CWL-izing your pipeline

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Why CWL

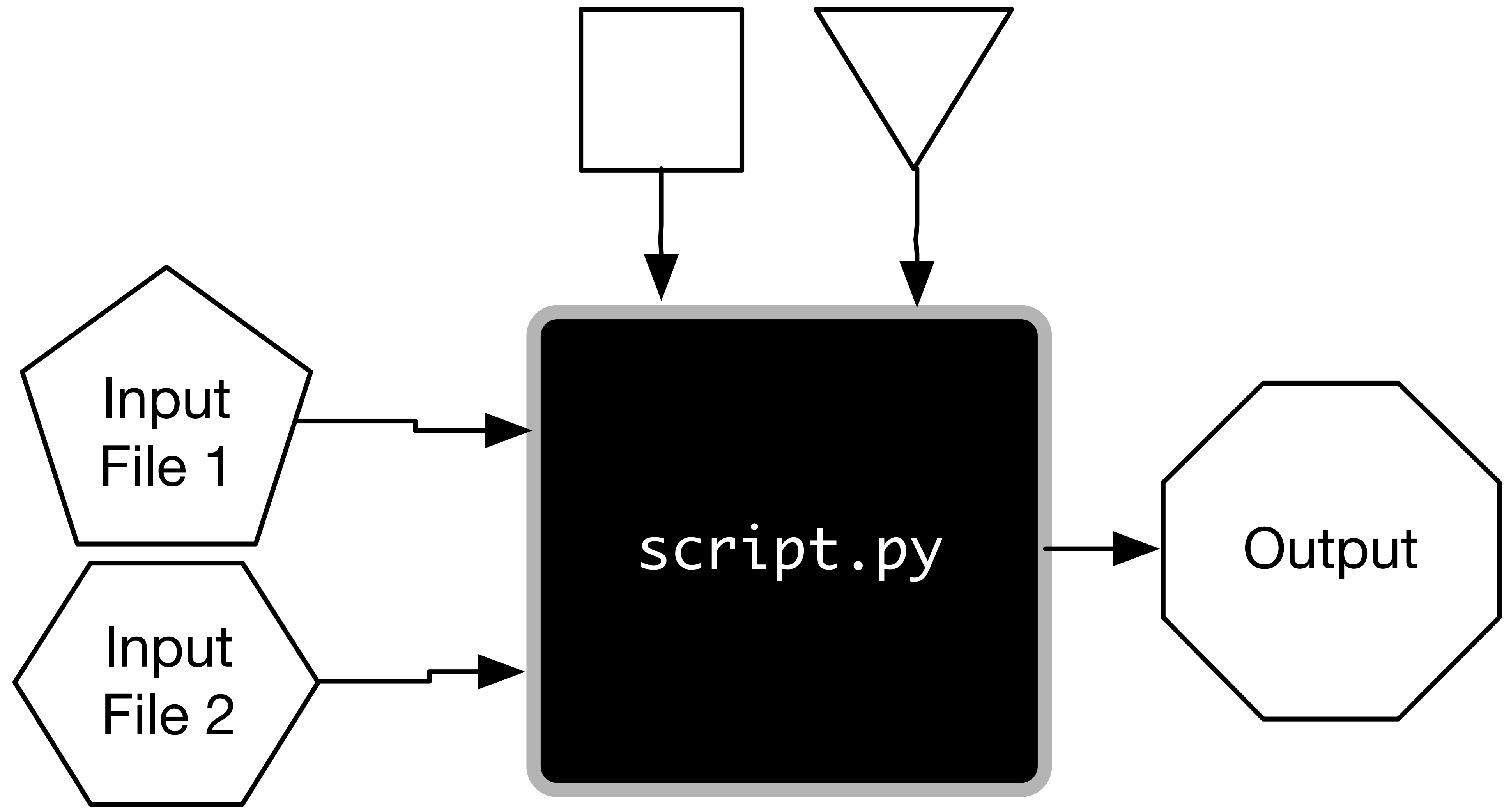
- Allow your tool or pipeline to be run easily on many systems
    - Laptop, Denali, MGI, CGC, Google Cloud
- Share, version workflows
    - Reproducibility

