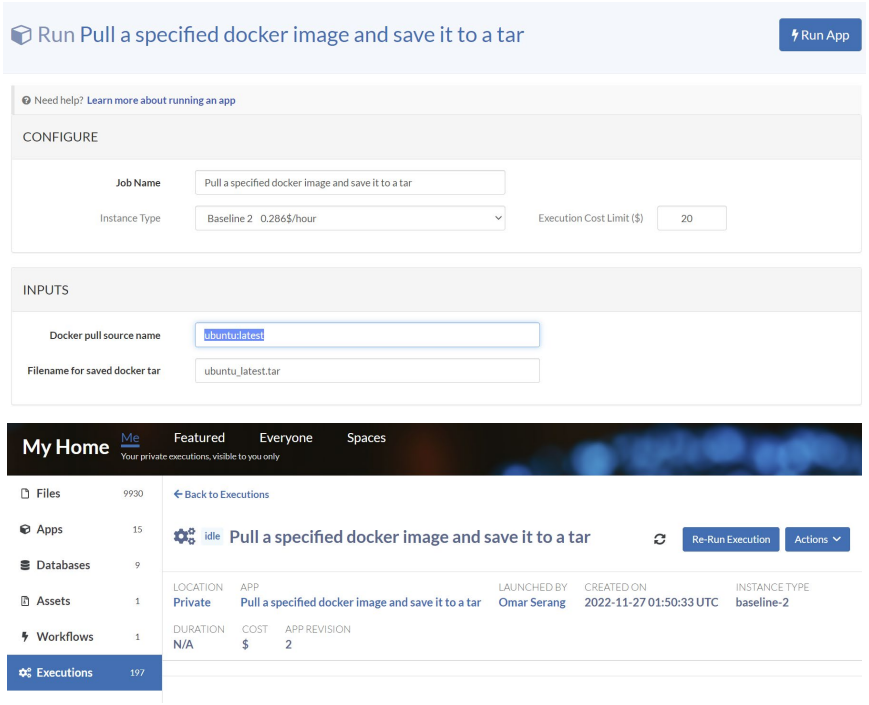


Select the Readme tab and describe your app, then hit the Create button to create your app.

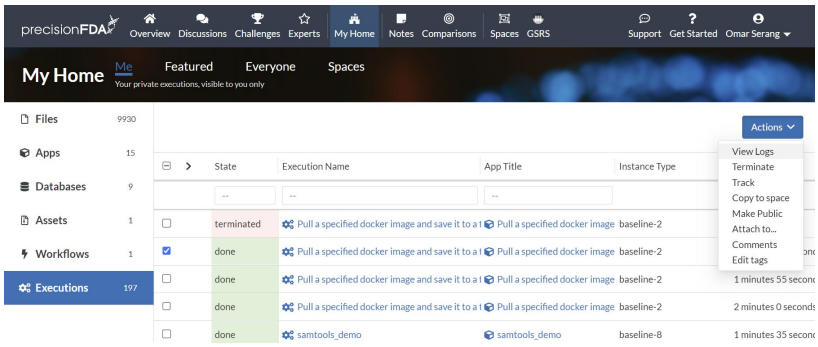


Run the docker_pull_and_save App

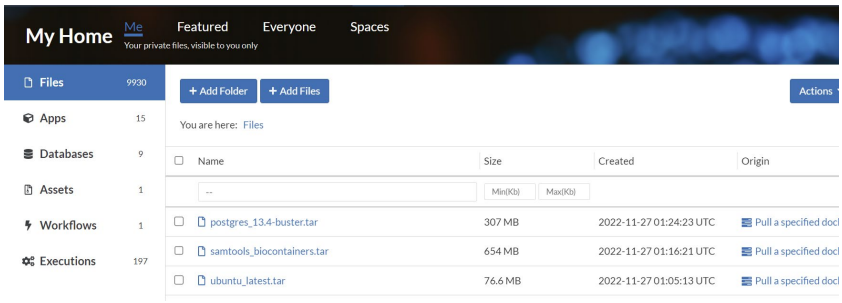
Run this app three times with the inputs listed above. You don't have to wait for one to finish to start the others as they will run in parallel.



Select one of the completed executions My Home / Executions for the app and View Logs using the Action dropdown menu and we can see the desired actions took place and the image .tar files appear in My Home / Files.




```
Downloading files using 2 threads++ set -euxo pipefail
++ sudo docker pull postgres:13.4-buster
13.4-buster: Pulling from library/postgres
.
.
.
Status: Downloaded newer image for postgres:13.4-buster
++ sudo docker save postgres:13.4-buster
++ emit docker_image_file postgres_13.4-buster.tar
```



Second App: *worker_layout_inspection*

Since assets are such a great app developer convenience, our second app, worker_layout_inspection, will illustrate the use of assets and inputs for presenting code and data to the app. First let's create some assets that will be incorporated into the app. Additionally, since Docker is also such a great app developer tool, the incorporation of Docker images into the app by packaging them in an asset or providing them as an input file, are both illustrated.

Create an asset with code and data

Layout your asset directories and files

The file system structure that you layout in your asset will be overlaid on the worker / (root) mount when the app is run. If you've include code in the asset's /usr/bin, it will be available to your app running on the worker. The app framework uses /work as the directory to present input files to apps so any files placed in the asset's /work directory will be available with other input files, though you could place files in whatever asset directory structure you want.

We going to construct our asset in a Linux shell, downloading from precisionFDA the following for inclusion in the asset:

- ubuntu_latest.tar (file-GK1FP9j05gK8z93Y1xGQpf5B-1)
- countries.txt (file-GK1F6j80Kj2XbJzx29f25y42-1)

Create your asset directory structure.

```
apt install tree
mkdir -p ~/fakeroot/work
mkdir -p ~/fakeroot/usr/bin
```

```
tree ~/fakeroot/
```

```
/home/dnanexus/fakeroot/
├── usr
│   └── bin
└── work
```

Create a shell script to install tree and run it, then move the script into the asset directory structure.

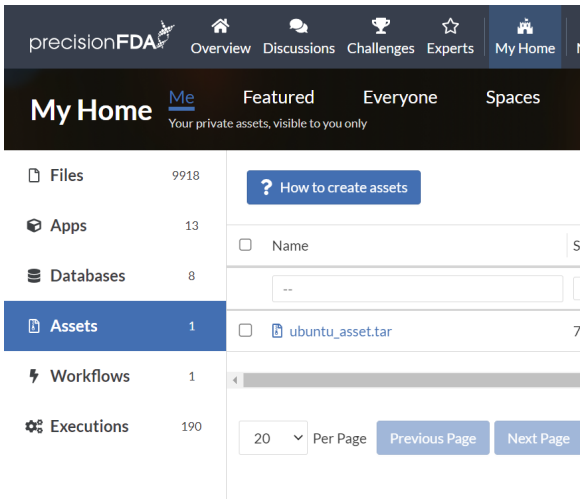
```
cat > tree_script.sh
      sudo apt install tree
      tree $1
```

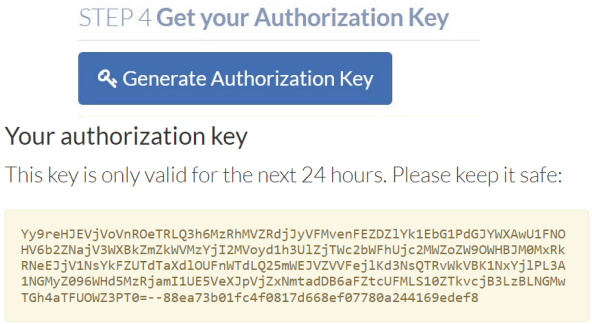
```
      CTRL-D
chmod ugo+x tree_script.sh
./tree_script.sh ~
/home/dnanexus
├── EHR_Sample_backup_nodbcreate_postgres.sql
├── datafiles
│   ├── manifest.txt
│   ├── observations.txt
│   └── patients.txt
└── db_backups
mv tree_script.sh ~/fakeroot/usr/bin
```

Create a Readme file as required for the asset. This doesn't need to reside in the asset /fakeroot directory structure.

```
echo "Assets for the worker layout inspection tutorial app" >
~/readme.txt
```

Download the Docker and data files and move them into the asset directory structure. Under My Home Assets, click on the How to create assets button to find links to the precisionFDA CLI, and the button to generate the temporary authorization key that you'll use with the CLI.





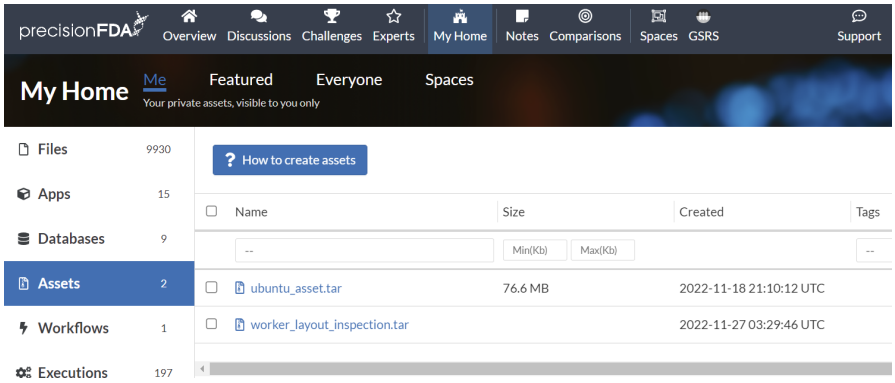

```
key="..."

pfda download -key $key -file-id file-GK1FP9j05gK8z93Y1xGQpf5B-1
pfda download -key $key -file-id file-GK1F6j80Kj2XbJzx29f25y42-1
ls *.tar *txt
countries.txt  foo2.txt  moo2.txt  ubuntu_latest.tar

mv countries.txt postgres_13.4-buster.tar ubuntu_latest.tar
~/fakeroot/work
tree ~/fakeroot
/home/dnanexus/fakeroot
├── usr
│   └── bin
```

```
│       └──── tree_script.sh
└──── work
    ├──── countries.txt
    └──── ubuntu_latest.tar
```

Create the asset using the CLI

Now that the asset contents have been laid out, creating the asset on precisionFDA is a straightforward process using the precision FDA CLI.

```
key="..."

pfda upload-asset --key $key --name worker_layout_inspection.tar --root
~/fakeroot --readme ~/readme.txt
>> Archiving asset...
>> Finalizing asset...
>> Done! Access your asset at
https://precision.fda.gov/home/assets/file-GK1JJB00Kj2fkz464yxB5zY2-1
```



Manually deploying an asset tar file

While this workflow should not be required, it is worth knowing to understand how assets work. Upload the asset tarball (e.g. *worker_layout_inspection.tar*) as a file, then in your app, add a file to the I/O Spec (e.g. "asset_tarball") and select this tarball as the default. Add the following line to the Script, right after the `set -euxo pipefail` command:

```
tar zxvf ${asset_tarball_path} -C / --strip-components=1 --no-same-owner
```

Everything that was installed in the fake_root/ in the tarball will be placed into the root directory of the worker, including any executable you may have. For example,

