Reproducible Science - Automation

Jul 22, 2020

Contents:

Tutorial on creating a reproducible python package.

CHAPTER 1

Introduction

This tutorial will teach you how to automate your data analysis using TAPIS.

1.1 Module Learning Objectives

In this example, we will show you how to setup automated analysis that is triggered when a file is uploaded to TACC.

Participants are **strongly encouraged** to follow along on the command line. After completing this module, participants should be able to:

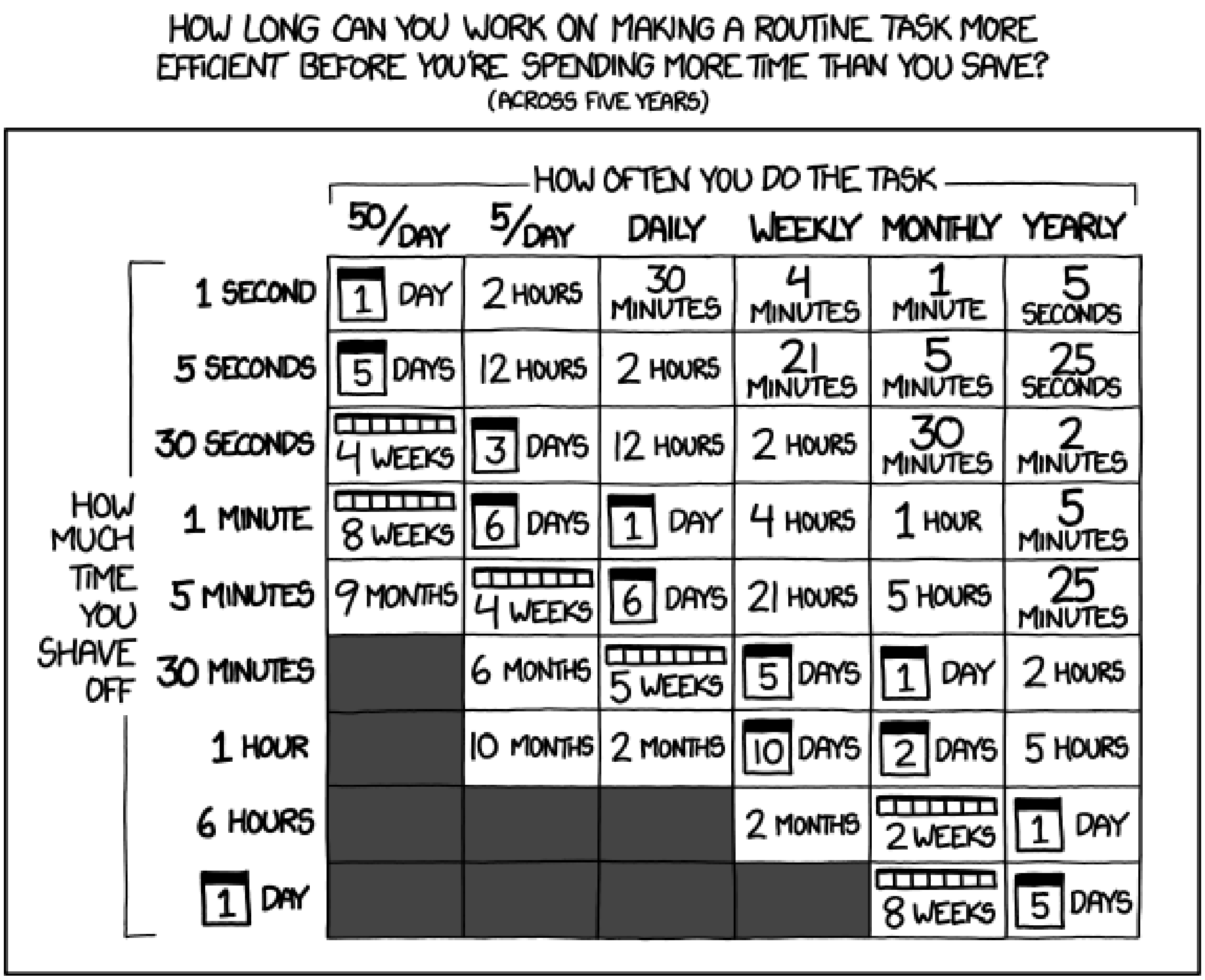
- Create a TAPIS notification when files are uploaded to a specific location
- Trigger an Abaco actor in response to a notification
- Use an Abaco actor to submit an job to an Application

And we're going to work backwards, first creating the tpp, then the actor, and finally the notification.