Four stages of development

- Core tool development
- Dockerization
- CWL Tool
- CWL Workflow

Core tool development

Input Parameters



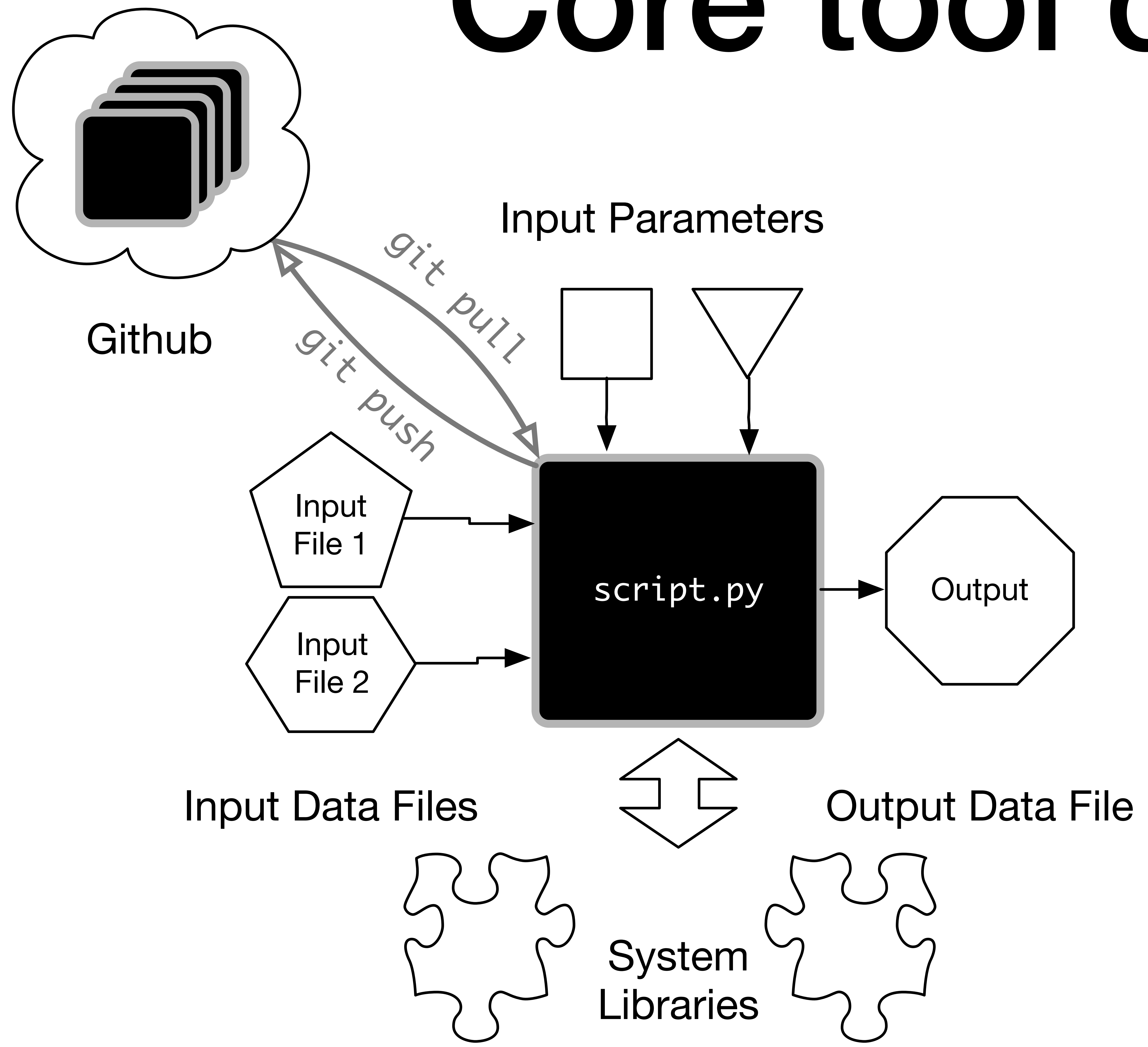
Input Data Files

Output Data File

```
python script.py -a -x vcf -o output.dat input1.bed input2.bam
```