`fake_root/usr/local/bin/sambamba`

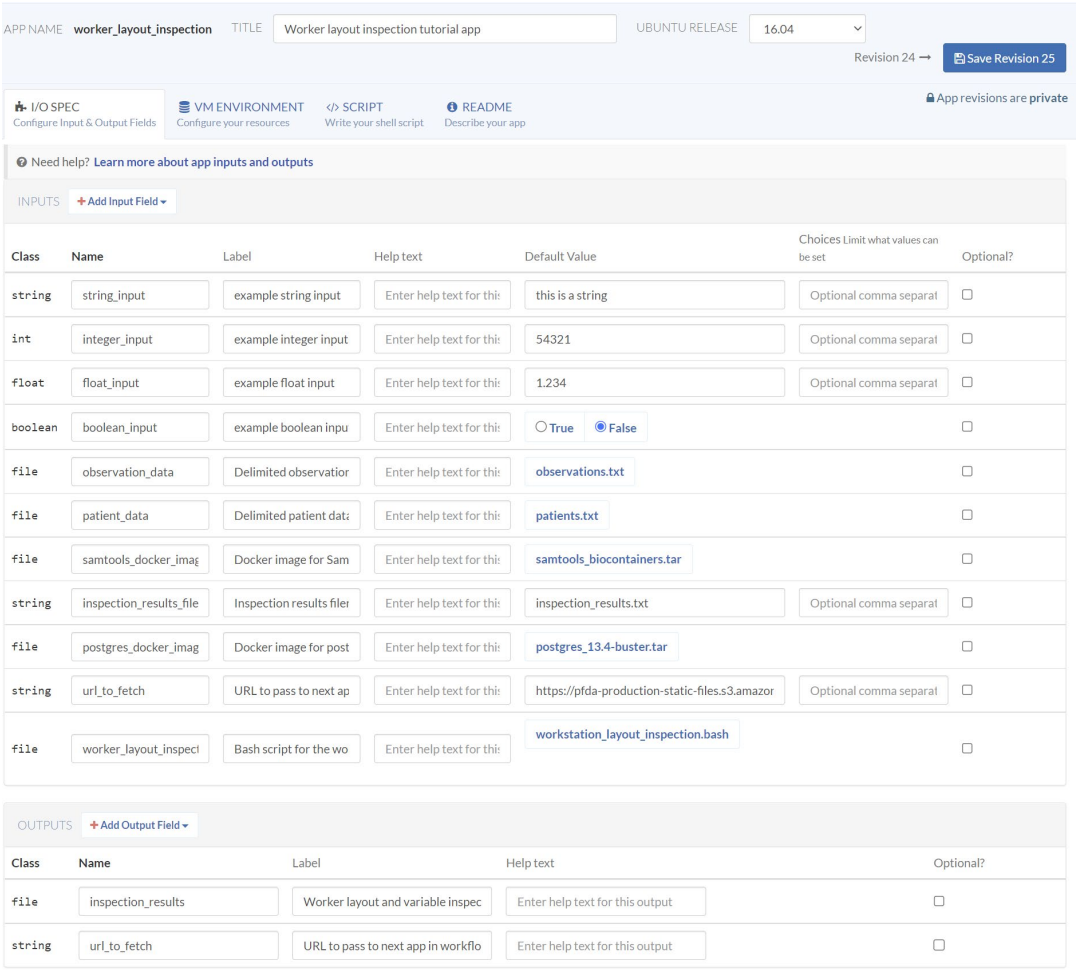
from the asset_tarball input, will be available in:

`/usr/local/bin/sambamba`

after the tar command above is run in the app script.

Create the App and Specify the I/O Spec

In My Home / Apps, click the Create App button to create the *worker_layout_inspection* app. In the I/O Spec tab, add the input and output fields.

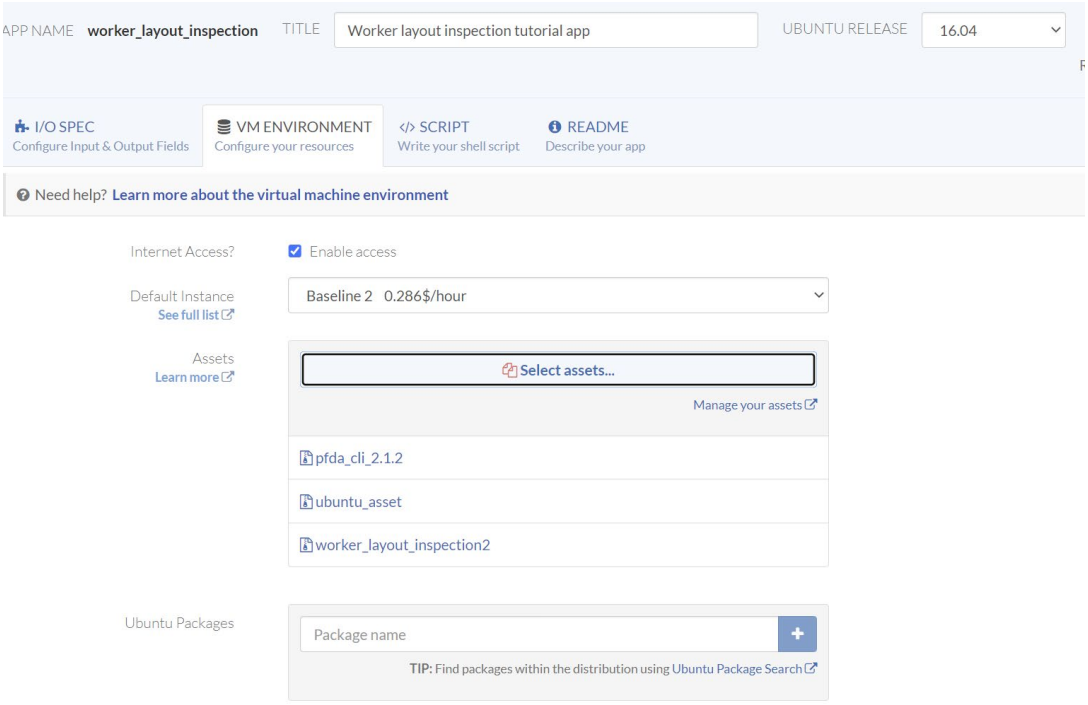


Class	Input Name	Label	Default Value
string	string_input	example string input	this is a string
int	integer_input	example integer input	54321
float	float_input	example float input	1.234
boolean	boolean_input	example boolean input	False
file	observation_data	Delimited observation data	observations.txt

file	patient_data	Delimited patient data	patients.txt
file	samtools_docker_image	Docker image for Samtools	samtools_biocontainers.tar
file	postgres_docker_image	Docker image for postgres server	postgres_13.4-buster.tar
string	inspection_results_filename	Inspection results filename	inspection_results.txt
string	url_to_fetch	URL to pass to next app in workflow	https://pfda-production-static-files.s3.amazonaws.com/cli/pfda-linux-2.2.tar.gz
Class	**Output Name**	**Label**	
file	Inspection_results	Worker layout and variable inspection results	
string	url_to_fetch	URL to pass to next app in workflow	

Specify the VM Environment

In the VM Environment tab, enable internet access, select default instance Baseline 2, and add the following assets: worker_layout_inspection, pfda_cli_2.2, and ubuntu_asset.



Specify the Script

Add the following code to the script tab:

```
set -euxo pipefail

# Append the worker OS information to the specified inspection results
file.
cat /etc/os-release  | tee -a "$inspection_results_filename"

# Install tree
sudo apt update
sudo apt install tree

# Inspect the scalar input variables.
echo "string_input" "$string_input"
echo "integer_input" "$integer_input"
echo "float_input" "$float_input"
echo "url_to_fetch" "$url_to_fetch"
echo ""

# Inspect the file input variables and the different
# operators for accessing them on the worker FS.
echo "patient_data" "$patient_data"
echo "patient_data_name" "$patient_data_name"
echo "patient_data_path" "$patient_data_path"
echo "patient_data_prefix" "$patient_data_prefix"
echo ""
echo "observation_data" "$observation_data"
```

```
echo "observation_data_name" "$observation_data_name"
echo "observation_data_path" "$observation_data_path"
echo "observation_data_prefix" "$observation_data_prefix"
echo ""
echo "samtools_docker_image" "$samtools_docker_image"
echo "samtools_docker_image_name" "$samtools_docker_image_name"
echo "samtools_docker_image_path" "$samtools_docker_image_path"
echo "samtools_docker_image_prefix" "$samtools_docker_image_prefix"

# Use the pfda CLI that was loaded with the pfda_cli_2.2 asset.
ls -al /usr/bin/pfda*
pfda --version

# Use the simple script that was loaded with the
worker_layout_inspection asset.
ls -al /usr/bin/tree_script.sh
tree_script.sh /work

# Using the Docker image that was loaded with the ubuntu_asset asset,
# we can run an up-to-date Ubuntu OS in a docker container on the
worker.
# Append the container OS information to the specified inspection
results file.
docker load -i /ubuntu_latest.tar
docker run --rm -v /work:/work -w /work ubuntu:latest cat /etc/os-
release | tee -a "$inspection_results_filename"

# Using the Docker image that was provided as an input file,
# we can run samtools. Add inputs and outputs to this script and
# pass them to the samtools invocation to create your own
# samtools app.
docker load -i "$samtools_docker_image_path"
docker run --rm biocontainers/samtools:v1.9-4-deb_cv1 samtools --version

docker images
docker ps

# Pass the URL to fetch input to the same output variable to pass
# to the next app in the tutorial workflow (i.e. url fetcher).
emit "url_to_fetch" "$url_to_fetch"

# Save the inspection results file with specified name.
emit "inspection_results" "$inspection_results_filename"
```

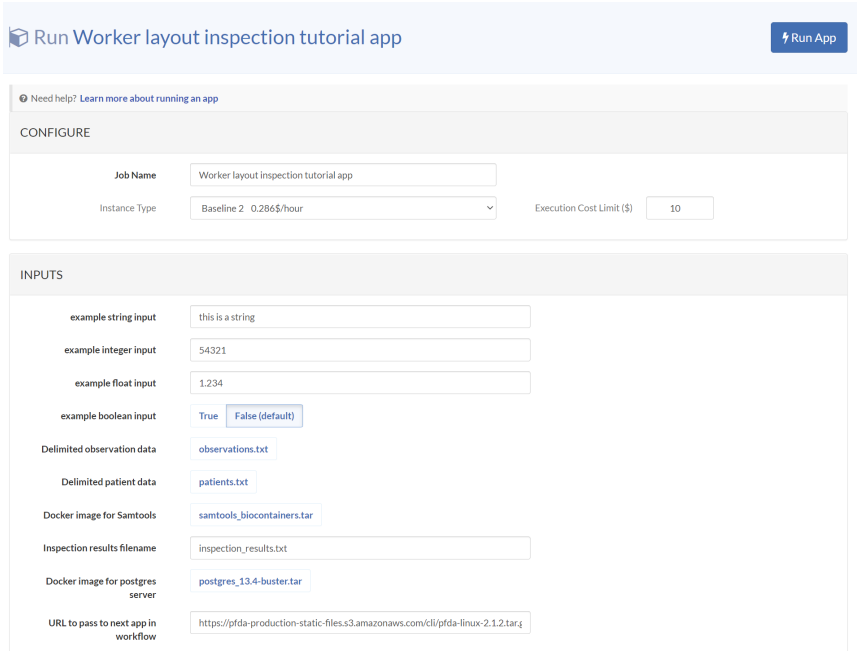
Specify the Readme

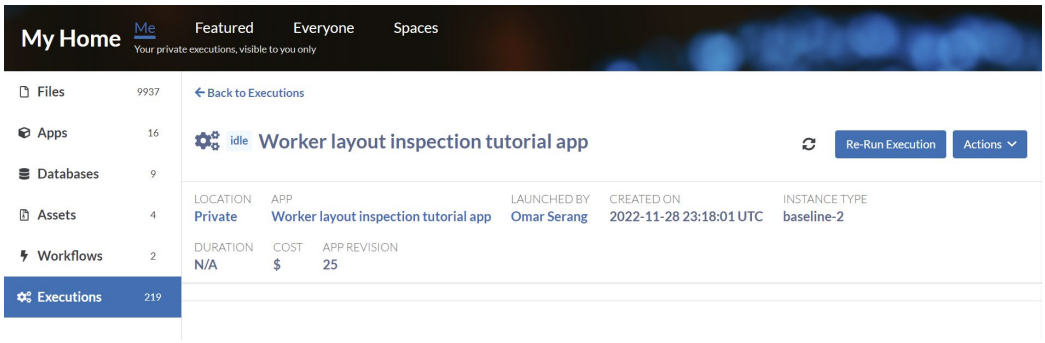
Add the following in the Readme tab:

```
Produce an inspection report of the worker filesystem and file inputs
from the context of the app.
Also provide the multiple representations available for file inputs.
Echo the non-file input variables.
```

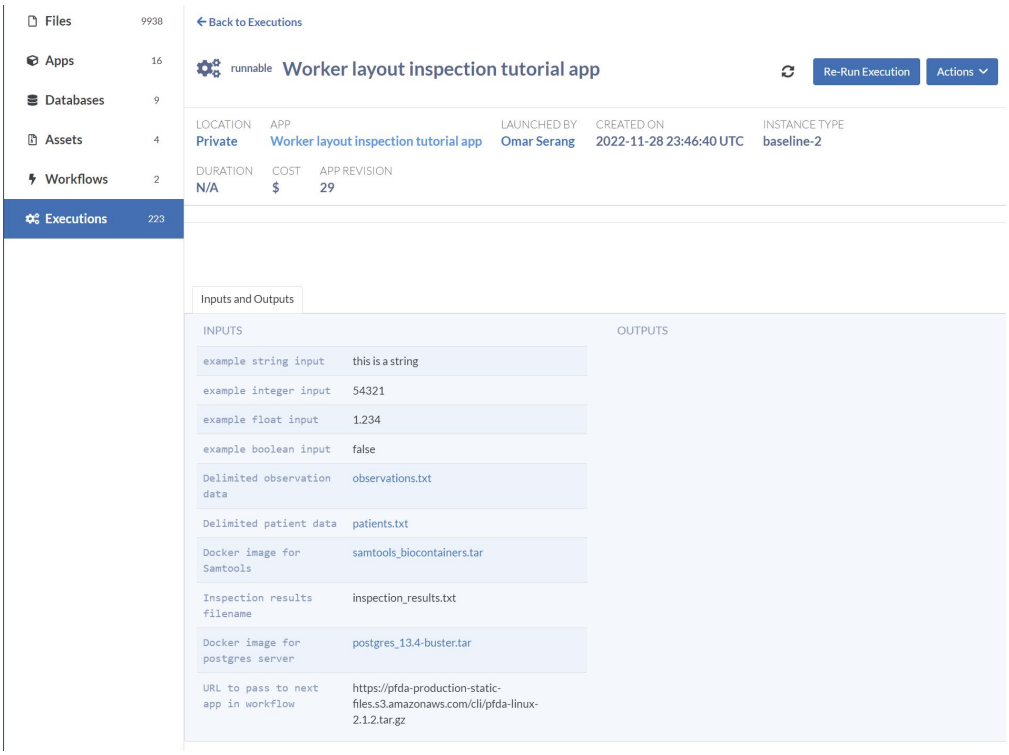
Run the app

In My Home / Apps, select the *worker_layout_inspection* app and click Run App to launch the latest version of the app with all default inputs.