1.2 Why is this important?

As you develop your computational skills, you will find that these skill are in high demand. Basic operations like moving files, interpreting metadata, initiating scripts, and formatting outputs will take up and inordinate amount of your time and are boring. If you can standardize your process for data ingest, you can automate the boring parts of your work. And can instead devote more time to interpreting your analysis and working on a new, improved version of your pipeline. Moreover, automating analysis will standardize the processing of your data, so in 6 months from now when your computational results have been verified experimentally you can go look back at what version of the application was run, what the parameters were, and write your methods section accordingly. Instead of having to guess or remember what you did, you can just check the records.

Don't underestimate the time-saving value of automation! Check out this informative chart from XKCD


HOW LONG CAN YOU WORK ON MAKING A ROUTINE TASK MORE EFFICIENT BEFORE YOU'RE SPENDING MORE TIME THAN YOU SAVE?
(ACROSS FIVE YEARS)

HOW MUCH TIME YOU SHAVE OFF	HOW OFTEN YOU DO THE TASK: 50/DAY	5/DAY	DAILY	WEEKLY	MONTHLY	YEARLY
1 SECOND	1 DAY	2 HOURS	30 MINUTES	4 MINUTES	1 MINUTE	5 SECONDS
5 SECONDS	5 DAYS	12 HOURS	2 HOURS	21 MINUTES	5 MINUTES	25 SECONDS
30 SECONDS	4 WEEKS	3 DAYS	12 HOURS	2 HOURS	30 MINUTES	2 MINUTES
1 MINUTE	8 WEEKS	6 DAYS	1 DAY	4 HOURS	1 HOUR	5 MINUTES
5 MINUTES	9 MONTHS	4 WEEKS	6 DAYS	21 HOURS	5 HOURS	25 MINUTES
30 MINUTES	▨	6 MONTHS	5 WEEKS	5 DAYS	1 DAY	2 HOURS
1 HOUR	▨	10 MONTHS	2 MONTHS	10 DAYS	2 DAYS	5 HOURS
6 HOURS	▨	▨	▨	2 MONTHS	2 WEEKS	1 DAY
1 DAY	▨	▨	▨	▨	8 WEEKS	5 DAYS

This module is about 90 minutes, so if this process shaves 30 seconds off of something you do once a week, or shaves 30 minutes off something you do once a year, then it's worth the time investment!

1.3 Requirements

- Accounts
  - GitHub
  - Docker Hub Account
- Software
  - Python 3
  - git
  - python pip
  - Tapis CLI
  - Docker CE
  - Storage and Execution systems setup from the TAPIS module

CHAPTER 2

Deploying An Application

We're going to take some of what we've learned from best practices and put it into, well, practice. Apps deploy is a CLI command that will build a docker container, push it to dockerhub, upload your app asset bundle to a deploymentSystem, and register your app on an executionSystem all in a single step. Apps deploy is a single command that replaces:

```
docker build -t $DOCKER_USERNAME/$DOCKER_REPO:$DOCKER_TAG -f Dockerfile
docker push $DOCKER_USERNAME/$DOCKER_REPO:$DOCKER_TAG
tapis files upload agave://$DEPLOYMENT_SYSTEM/$DEPLOYMENT_PATH/ runner.sh
tapis apps create -F app.json
```

And we plan on adding even more in the future! Namely an automatic upload to GitHub so there's a source controlled snapshot of each deployment.

2.1 Setup Tapis CLI

Let's go ahead and install the TAPIS CLI on your host system:

```
pip install tapis-cli
```

And re-run:

```
tapis auth init
```

Or, if you want to be clever, move over the authentication directory we created last week:

```
cp -R ~/.tapis ~/.agave
```

To check Tapis is setup correctly, you can run:

```
tapis systems search --public eq false
```

and you should see the storage and executions systems we setup last week.

2.2 Docker CLI Tangent

You might be wondering: "Can I just re-use the TAPIS container the same way we did last week?". And yes, you can, but there are some caveats. See this tangent for more info.

2.3 Copy an Application from Github

Let's create a Tapis app to perform some analysis. For this example we'll create a fastqc application that is triggered when `.fastq` files are uploaded to a certain directory, but you can use any application or file type for this.