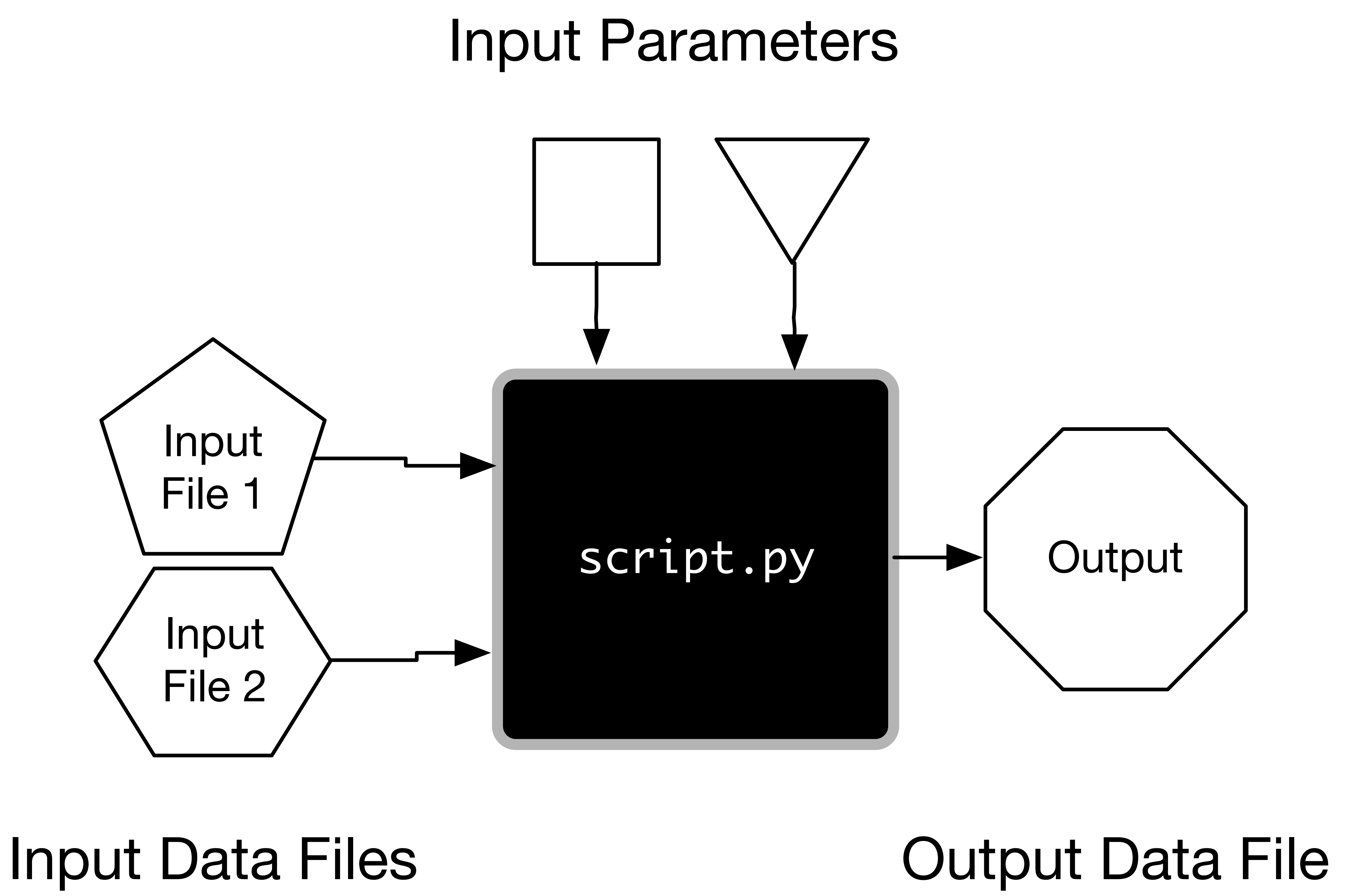
- Starting point is command line tool which:
  - Accepts input parameters
  - Accepts input files (data)
  - Writes defined set of results
- Generally processes one sample / dataset
- No queuing or LSF support