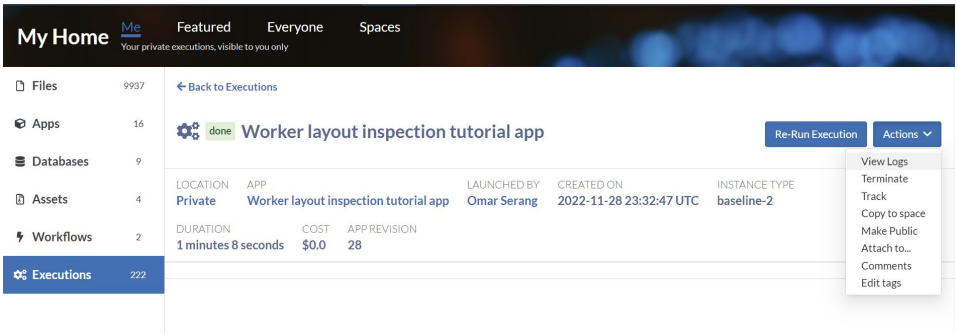


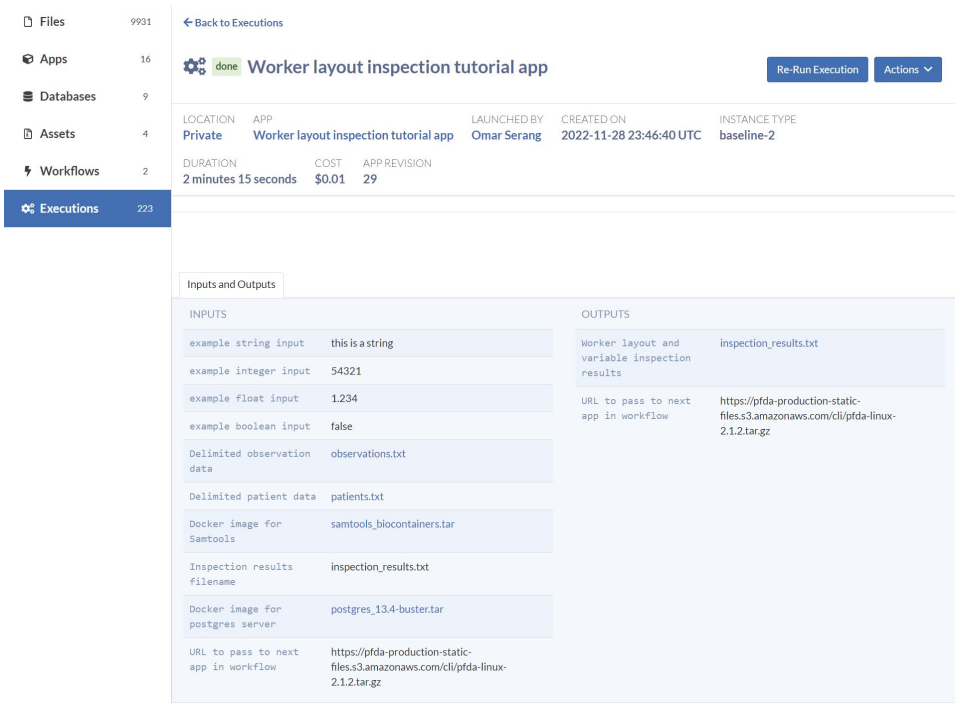
Refresh the execution status using the button until the job is first idle, runnable, running, and done, (or failed).



Inspect the execution logs and the inspection results file

Note that the execution of the app took just over a minute and produced inspection_results.txt file and URL string outputs.





Select View Logs from the the Actions dropdown menu. Let's look at a condensed and annotated version of the log output to understand what our app just did.

```
# Worker initialization
Logging initialized (priority)
CPU: 20% (2 cores) * Memory: 779/3720MB * Storage: 32GB free * Net: 0↓
/0↑MBps
umount: /proc/diskstats: not mounted
dxpy/0.331.0 (Linux-5.4.0-1088-aws-x86_64-with-Ubuntu-16.04-xenial)
/usr/sbin/rsyslogd already running.
bash running (job ID job-GK2ZQj00Kj2z9q76KbZbkG3G)

# Fetch the app's assets.
Fetching asset ubuntu_asset.tar (file-GJqz9J00Kj2zZQPGKVZBg436)
Fetching asset pfda_cli_2.2.tar (file-GJv0kFQ0Kj2YzFb86g4B8px5)
Fetching asset worker_layout_inspection2.tar (file-
GK1xxbQ0Kj2gBZjxF244F21k)

# Download the input files.
downloading file: file-GK1F6jj0Kj2gyF8jG8jPjGpV to filesystem:
/work/in/patient_data/patients.txt
downloading file: file-GK1F6jQ0Kj2v90jxPV0ZBQ5G to filesystem:
/work/in/observation_data/observations.txt
downloading file: file-GK1FXK80pyBj68X3K6jVX55b to filesystem:
/work/in/samtools_docker_image/samtools_biocontainers.tar
downloading file: file-GK1Fg68072kf3ZXYGJvxPGPj to filesystem:
/work/in/postgres_docker_image/postgres_13.4-buster.tar

# The worker's OS release information.
```

```
cat /etc/os-release
NAME="Ubuntu"
VERSION="16.04.7 LTS (Xenial Xerus)"
ID=ubuntu
ID_LIKE=debian
PRETTY_NAME="Ubuntu 16.04.7 LTS"
VERSION_ID="16.04"
HOME_URL="http://www.ubuntu.com/"
SUPPORT_URL="http://help.ubuntu.com/"
BUG_REPORT_URL="http://bugs.launchpad.net/ubuntu/"
VERSION_CODENAME=xenial
UBUNTU_CODENAME=xenial

# Install tree
sudo apt update
apt install tree
Unpacking tree (1.7.0-3) ...
Processing triggers for man-db (2.7.5-1) ...
Setting up tree (1.7.0-3) ...

# Resolution of each scalar input variable
string_input this is a string
integer_input 54321
float_input 1.234
url_to_fetch https://pfda-production-static-
files.s3.amazonaws.com/cli/pfda-linux-2.2.tar.gz

# Resolution of each file input variable into the four
# types of references available
patient_data file-GK1F6jj0Kj2gyF8jG8jPjGpV
patient_data_name patients.txt
patient_data_path /work/in/patient_data/patients.txt
patient_data_prefix patients

observation_data file-GK1F6jQ0Kj2v90jxPV0ZBQ5G
observation_data_name observations.txt
observation_data_path /work/in/observation_data/observations.txt
observation_data_prefix observations

samtools_docker_image file-GK1FXK80pyBj68X3K6jVX55b
samtools_docker_image_name samtools_biocontainers.tar
samtools_docker_image_path
/work/in/samtools_docker_image/samtools_biocontainers.tar
samtools_docker_image_prefix samtools_biocontainers

# View the pfda CLI that was installed with the pfda CLI asset and run
it.
ls -al /usr/bin/pfda
-rwxr-xr-x 1 root root 11810776 Aug  3 08:07 /usr/bin/pfda

pfda --version
```

```
pFDA CLI Info
  Commit ID   :    e2325fdba10e06ee32a8035fb6b7161f1e82ffe6
  CLI Version :    2.2
  Os/Arch     :    linux/amd64
  Build Time  :    2022-08-03-100606
  Go Version  :    go1.16.7b7
  TLS Version :    TLS 1.2
  FIPS        :    +crypto/tls/fipsonly verified

# View the tree script that was installed with the workstation asset and
run it.
# Note the countries.txt file in /work as it was packaged in the
worker_layout_inspection asset.
# Note the directory layout of the file input types.

ls -al /usr/bin/tree_script.sh
-rwxr-xr-x 1 root root 30 Nov 27 21:32 /usr/bin/tree_script.sh

tree_script.sh /work
/work
├──── countries.txt
├──── in
│    ├──── observation_data
│    │    └──── observations.txt
│    ├──── patient_data
│    │    └──── patients.txt
│    ├──── postgres_docker_image
│    │    └──── postgres_13.4-buster.tar
│    └──── samtools_docker_image
│         └──── samtools_biocontainers.tar
└──── inspection_results.txt

# Load the docker image that was installed with ubuntu asset and run it,
# presenting the container OS release information.
docker load -i /ubuntu_latest.tar

5 directories, 6 files
Loaded image: ubuntu:latest
docker run --rm -v /work:/work -w /work ubuntu:latest cat /etc/os-
release | tee -a inspection_results.txt

PRETTY_NAME="Ubuntu 22.04.1 LTS"
NAME="Ubuntu"
VERSION_ID="22.04"
VERSION="22.04.1 LTS (Jammy Jellyfish)"
VERSION_CODENAME=jammy
ID=ubuntu
ID_LIKE=debian
HOME_URL="https://www.ubuntu.com/"
```

```
SUPPORT_URL="https://help.ubuntu.com/"
BUG_REPORT_URL="https://bugs.launchpad.net/ubuntu/"
PRIVACY_POLICY_URL="https://www.ubuntu.com/legal/terms-and-
policies/privacy-policy"
UBUNTU_CODENAME=jammy

# Load the samtools docker image that was provided as an input file and
run it.
docker load -i /work/in/samtools_docker_image/samtools_biocontainers.tar
Loaded image: biocontainers/samtools:v1.9-4-deb_cv1

docker run --rm biocontainers/samtools:v1.9-4-deb_cv1 samtools --version
samtools 1.9
Using htslib 1.9
Copyright (C) 2018 Genome Research Ltd.

# Docker images and running containers on the worker
docker images
REPOSITORY               TAG                 IMAGE ID            CREATED
SIZE
ubuntu                   latest              a8780b506fa4        3 weeks
ago         77.8MB
biocontainers/samtools   v1.9-4-deb_cv1      f210eb625ba6        3 years
ago         666MB

docker ps
CONTAINER ID        IMAGE               COMMAND             CREATED
STATUS              PORTS               NAMES

# Emit the URL string output variable.
emit url_to_fetch https://pfda-production-static-
files.s3.amazonaws.com/cli/pfda-linux-2.2.tar.gz

# Emit the inspection results file.
emit inspection_results inspection_results.txt
```

Utility Apps: *untar_files, tar_files_from_manifest*

We are going to use the pfda_cli_2.2.tar asset to create two very useful apps that demonstrate a design pattern that is readily extensible. The precisionFDA app I/O specification supports scalar and file and output types but does not support arrays for input or output variables. This means that using the app input variable and output emit framework, you cannot create apps with an arbitrary number of inputs or outputs. For instance, you really can't even create an untar app due to this limitation. These two apps demonstrate a design pattern to overcome this limitation.