You can clone the fastqc example app from here:

```
git clone https://github.com/JoshuaUrrutia/fastqc_app.git
cd fastqc_app
```

Or, if you'd like, you're welcome to use application that was created last week: https://tacc.github.io/summer-institute-2020-tapis/block2/apps/

2.4 Find deploymentPath

Remember the storage system we created last week?

```
{
"id": "UPDATEUSERNAME.stampede2.storage",
"name": "Storage system S2",
"status": "UP",
"type": "STORAGE",
"description": "Storage system for TACC cloud storage on S2",
"site": "www.tacc.utexas.edu",
"public": false,
"default": true,
"storage": {
  "host": "stampede2.tacc.utexas.edu",
  "port": 22,
  "protocol": "SFTP",
  "rootDir": "/",
  "homeDir": "/work/dir../UPDATEUSERNAME/stampede2",
  "auth": {
    "username": "UPDATEUSERNAME",
    "publicKey":"paste public key here",
    "privateKey":"paste private key here",
    "type": "SSHKEYS"
  }
}
}
```

By default our write operations when we run `tapis apps deploy` will write to the `rootDir` above. If you plan on deploying lots of apps, it's a good idea to redefine the rootDir on your system to be a directory where you have write access, for example replacing the rootDir with your homeDir: `/work/dir../UPDATEUSERNAME/stampede2`. This will simplify the structure of your `app.ini` file, and you won't have to lookup or remember your directory number when listing and uploading files.

But, since this system is already created, we'll just grab the absolute path to the `homeDir` directory where we have write access.

To get a full listing of your system, run:

```
tapis systems show -f json $USERNAME.stampede2.storage
```

And look for the "homeDir" key in the json response:

```
"homeDir": "/work/05369/urrutia/stampede2/"
```

Ok and now we'll create a directory called *apps* where we'll store all our app bundles.

```
# tapis files mkdir agave://urrutia.stampede2.storage/work/05369/urrutia/stampede2/␣
↪apps
tapis files mkdir agave://$USERNAME.stampede2.storage/$HOME_DIR apps
```

2.5 Edit the app.ini file

Replace the docker username and storage_path in the app.ini, with your docker username and your homeDir (the location on your storage system where you have write access).

```
[app]
name = fastqc
label = fastqc
description = FastQC app to assess fastq quality
version = 0.11.9
storage_system = stampede2.storage
storage_path = /work/05369/urrutia/stampede2/
hpc_system = stampede2.execution
bundle = assets



[docker]
dockerfile = Dockerfile
namespace = jurrutia
repo = fastqc_app
tag = 0.11.9

[env]

[git]
branch = main
```

The contents of the app.ini file will be injected into your app definition (app.json):

```
{
  "name": "{{ agave.username }}-{{ app.name }}",
  "version": "{{ app.version }}",
  "executionType": "HPC",
  "executionSystem": "{{ agave.username }}.{{ app.hpc_system}}",
  "parallelism": "SERIAL",
  "deploymentPath": "{{ app.storage_path}}/apps/{{ app.name }}-{{ app.version }}",
  "deploymentSystem": "{{ agave.username }}.{{ app.storage_system}}",
  "defaultProcessorsPerNode": 1,
  "defaultNodeCount": 1,
  "defaultQueue": "normal",
```

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```
  "label": "FastQC",
  "modules": ["load tacc-singularity"],
  "shortDescription": "{{ app.description }}",
  "templatePath": "runner-template.sh",
  "testPath": "tester.sh",
  "inputs": [
  {
  "id": "fastq",
  "value": {
    "default": "agave://data.iplantcollaborative.org/urrutia//sample/reads1.fastq.gz",
    "visible": true,
    "required": true
  },
  "semantics": {
    "ontology": [
      "http://edamontology.org/format_1930"
    ]
  },
  "details": {
    "label": "FASTQ sequence file"
  }
}
  ],
  "parameters": [{
    "id": "CONTAINER_IMAGE",
    "value": {
      "default": "{{ docker.organization }}/{{ docker.repo }}:{{ docker.tag }}",
      "description": "Container Image. Do not edit.",
      "type": "string",
      "visible": false,
      "required": true
    }
  }],
  "outputs": []
}
```

2.6 Deploy the Application

All that's left now is to deploy the application from the FastQC repo:

```
tapis apps deploy
```

Which should print out a table like this:

```
+--------+----------------------------------------------------------------------------
↪------------------------------------------------------------------------------------
↪-----------------------------+
| stage  | message                                                                    ␣
↪                                                                                    ␣
↪                             |
+--------+----------------------------------------------------------------------------
↪------------------------------------------------------------------------------------
↪-----------------------------+
| build  | Step 1/4 : FROM python:3.8                                                 ␣
↪                                                                                    ␣
↪                             |
```

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```
| build   |  ---> ea8c3fb3cd86                                                        ␣
↪                                                                                   ␣
↪                               |
|         |                                                                         ␣
↪                                                                                   ␣
↪                               |
| build   | Step 2/4 : RUN apt-get update     && apt-get upgrade -y     && apt-get␣
↪install wget -y     && apt-get install zip -y     && apt-get install default-jre -y␣
↪                                   |
| build   |  ---> Using cache                                                         ␣
↪                                                                                   ␣
↪                               |
|         |                                                                         ␣
↪                                                                                   ␣
↪                               |
| build   |  ---> f0f2bd1f3194                                                        ␣
↪                                                                                   ␣
↪                               |
|         |                                                                         ␣
↪                                                                                   ␣
↪                               |
| build   | Step 3/4 : RUN wget https://www.bioinformatics.babraham.ac.uk/projects/
↪fastqc/fastqc_v0.11.9.zip     && unzip fastqc_v0.11.9.zip     && rm fastqc_v0.11.9.
↪zip     && chmod +x FastQC/fastqc |
| build   |  ---> Using cache                                                         ␣
↪                                                                                   ␣
↪                               |
|         |                                                                         ␣
↪                                                                                   ␣
↪                               |
| build   |  ---> 3bea8add49b6                                                        ␣
↪                                                                                   ␣
↪                               |
|         |                                                                         ␣
↪                                                                                   ␣
↪                               |
| build   | Step 4/4 : ENV PATH "/FastQC/:$PATH"                                      ␣
↪                                                                                   ␣
↪                               |
| build   |  ---> Using cache                                                         ␣
↪                                                                                   ␣
↪                               |
|         |                                                                         ␣
↪                                                                                   ␣
↪                               |
| build   |  ---> cfafe349377a                                                        ␣
↪                                                                                   ␣
↪                               |
|         |                                                                         ␣
↪                                                                                   ␣
↪                               |
| build   | Successfully built cfafe349377a                                           ␣
↪                                                                                   ␣
↪                               |
|         |                                                                         ␣
↪                                                                                   ␣
↪                               |
```

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```
| build  | Successfully tagged jurrutia/fastqc_app:0.11.9                                    ␣
↪                                                                                            ␣
↪                              |
|        |                                                                                   ␣
↪                                                                                            ␣
↪                              |
| push   | The push refers to repository [docker.io/jurrutia/fastqc_app]                     ␣
↪                                                                                            ␣
↪                              |
| push   | 0.11.9: digest:␣
↪sha256:4ee48dae892538f83b69d6a1a7dbf099c51d3d032e44d0241518984897b5274f size: 2642 ␣
↪                                                                                            ␣
↪     |
| upload | assets/runner-template.sh                                                         ␣
↪                                                                                            ␣
↪                              |
| upload | assets/tester.sh                                                                  ␣
↪                                                                                            ␣
↪                              |
| upload | assets/_lib/CONTAINER_IMAGE                                                       ␣
↪                                                                                            ␣
↪                              |
| upload | assets/_lib/extend-runtime.sh                                                     ␣
↪                                                                                            ␣
↪                              |
| create | Created Tapis app urrutia-fastqc-0.11.9 revision 1                                ␣
↪                                                                                            ␣
↪                              |
+--------+------------------------------------------------------------------------------------
↪------------------------------------------------------------------------------------
↪-----------------------------+
```

CHAPTER 3

Deploying an Actor

What is an actor? See more info in our documentation:

- Abaco documentation
- Abaco swagger guide

Basically a Tapis actor is a script, that lives in the cloud, and does something for you. It's not for compute intensive jobs, that's what apps are for, it's designed to be quick, responsive, and lightweight.

We're going to deploy an actor that will receive a notification when a file is uploaded, create a Tapis `job.json`, and submit that job to our FastQC application.

3.1 Copy a Reactor from Github

Clone a Abaco reactor I created to submit FastQC jobs:

```
git clone https://github.com/JoshuaUrrutia/fastqc_router_reactor.git
```

3.2 Edit actor.ini and config.yml

We'll need to make edits to actor.ini so that it points to your dockerhub username:

```
[actor]
name = fastqc_router
token = True

[docker]
dockerfile = Dockerfile
namespace = jurrutia
repo = fastqc_router
tag = 0.2
```

And change the name of the app in `config.yml`, so it matches your app id. And change the email address there so the notification is sent to your email:

```
---
logs:
  level: DEBUG
  token: ~
fastqc:
  appId: urrutia-fastqc-0.11.9
  name: fastqc_test
  archive: true
  archivePath: ""
  archiveSystem: ""
  inputs:
    fastq: ""
  notifications:
    -
      event: FINISHED
      url: your@email.com
```

Now we create an empty `secrets.json` file. It's just empty in this example, but if you had passwords or credentials you wanted to be available in your actor, you could add those to the secrets.json. It is included in the `.gitignore` file for this repo so you don't accidentally push a password to github.

```
cp secrets.json.sample secrets.json
```

3.3 Deploy the Actor

All that's left is to deploy our reactor:

```
tapis actors deploy
```

You should see a response like:

```
Building jurrutia/fastqc_router:0.1
Finished (27932 msec)
Pushing jurrutia/fastqc_router:0.1
Finished (9354 msec)
+--------+-----------------------------------------------------------------------------
↪---------------------+
| stage  | message                                                                    ␣
↪                     |
+--------+-----------------------------------------------------------------------------
↪---------------------+
| build  | Step 1/1 : FROM jurrutia/reactors:python2-edge                             ␣
↪                     |
| build  | # Executing 5 build trigger                                                ␣
↪                     |
| build  | s                                                                          ␣
↪                     |
| build  |  ---> Running in 34bf66e2e455                                              ␣
↪                     |
|        |                                                                            ␣
↪                     |
| build  | You must give at least one requirement to install (see "pip help install")␣
↪                     |
```

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```
|         |                                                                                    ␣
↪                       |
| build   | Removing intermediate container 34bf66e2e455                                       ␣
↪                       |
|         |                                                                                    ␣
↪                       |
| build   |  ---> ca9ae97aef39                                                                 ␣
↪                       |
|         |                                                                                    ␣
↪                       |
| build   | Successfully built ca9ae97aef39                                                    ␣
↪                       |
|         |                                                                                    ␣
↪                       |
| build   | Successfully tagged jurrutia/fastqc_router:0.1                                     ␣
↪                       |
|         |                                                                                    ␣
↪                       |
| push    | The push refers to repository [docker.io/jurrutia/fastqc_router]                   ␣
↪                       |
| push    | 0.1: digest:␣
↪sha256:844f0ce2de5e03f1f15fedb64b7f5354bf64da453a18c87c6cb5c9981e6e8991 size: 6978 |
| create  | Created Tapis actor X4blX3Ez65qQZ                                                  ␣
↪                       |
| cache   | Cached actor identifier to disk                                                    ␣
↪                       |
+---------+-----------------------------------------------------------------------------------
↪---------------------+
```

Copy your actor id (`X4blX3Ez65qQZ` in the above example). If you forget the id, you can always list out your actors with `tapis actors list`.

3.4 Create a FastQC Folder

Now we'll create the `fastqc` folder on our storage system. After we create our notification, any file that is uploaded here will be analyzed automatically by our FastQC app!

```
# tapis files mkdir agave://urrutia.stampede2.storage/work/05369/urrutia/stampede2␣
↪fastqc
tapis files mkdir agave://$USERNAME.stampede2.storage/$HOME_DIR fastqc
```

3.5 Create File System Notifications

Now you're ready to create a file system notification. This notification will pass a message to the `fastqc_router_reactor` when a file is uploaded to the `fastqc` directory on your storage system. The `fastqc_router_reactor` takes this notification, crafts a `job.json`, and submits a job to the `fastqc_app`. We've created a python wrapper to help setup the file system notifications, you can download the python scripts here:

```
git clone https://github.com/JoshuaUrrutia/abaco_notifications.git
cd abaco_notifications
```

From the `abaco_notifications` directory, you can run `add_notify_reactor.py` to setup a notification. For example:

```
# python add_notify_reactor.py urrutia.stampede2.storage /work/05369/urrutia/
↪stampede2/fastqc X4blX3Ez65qQZ
python add_notify_reactor.py $AGAVE_SYSTEM_NAME $PATH_TO_DIRECTORY $ACTOR_ID
```