Core tool development



- Core tool typically stored on Github
- System libraries accessed implicitly
    - OS, installed software, etc
    - Maintaining uniform environment important but difficult

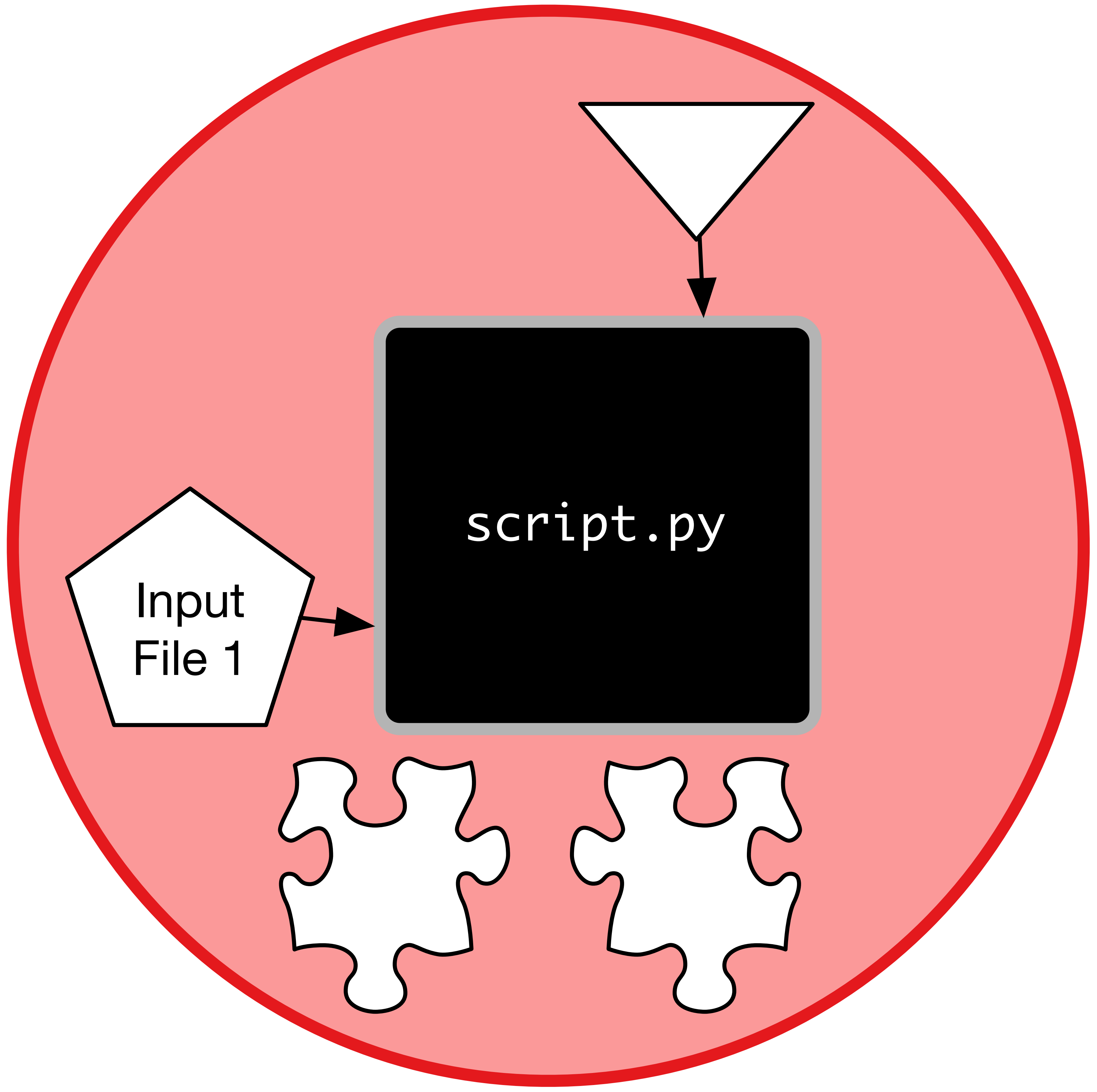
Core tool lessons



```
python script.py -a -x vcf -o output.dat input1.bed input2.bam
```