Note that these apps require a temporary authorization key that you'll use with the CLI and this key will appear in the execution log files. Thus you should only run this app in your My Home or Private Space contexts so as not to expose the key to other users.

Your authorization key

This key is only valid for the next 24 hours. Please keep it safe:

```
Yy9reHJEVjVoVnROeTRLQ3h6MzRhMVZRdjJyVFMvenFEZDZlYk1EbG1PdGJYWXAwU1FNO
HV6b2ZNajV3WXBkZmZkWVMzYjI2MVoyd1h3UlZjTWc2bWFhUjc2MWZoZW9OWHBJM0MxRk
RNeEJjV1NsYkFZUTdTaXdlOUFnWTdLQ25mWEJVZVVFejlKd3NsQTRvWkVBK1NxYjlPL3A
1NGMyZ096WHd5MzRjamI1UE5VeXJpVjZxNmtadDB6aFZtcUFMLS10ZTkvcjB3LzBLNGMw
TGh4aTFUOWZ3PT0=--88ea73b01fc4f0817d668ef07780a244169edef8
```

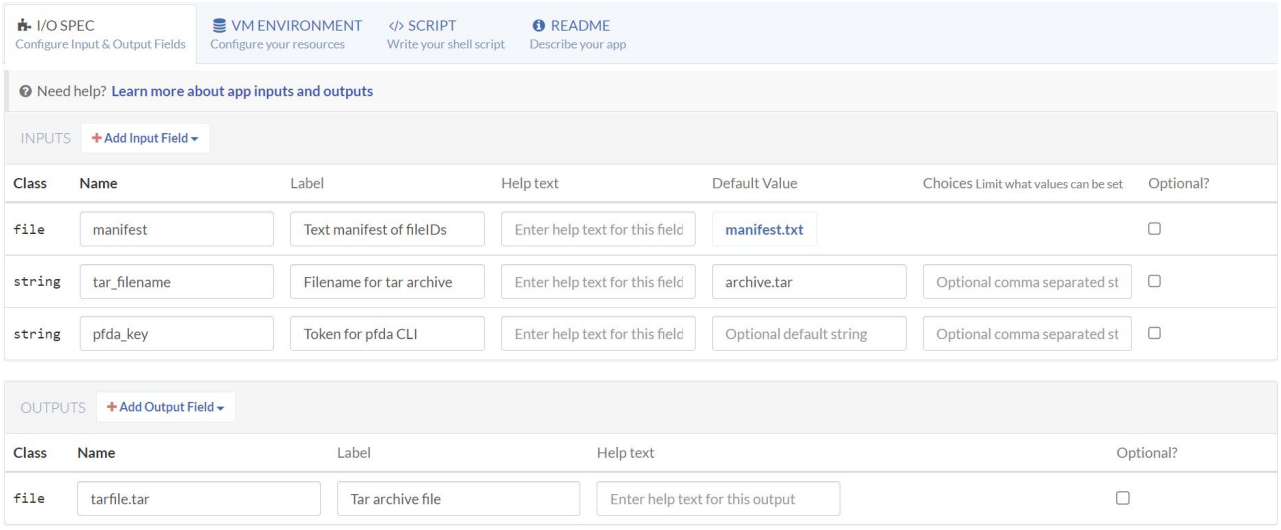
tar_files_from_manifest: Tar a manifest of fileIDs

From My Home / Files, select the detail page and copy the file ID for a number of files. Create and upload *manifest.txt* with the list to be incorporated into an archive file (e.g.):

```
cat manifest.txt
file-GJv1zKj0Kj2vzFP4Gg475ZyX-1
file-GJv1zKj0Kj2XY800GgJY2f4G-1
file-GJv1zKQ0Kj2vfZkVFxp436B9-1

key="..."
pfda upload-file -key $key -file manifest.txt
```

Create a *tar_files_from_manifest* app titled "Tar a manifest of fileIDs", with the following I/O Spec.

Class	Input Name	Label	Default Value
file	manifest	Text manifest of fileIDs	manifext.file
string	tar_filename	Filename for tar archive	archive.tar
string	pfda_key	Token for pfda CLI	
Class	**Output Name**	**Label**	
file	tarfile	Tar archive file	



Setup the VM environment with internet access enabled, Baseline 2 default instance type, and select the pfda_cli_2.2 asset. Note that it can take minutes for the list of assets to loaded before they can be searched.

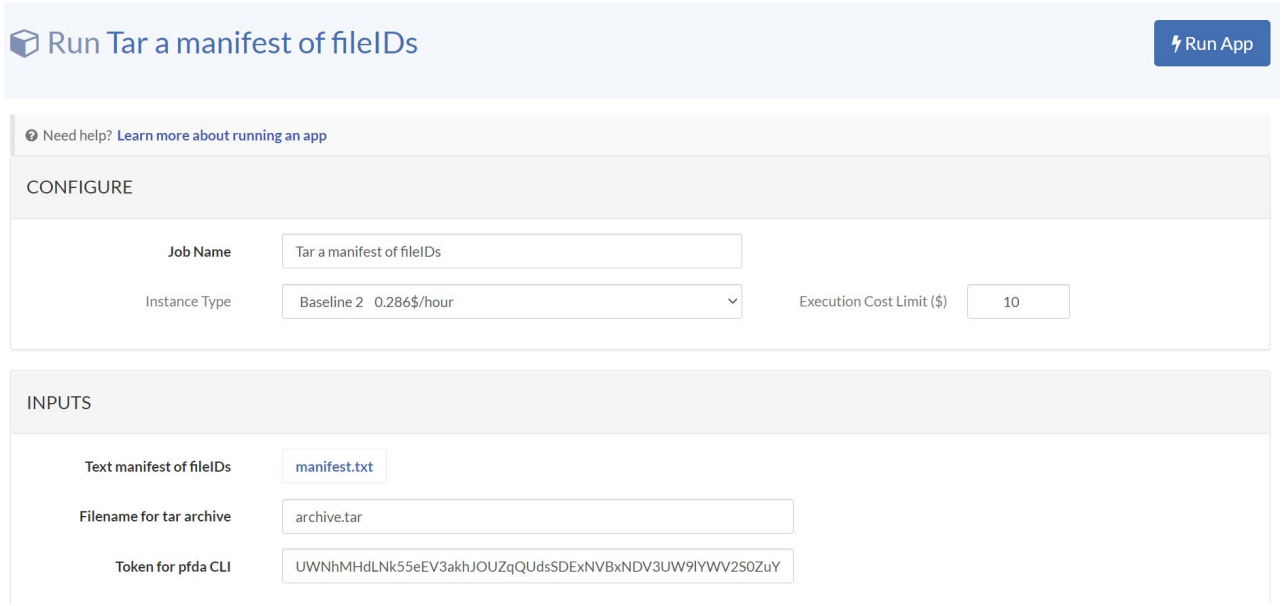
Enter the following Script:

```
set -euxo pipefail
echo "$pfda_key"
echo "$tar_filename"
echo "$manifest"
sudo apt-get update
sudo apt-get install -y dos2unix
pfda -version
mkdir temp
cd temp
dos2unix "$manifest_path"
for file in $(cat "$manifest_path"); do pfda download -key "$pfda_key" -
file-id $file; done
cd ..
tar cvf "$tar_filename" temp/*
emit "tarfile" "$tar_filename"
```

Enter a Readme and Create the app.

```
Input a manifest file containing a list of fileIDs and the name of tar
archive file. You'll need to provide a temporary authorization key
for use with the pfda CLI and thus you should only run this app in
your My Home or Private Spaces.
```

Run the app with the default inputs and a fresh authorization token for the pfda CLI and observe the new archive.tar file.



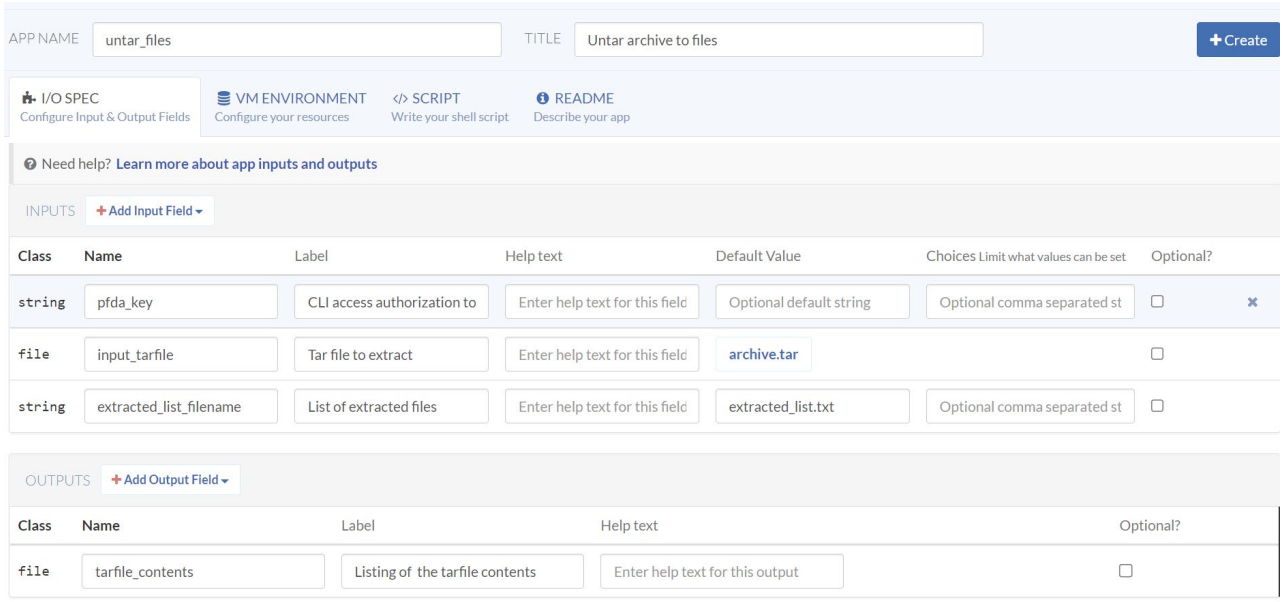
When the execution is done, download the archive.tar file to verify its contents.

```
tar tvf archive.tar
-rw-r--r-- root/root         15 2022-11-29 02:22 temp/foo.txt
-rw-r--r-- root/root         15 2022-11-29 02:22 temp/foo2.txt
-rw-r--r-- root/root         15 2022-11-29 02:22 temp/foo3.txt
```

untar_files: Untar archive to files

Create a *untar_files* app titled "Untar archive to files", with the following I/O Spec.

Class	Input Name	Label	Default Value
string	pfda_key	CLI access authorization token	
file	input_tarfile	Tar file to extract	archive.tar
string	extracted_list_filename	List of extracted files	extracted_list.txt
Class	**Output Name**	**Label**	
file	tarfile_contents	Listing of the tarfile contents	



Setup the VM environment with internet access enabled, Baseline 2 default instance type, and select the pfda_cli_2.2 asset. Note that it can take minutes for the list of assets to loaded before they can be searched.