If it runs successfully your response should look like:

```
assocationIds = 8216966626126028310-242ac112-0001-002
notification id: 18251060861323945066-242ac116-0001-011
notification url: https://portals-api.tacc.utexas.edu/actors/v2/X4blX3Ez65qQZ/
↪messages?x-nonce=PORTALS_baTEq5E5oylx
```

If there are incompatibilities with your version of python you can also use a containerized version of `add_notify_reactor.py`:

```
docker run --rm -it \
           -v ${HOME}/.agave:/root/.agave \
           jurrutia/add_notify_reactor:0.1 \
           python /opt/add_notify_reactor.py \
           $AGAVE_SYSTEM_NAME \
           $PATH_TO_DIRECTORY \
           $ACTOR_ID
```

And you can see all your notification using the `notifications` endpoint:

```
tapis notifications list
```

3.6 Upload and Test

Now the only thing left to do is to test and see if our `upload -> notification -> reactor -> app` chain is functioning.

Upload a fastq file to your FastQC directory (you can find a copy of this file in the `fastqc_app/tests/` repo):

```
# tapis files upload agave://urrutia.stampede2.storage/work/05369/urrutia/stampede2/
↪fastqc reads1.fastq.gz
tapis files upload agave://$SYSTEM/$PATH/ $FILE
```

Now that we've uploaded lets see if our actor was triggered:

```
tapis actors execs list $ACTOR_ID
```

The response should look like:

```
urrutia$ tapis actors execs list X4blX3Ez65qQZ
+---------------+----------+
| executionId   | status   |
+---------------+----------+
| AqDao7YgEYZ6Z | COMPLETE |
+---------------+----------+
```

If you want to see the logs from your actor execution you can run:

```
tapis actors execs logs $ACTOR_ID $EXECUTION_ID
```

Finally, let's check to see if a job was submitted to our application:

```
tapis jobs list
+------------------------------------------+--------------------------------+---------
↪-+
| id                                       | name                           | status ␣
↪ |
+------------------------------------------+--------------------------------+---------
↪-+
| 485458bc-335d-4d05-ae30-70de2583b6d5-007 | fastqc_test                    |␣
↪FINISHED |
+------------------------------------------+--------------------------------+---------
↪-+
```

And go ahead and download the outputs of that job:

```
# tapis jobs outputs download 485458bc-335d-4d05-ae30-70de2583b6d5-007
# cd 485458bc-335d-4d05-ae30-70de2583b6d5-007
tapis jobs outputs download $JOB_ID
cd $JOB_ID
open reads1_fastqc.html
```

Congratulations, you successfully automated part of your workflow with Tapis! But there is no reason to stop here, you can add a notification to your FastQC jobs to trigger a new reactor (and perform an alignment maybe?), and build an entirely automated workflow by chaining together reactors and apps.

CHAPTER 4

Troubleshooting

4.1 Notifications

If the reactor never executed, you can check the notifications are working by posting notifications to `PostBin` using the `add_notify_requestbin.py` script in the `abaco_notifications` directory:

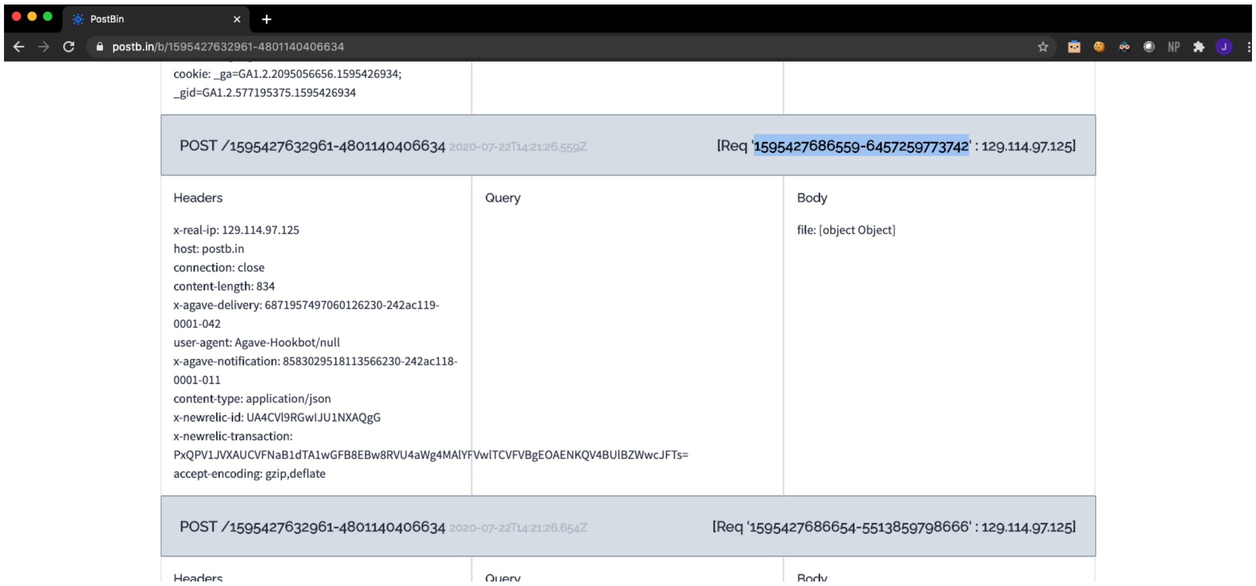
```
python add_notify_requestbin.py $AGAVE_SYSTEM_NAME $PATH_TO_DIRECTORY
assocationIds = 344770698063965720-242ac112-0001-002
notification id: 8583029518113566230-242ac118-0001-011
notification url: https://postb.in/b/1595427632961-4801140406634
```

You can re-upload the file and check the requestbin url to see if it receives the notification:

```
# tapis files upload agave://urrutia.stampede2.storage/work/05369/urrutia/stampede2/
↪fastqc reads1.fastq.gz
tapis files upload agave://$SYSTEM/$PATH/ $FILE
```

You can go to the PostBin URL to see all the requests, and to get more information about a specific request you can copy/paste the Request ID into a browser in this format:

```
# https://postb.in/api/bin/1595427632961-4801140406634/req/1595427686559-6457259773742
https://postb.in/api/bin/$BIN_ID/req/$REQUEST_ID
```



```
PostBin
postb.in/b/1595427632961-4801140406634

cookie: _ga=GA1.2.2095056656.1595426934;
_gid=GA1.2.577195375.1595426934

POST /1595427632961-4801140406634 2020-07-22T14:21:26.559Z        [Req '1595427686559-6457259773742' : 129.114.97.125]

Headers                                   Query        Body

x-real-ip: 129.114.97.125                              file: [object Object]
host: postb.in
connection: close
content-length: 834
x-agave-delivery: 6871957497060126230-242ac119-
0001-042
user-agent: Agave-Hookbot/null
x-agave-notification: 8583029518113566230-242ac118-
0001-011
content-type: application/json
x-newrelic-id: UA4CVl9RGwIJU1NXAQgG
x-newrelic-transaction:
PxQPV1JVXAUCVFNaB1dTA1wGFB8EBw8RVU4aWg4MAlYFVwlTCVFVBgEOAENKQV4BUlBZWwcJFTs=
accept-encoding: gzip,deflate

POST /1595427632961-4801140406634 2020-07-22T14:21:26.654Z        [Req '1595427686654-5513859798666' : 129.114.97.125]

Headers                                   Query        Body
```

Added to many notificatons? You can delete them individually with:

```
tapis notifications delete $NOTIFICATON_ID
```

Or, if you just want to git rid of all your notifications, you can run:

```
tapis notifications list -c id  -f value | xargs -n 1 tapis notifications delete
```

4.2 Reactor

If the reactor executed, but did not launch your app, you can check the reactor logs:

```
tapis actors execs logs $ACTOR_ID $EXECUTION_ID
```

You can then edit your `reactor.py` or `config.yml` as needed, and redeploy the actor. If you want to redeploy your reactor but don't want to re-create the notification, you can deploy your reactor to the same actor id with:

```
# tapis actors deploy -I X4blX3Ez65qQZ
tapis actors deploy -I $ACTOR_ID
```

4.3 Application

If the app launched, but you are not getting the output you expect, you can check the app logs. Run jobs-list to find the relevant job_ID, then you can run:

```
# tapis jobs outputs download 485458bc-335d-4d05-ae30-70de2583b6d5-007
tapis jobs show $JOB_ID
# and check the lastStatusMessage
tapis jobs outputs download $JOB_ID
# and check the .err and .our files
```