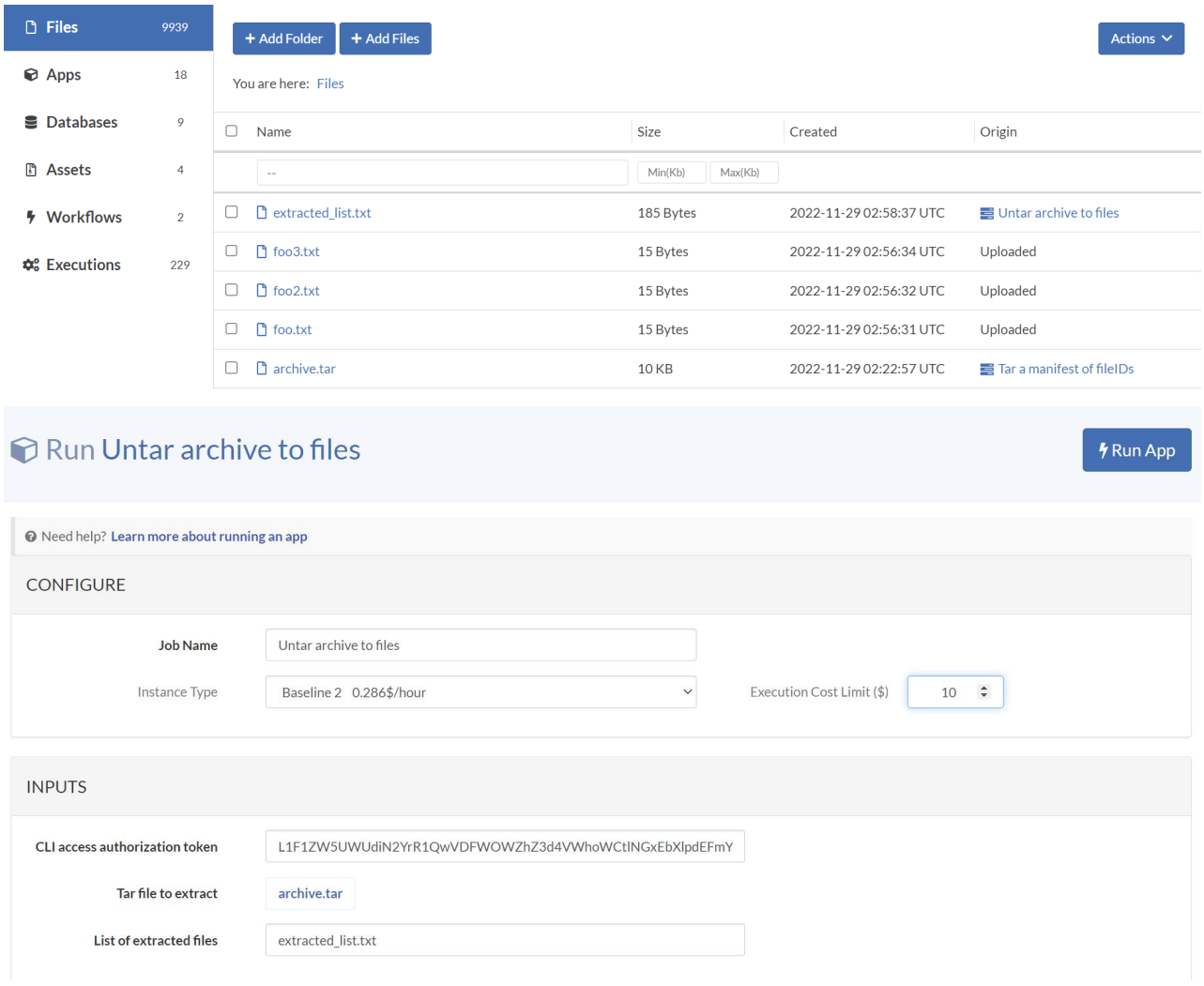
Enter the following Script:

```
set -euxo pipefail
echo "$pfda_key"
echo "$input_tarfile"
echo "$extracted_list_filename"
pfda -version
tar tvf "$input_tarfile_path" > "$extracted_list_filename"
mkdir temp
tar xvf "$input_tarfile_path" --directory temp
ls temp
for FILE in $(find ./temp -type f -print); do echo $FILE; done
emit "tarfile_contents" "$extracted_list_filename"
```

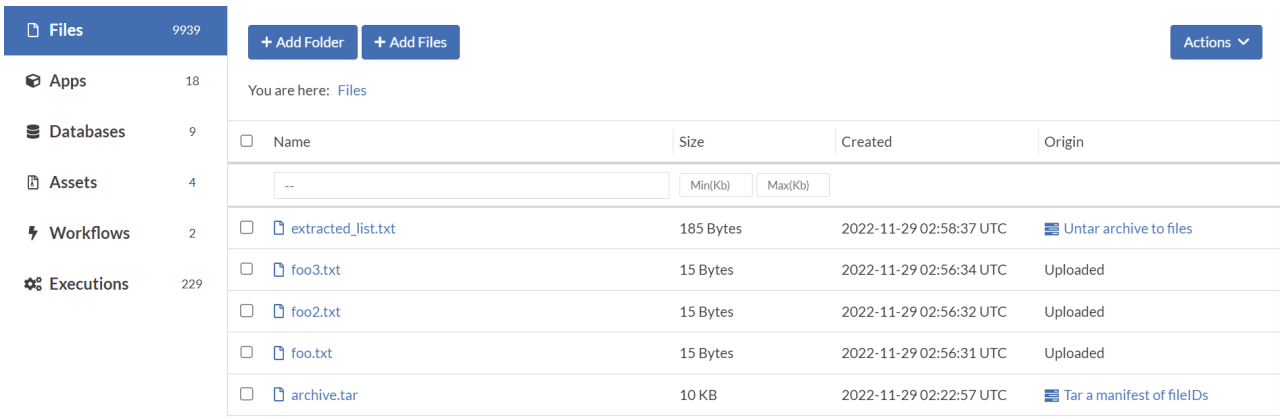
Enter a Readme and Create the app.

```
Input a tar archive file to extract into individual files. You'll need
to provide a temporary authorization key for use with the pfda CLI and
thus you should only run this app in your My Home or Private Spaces.
```

Run the app with the default inputs and a fresh authorization token for the pfda CLI.

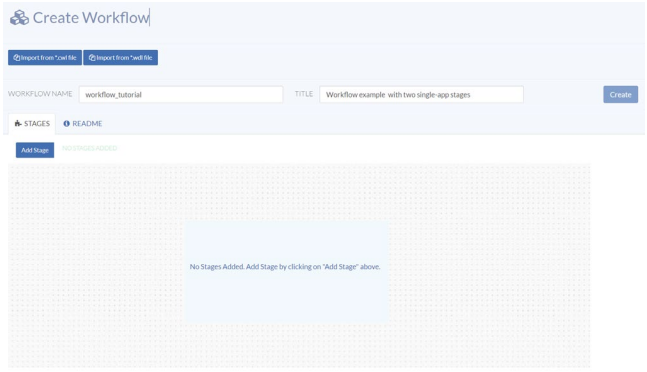


When the execution is done, observe the new extracted files, and open the extracted_list.txt file to see the list of extracted files.



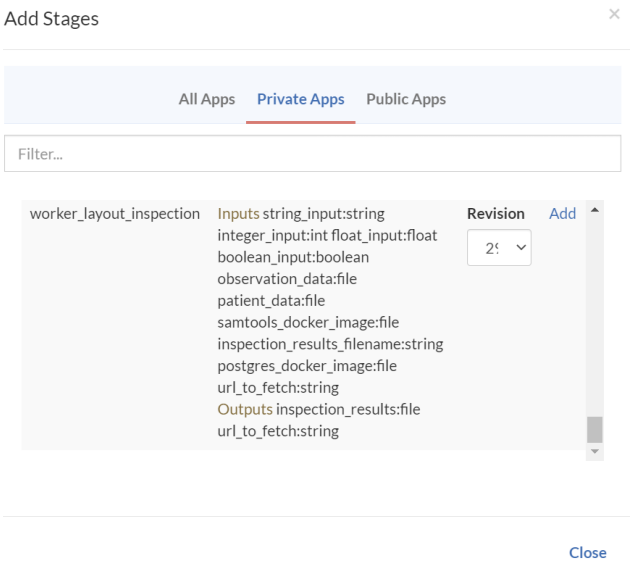
First Workflow: *simple_workflow*

Workflows enable you to string together multiple stages, each running on its own instance type and its own app(s). Outputs from a given stage can be routed to inputs in the next stage. We will create this workflow using the web interface. In My Home / Workflows, click Create Workflow and name it *simple_workflow* with a title "Workflow example with two single-app stages".

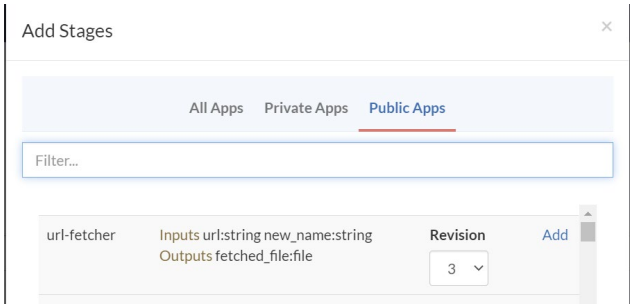


Add the workflow stages

Click the Add Stage button and add the private workflow_layout_inspection app to the stage.

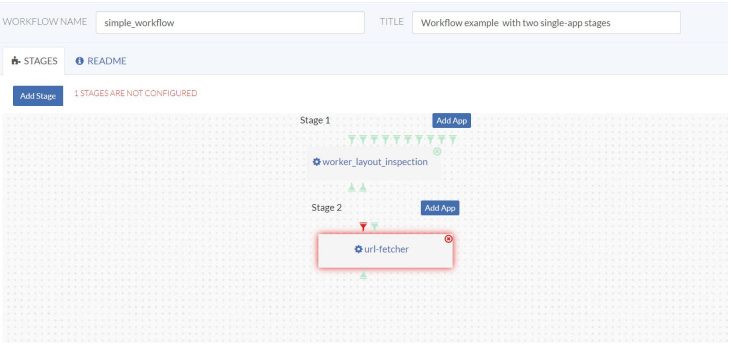


Add a second stage with the public url-fetcher app.

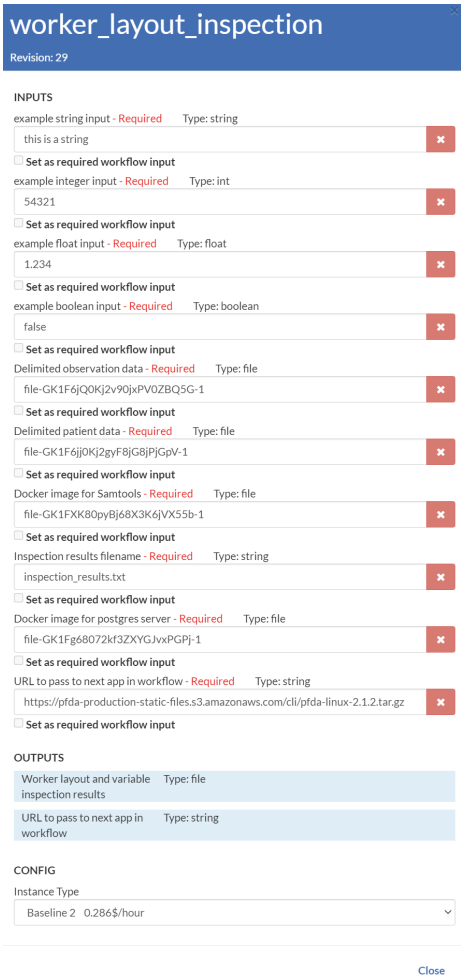


Configure the workflow stages

Now we are ready to configure the stages.

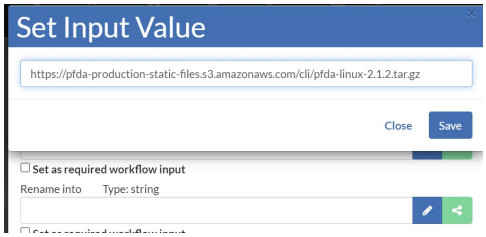


Click on Stage 1 to display the worker_layout_inspection app's configuration; we will accept all the default values provided in the app so there is nothing more that needs to be configured for Stage 1.

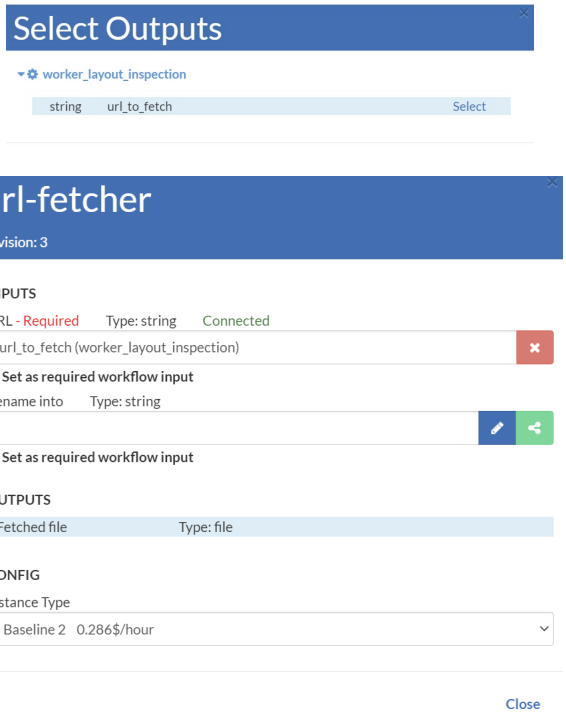


Click on Stage 2 to display the url-fetcher app's configuration. Note the red color indicating that a required input has not been specified either from the output of a previous stage, or explicitly in the workflow stage's input spec.

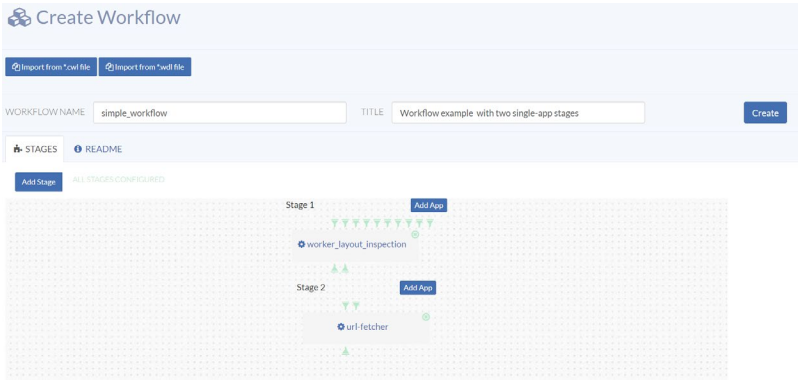
Click the  button to enter an explicit URL for this Stage.



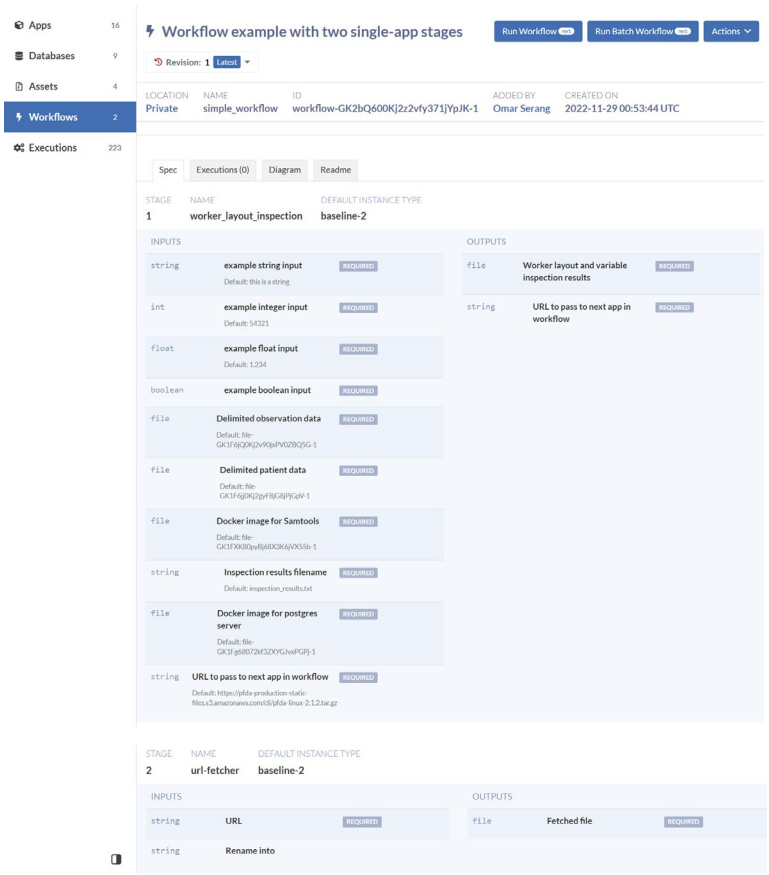
However, we want to specify this input field using the output field from the previous stage by clicking on the  button.



Select the Baseline 2 instance type to override the app default value and close the stage. Note that everything is green now and ready to Create.

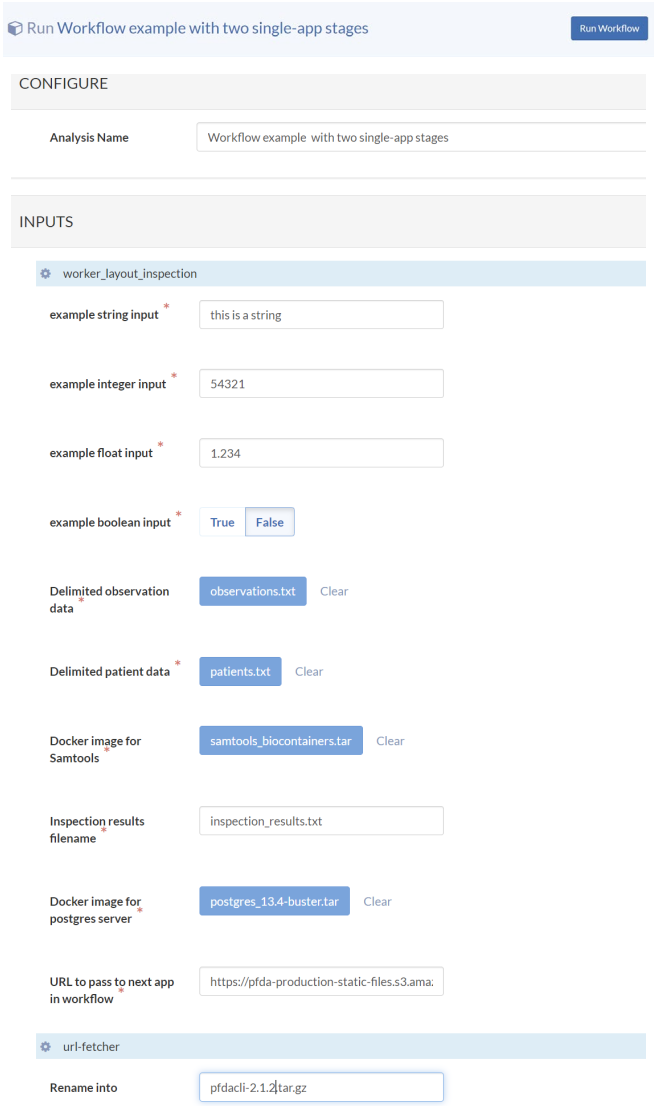


You can view the two stages of your new workflow.

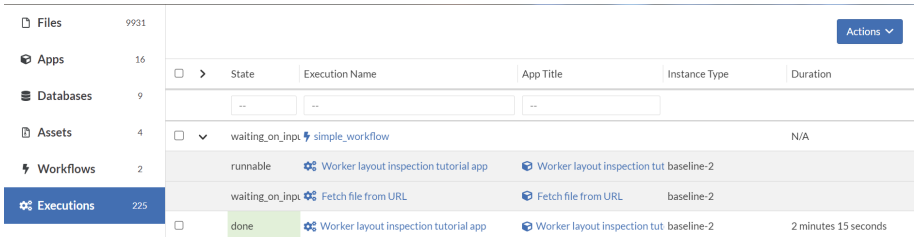

Apps 16
Databases 9
Assets 4
Workflows 2
Executions 223
Workflow example with two single-app stages
Run Workflow
Run Batch Workflow
Actions
Revision: 1 Latest
LOCATION NAME ID ADDED BY CREATED ON
Private simple_workflow workflow-GK2bQ600Kj2z2vfy371jYpJK-1 Omar Serang 2022-11-29 00:53:44 UTC
Spec
Executions (0)
Diagram
Readme
STAGE NAME DEFAULT INSTANCE TYPE
1 worker_layout_inspection baseline-2
INPUTS
string example string input REQUIRED
Default: this is a string
int example integer input REQUIRED
Default: 54321
float example float input REQUIRED
Default: 1.234
boolean example boolean input REQUIRED
file Delimited observation data REQUIRED
Default: file-GK1F6jQ0KJ2v90jxPV0ZBQ5G-1
file Delimited patient data REQUIRED
Default: file-GK1F6jQ0KJ2pvF8JG8jPJGpV-1
file Docker image for Samtools REQUIRED
Default: file-GK1FXK80qvBj68X3K6JVX55b-1
string Inspection results filename REQUIRED
Default: inspection_results.txt
file Docker image for postgres server REQUIRED
Default: file-GK1Fg66072f3ZXYGJvxPGPJ-1
string URL to pass to next app in workflow REQUIRED
Default: https://pfda-production-static-files.s3.amazonaws.com/cli/pfda-linux-2.1.2.tar.gz
OUTPUTS
file Worker layout and variable inspection results REQUIRED
string URL to pass to next app in workflow REQUIRED
STAGE NAME DEFAULT INSTANCE TYPE
2 url-fetcher baseline-2
INPUTS
string URL REQUIRED
string Rename into
OUTPUTS
file Fetched file REQUIRED

Run the workflow

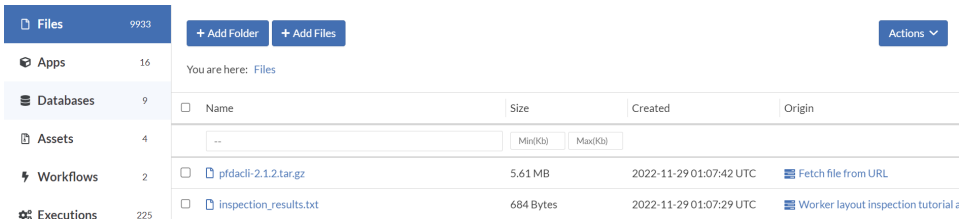
Click on the Run Workflow button, accept all the default values for the workflow_layout_inspection stage, but enter *pfdacl.tar.gz* in the *Rename into* field in the second stage, then run the workflow.



In the Executions tab, expand the simple_workflow listing to see the two executions associated with the workflow.



Once the stages have completed, the workflow is done and we can open the executions associated with the stages and inspect the logs. Also note the inspection results file from stage 1 and the renamed fetched URL file from stage 2.

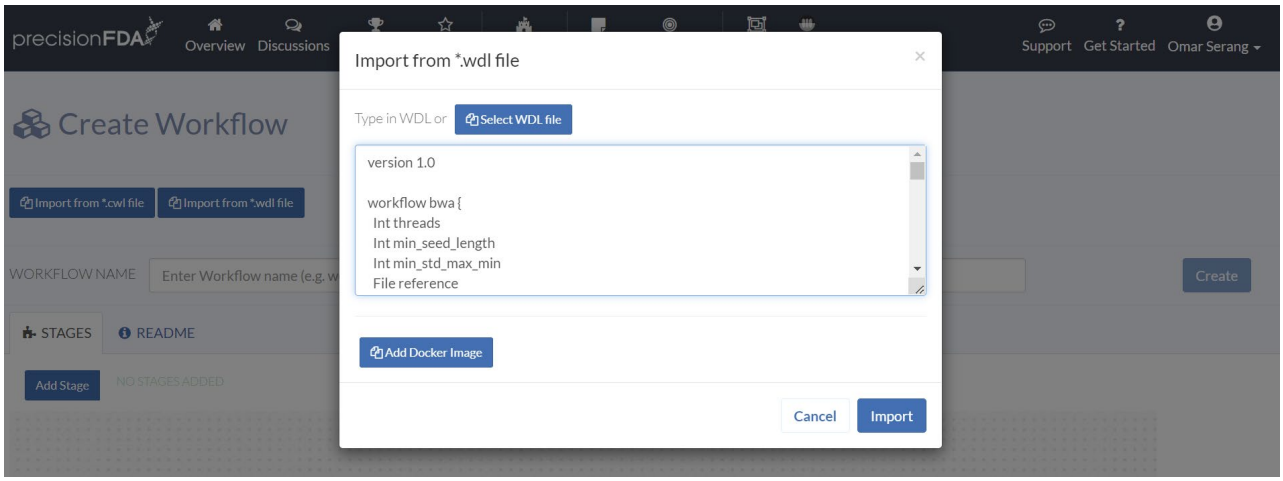


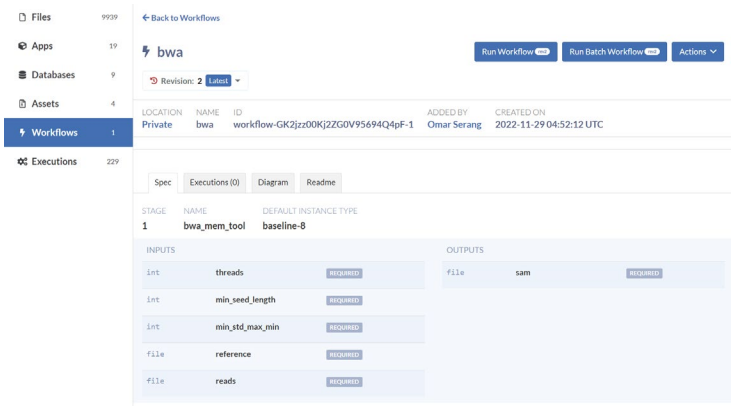
Second Workflow: *workflow_from_wdl*

Importing a workflow from a WDL specification based on Docker images provides convenient way to express precisionFDA workflows in a serialized textual format. From My Home / Workflows, click the Create Workflow button, and click the Import from *.wdl file button. Enter the following WDL in the text input and click Import.

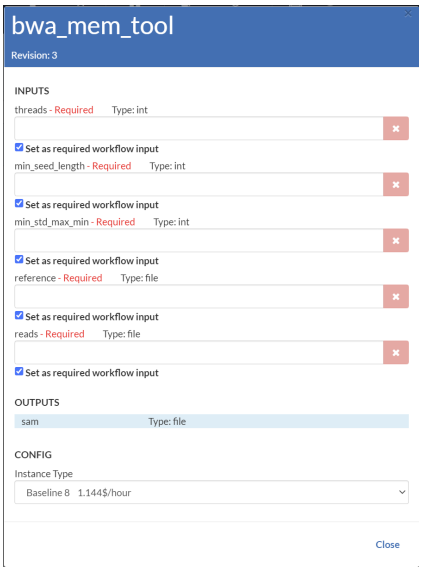
```
version 1.0

workflow bwa {
  Int threads
  Int min_seed_length
  Int min_std_max_min
  File reference
  File reads

 call bwa_mem_tool {
   threads = threads,
   min_seed_length = min_seed_length,
   min_std_max_min =  min_std_max_min,
   reference = reference,
   reads = reads
 }
}

task bwa_mem_tool {
  Int threads
  Int min_seed_length
  Int min_std_max_min
  File reference
  File reads

  command {
     bwa mem -t ${threads} \
     -k ${min_seed_length} \
     -I ${sep=',' min_std_max_min+} \
     ${reference} \
     ${sep=' ' reads+} > output.sam
  }
```

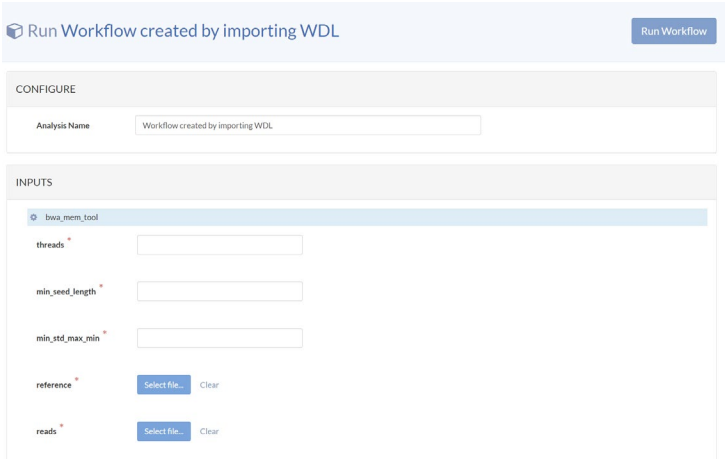
```
  output {
    File sam = "output.sam"
  }

  runtime {
    docker: "broadinstitute/baseimg"
  }
}
```





Like workflows created through the web inteface, WDL-based workflows can be updated and run.



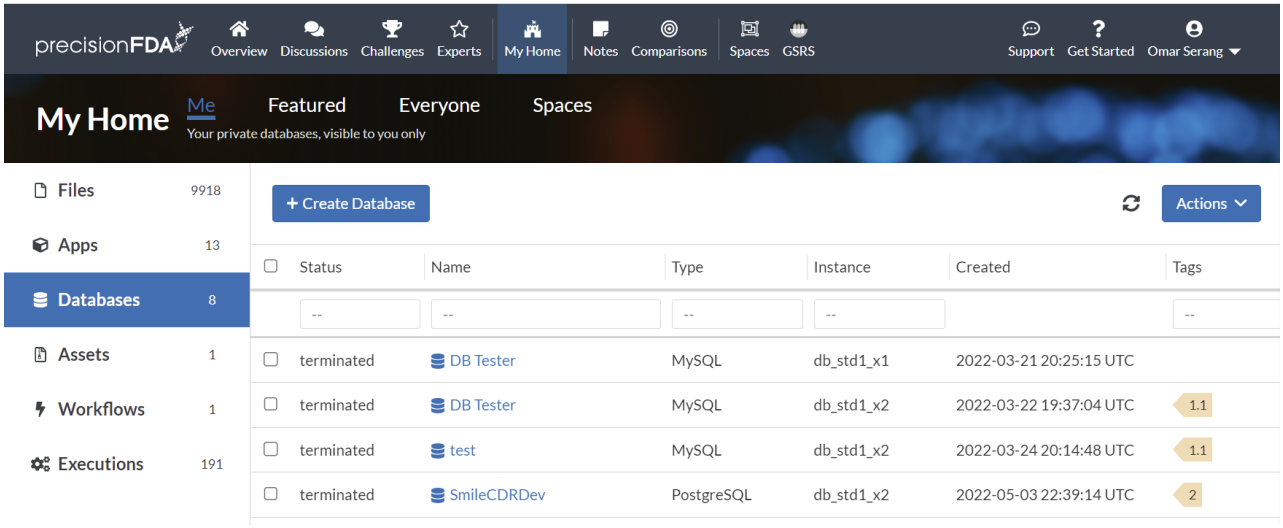


Database App: *worker_database*

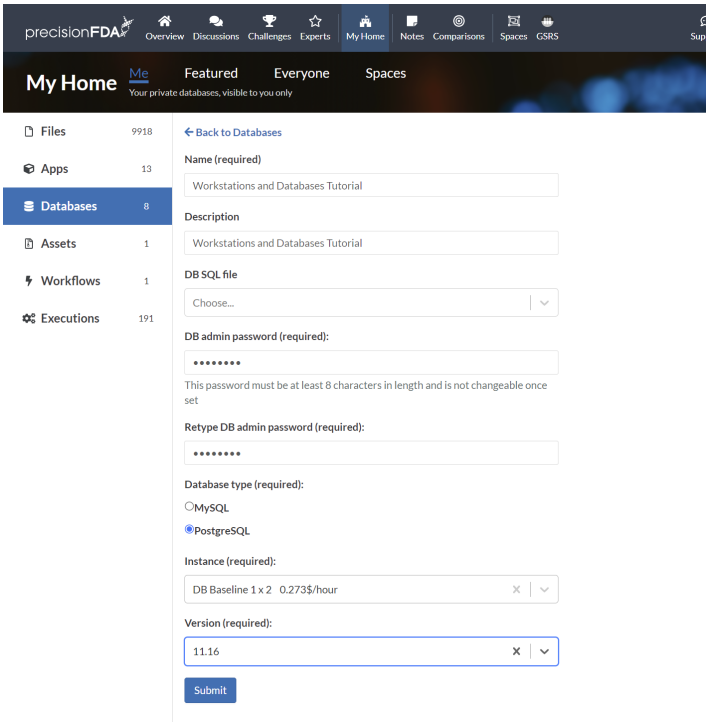
This app demonstrates the use of a precisionFDA Database cluster (PostgreSQL), a convenient and very power resource for RDBMS-based analytics. You will need to be authorized for DB Clusters in order to create the database for this app.

Create the Database

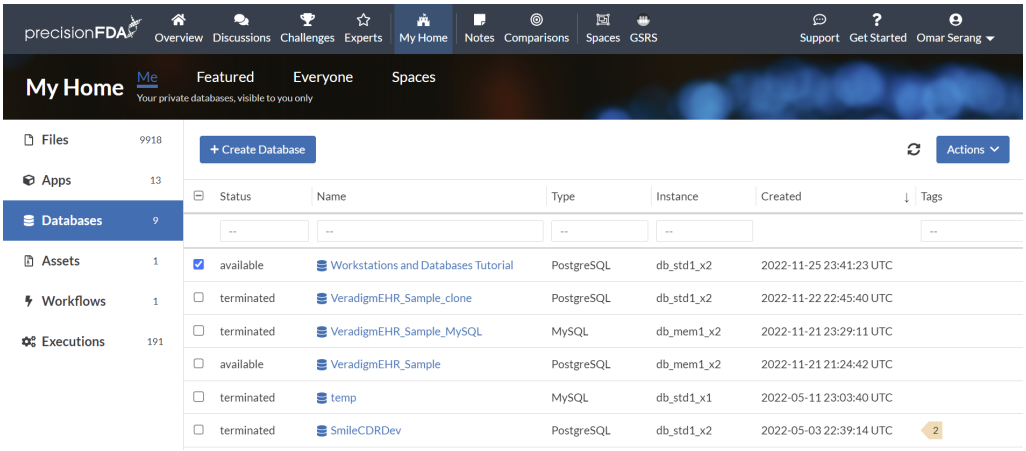
Select the Databases tab in My Home and click the Create Database button.



Create a “Workstations and Databases Tutorial” database, “password”, PostgreSQL 11.16 on the smallest available database instance type, and click the Submit button.



Refresh the database status using the button until the database is available.



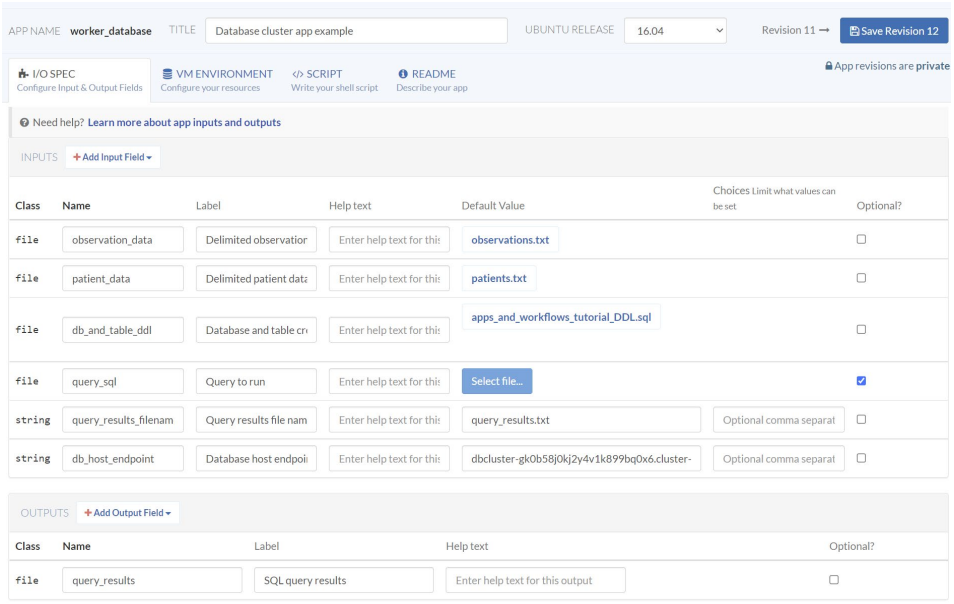
Fork *workstation_layout_inspection* to *workstation_database* app

Using My Home / Apps, select the worker_layout_inspection app and select Fork. Name the new application *worker_database* titled "Database cluster app example".

Specify the I/O Spec

Update the I/O spec to the following:

Class	Input Name	Label	Default Value
file	observation_data	Delimited data file for ETL into OBSERVATION table.	observations.txt
file	patient_data	Delimited data file for ETL into PATIENT table.	patients.txt
file	db_and_table_ddl	Database and table creation DDL	
file	query_sql	Query to run	(optional)
string	db_endpoint_url	Database host endpoint	
string	query_results_filename	Query results file name	query_results.txt
Class	**Output Name**	**Label**	
file	query_results	SQL query results	



Specify the VM Environment

Update the VM environment to keep internet access enabled, Baseline 2 default instance type, and remove the pfda_cli_2.2 and ubuntu_asset assets so that only the worker_layout_inspection asset remains. Note that it can take minutes for the list of assets to loaded before they can be searched.

Specify the Script

Enter the following Script:

```
set -euxo pipefail

# Install postgres client
sudo apt install -y postgresql-client
psql --version

# Inspect the database and table DDL
# and the three data files for ETL.
# Two data files specified as inputs.
#cat "$db_and_table_ddl_path"
#cat "$observation_data_path"
#cat "$patient_data_path"

# Third data file installed with the worker_layout_inspection asset
#cat /work/countries.txt

# Connect to the DB cluster and list the databases
PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d postgres -c
'\l'

# Create the apps_and_workflows_tutorial_db and three tables
PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d postgres -f
"$db_and_table_ddl_path"
```

```
PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d
apps_and_workflows_tutorial_db -c '\d'

# ETL the OBSERVATION table data
PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d
apps_and_workflows_tutorial_db -c "\copy public.\"OBSERVATION\" from
'/work/in/observation_data/observations.txt' delimiter '|' NULL ''"

PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d
apps_and_workflows_tutorial_db -c "select * from public.\"OBSERVATION\""

# ETL the PATIENT table data
PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d
apps_and_workflows_tutorial_db -c "\copy public.\"PATIENT\" from
'/work/in/patient_data/patients.txt' delimiter '|' NULL ''"

PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d
apps_and_workflows_tutorial_db -c "select * from public.\"PATIENT\""

# ETL the COUNTRY table data
PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d
apps_and_workflows_tutorial_db -c "\copy public.\"COUNTRY\" from
'/work/countries.txt' delimiter '|' NULL ''"

PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d
apps_and_workflows_tutorial_db -c "select * from public.\"COUNTRY\""

# Run the specified query and put the results into the specified
filename.
PGPASSWORD="password" psql -h "$db_host_endpoint" -U root -d
apps_and_workflows_tutorial_db -f "$query_sql_path" | tee -a
"$query_results_filename"

emit "query_results" "$query_results_filename"
```

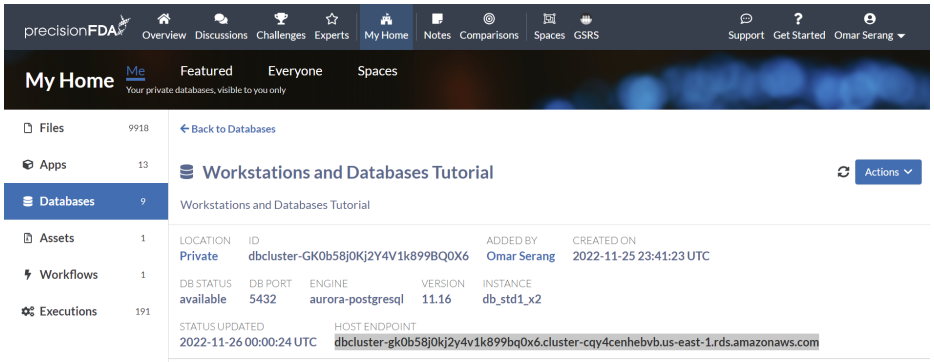
Specify the Readme

Enter a Readme and Create the app.

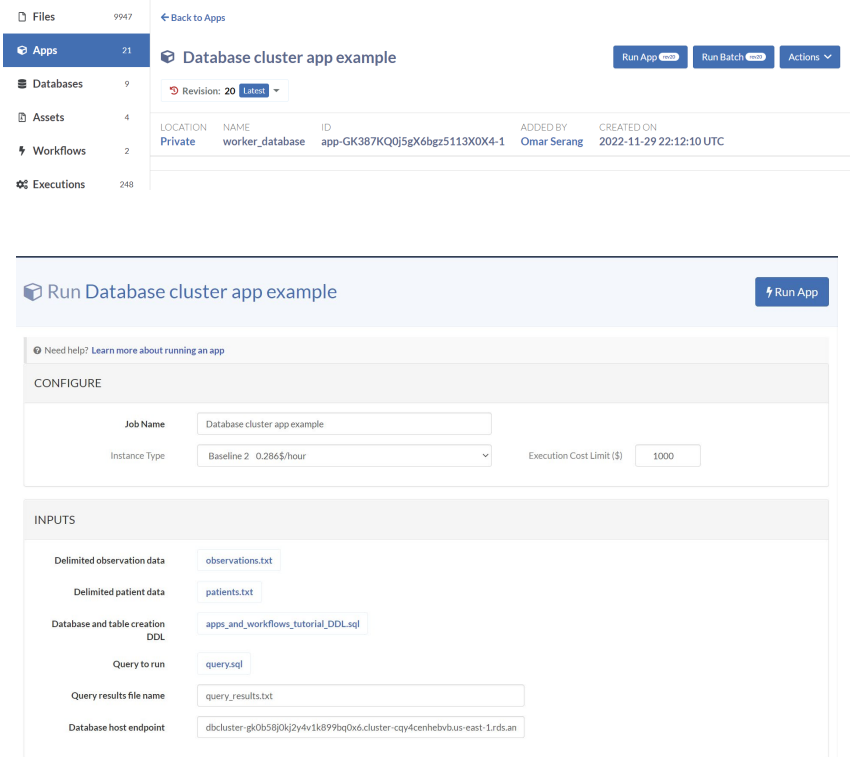
```
Connect to a database cluster and create a database and three tables.
Load two tables with data provided as input files, and the third table
with data from an asset. Present a specified query file and retrieve the
query results file.
```

Run the app

Click on the Workstations and Databases Tutorial database to open the detail page and copy the host endpoint URL.



Run the app providing the database host endpoint URL copied above, and leave the remaining inputs at their default values.



Inspect the execution logs

View the logs for the *Database cluster app example* execution using the Actions dropdown menu. Let's look at a condensed and annotated version of the log output to understand what our app just did.

```
# Install the assets and file inputs on the worker filesystem
Fetching asset worker_layout_inspection2.tar (file-
GK1xxbQ0Kj2gBZjxF244F21k)
downloading file: file-GK2xgy80Kj2x48j54fXGqF1V to filesystem:
/work/in/query_sql/query.sql
```

```
downloading file: file-GK1F6jj0Kj2gyF8jG8jPjGpV to filesystem:
/work/in/patient_data/patients.txt
downloading file: file-GK2v2Zj0Kj2gk9GB1920BYP3 to filesystem:
/work/in/db_and_table_ddl/apps_and_workflows_tutorial_DDL.sql
downloading file: file-GK1F6jQ0Kj2v90jxPV0ZBQ5G to filesystem:
/work/in/observation_data/observations.txt

# Install postgres CLI client and display version
++ sudo apt install -y postgresql-client
++ psql --version
psql (PostgreSQL) 9.5.25

# Providing the password, connect to the specified host,
# user root, database postgres, and list the databases on the cluster.
++ PGPASSWORD=password
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d postgres -c '\l'
                                                  List of databases
                  Name                  |  Owner   | Encoding |
Collate   |    Ctype    |   Access privileges
----------------------------------------+----------+----------+---------
----+-------------+-----------------------
 apps_and_workflows_tutorial_db         | root     | UTF8     |
en_US.UTF-8 | en_US.UTF-8 |
 postgres                               | root     | UTF8     |
en_US.UTF-8 | en_US.UTF-8 |
 rdsadmin                               | rdsadmin | UTF8     |
en_US.UTF-8 | en_US.UTF-8 | rdsadmin=CTc/rdsadmin
 template0                              | rdsadmin | UTF8     |
en_US.UTF-8 | en_US.UTF-8 | =c/rdsadmin          +
                                        |          |          |
|             | rdsadmin=CTc/rdsadmin

# Create a new database and tables
++ PGPASSWORD=password
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d postgres -f
/work/in/db_and_table_ddl/apps_and_workflows_tutorial_DDL.sql
 template1                              | root     | UTF8     |
en_US.UTF-8 | en_US.UTF-8 | =c/root              +
                                        |          |          |
|             | root=CTc/root
 workstations_and_databases_tutorial_db | root     | UTF8     |
en_US.UTF-8 | en_US.UTF-8 |
(6 rows)

 pg_terminate_backend
----------------------
(0 rows)

DROP DATABASE
```

```
CREATE DATABASE
You are now connected to database "apps_and_workflows_tutorial_db" as
user "root".
CREATE TABLE
CREATE TABLE
CREATE TABLE

# Connect to the new database and list the new tables
++ PGPASSWORD=password
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d apps_and_workflows_tutorial_db -c
'\d'
          List of relations
 Schema |    Name     | Type  | Owner
--------+-------------+-------+-------
 public | COUNTRY     | table | root
 public | OBSERVATION | table | root
 public | PATIENT     | table | root
(3 rows)

# ETL the OBSERVATION table from the specified file.
++ PGPASSWORD=password
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d apps_and_workflows_tutorial_db -c
'\copy public."OBSERVATION" from
'\''/work/in/observation_data/observations.txt'\'' delimiter '\''|'\''
NULL '\''''\'''
COPY 5
++ PGPASSWORD=password
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d apps_and_workflows_tutorial_db -c
'select * from public."OBSERVATION"'
 observation_id | patient_id | observation_name |   loinc   |
created_date
---------------+------------+------------------+-----------+-----------
---
           9870 |      12345 | Annual check up  | 66678-4   | 2022-11-01
           9871 |      12345 | Emergency        | LG32756-5 | 2022-11-02
           9872 |      12346 | Clinic visit     | 66678-4   | 2022-11-03
           9873 |      12347 | Lab results      | 74418-5   | 2022-11-04
           9874 |      12347 | Post-op checkup  | 65375-8   | 2022-11-05
(5 rows)

# ETL the PATIENT table from the specified file.
++ PGPASSWORD=password
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d apps_and_workflows_tutorial_db -c
'\copy public."PATIENT" from '\''/work/in/patient_data/patients.txt'\''
delimiter '\''|'\'' NULL '\''''\'''
COPY 3
++ PGPASSWORD=password
```

```
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d apps_and_workflows_tutorial_db -c
'select * from public."PATIENT"'
 patient_id |     name      | gender |  zip  | country_id | created_date
------------+---------------+--------+-------+------------+-------------
-
      12345 | Fred Foobar   | M      | 94040 |       1001 | 2022-10-25
      12346 | Mary Merry    | F      | 94040 |       1002 | 2022-09-24
      12347 | Barney Rubble | M      | 94040 |       1003 | 2022-08-23
(3 rows)

# ETL the COUNTRY table as installed from the asset.
++ PGPASSWORD=password
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d apps_and_workflows_tutorial_db -c
'\copy public."COUNTRY" from '\''/work/countries.txt'\'' delimiter
'\''|'\'' NULL '\''''\'''
COPY 3
++ PGPASSWORD=password
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d apps_and_workflows_tutorial_db -c
'select * from public."COUNTRY"'
 country_id | country_name
------------+--------------
       1001 | USA
       1002 | CAN
       1003 | EU
(3 rows)

# Run the specified query.
++ PGPASSWORD=password
++ psql -h dbcluster-gk0b58j0kj2y4v1k899bq0x6.cluster-cqy4cenhebvb.us-
east-1.rds.amazonaws.com -U root -d apps_and_workflows_tutorial_db -f
/work/in/query_sql/query.sql
++ tee -a query_results.txt
Expanded display is on.
-[ RECORD 1 ]----+----------------
patient_id       | 12345
name             | Fred Foobar
gender           | M
zip              | 94040
country_id       | 1001
created_date     | 2022-10-25
observation_id   | 9870
observation_name | Annual check up
loinc            | 66678-4
created_date     | 2022-11-01
country_id       | 1001
country_name     | USA
-[ RECORD 2 ]----+----------------
patient_id       | 12345
```

```
name              | Fred Foobar
gender            | M
zip               | 94040
country_id        | 1001
created_date      | 2022-10-25
observation_id    | 9871
observation_name  | Emergency
loinc             | LG32756-5
created_date      | 2022-11-02
country_id        | 1001
country_name      | USA
-[ RECORD 3 ]----+----------------
patient_id        | 12346
name              | Mary Merry
gender            | F
zip               | 94040
country_id        | 1002
created_date      | 2022-09-24
observation_id    | 9872
observation_name  | Clinic visit
loinc             | 66678-4
created_date      | 2022-11-03
country_id        | 1002
country_name      | CAN
-[ RECORD 4 ]----+----------------
patient_id        | 12347
name              | Barney Rubble
gender            | M
zip               | 94040
country_id        | 1003
created_date      | 2022-08-23
observation_id    | 9873
observation_name  | Lab results
loinc             | 74418-5
created_date      | 2022-11-04
country_id        | 1003
country_name      | EU
-[ RECORD 5 ]----+----------------
patient_id        | 12347
++ emit query_results query_results.txt
name              | Barney Rubble
gender            | M
zip               | 94040
country_id        | 1003
created_date      | 2022-08-23
observation_id    | 9874
observation_name  | Post-op checkup
loinc             | 65375-8
created_date      | 2022-11-05
country_id        | 1003
country_name      | EU
```