- Script must accept any input filename
    - Cannot assume what it is
- Files are staged, directories are not
    - Can pass .tar.gz if necessary
- Output path independent of input path
    - Default output filenames useful

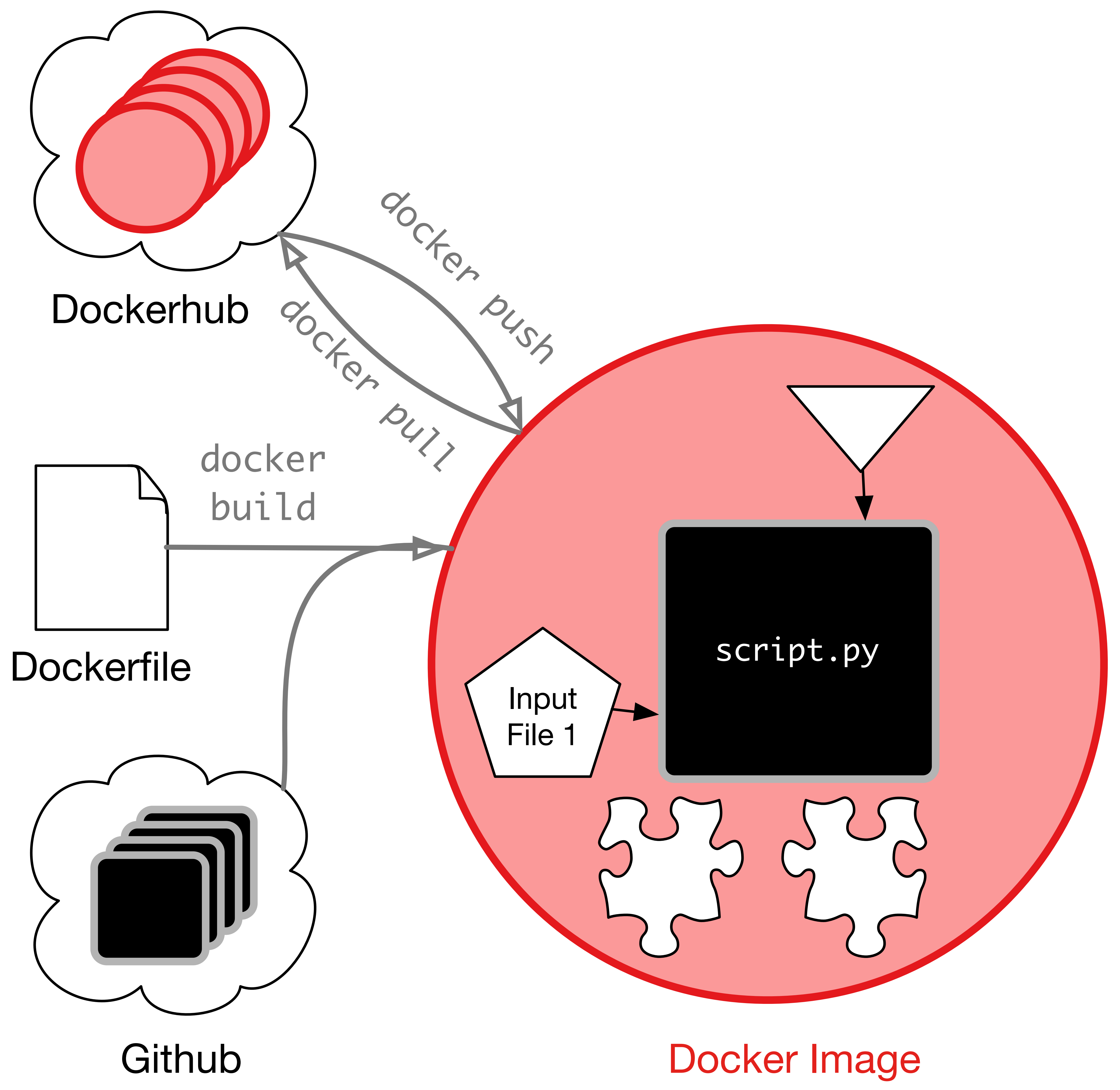
Docker



Docker Image

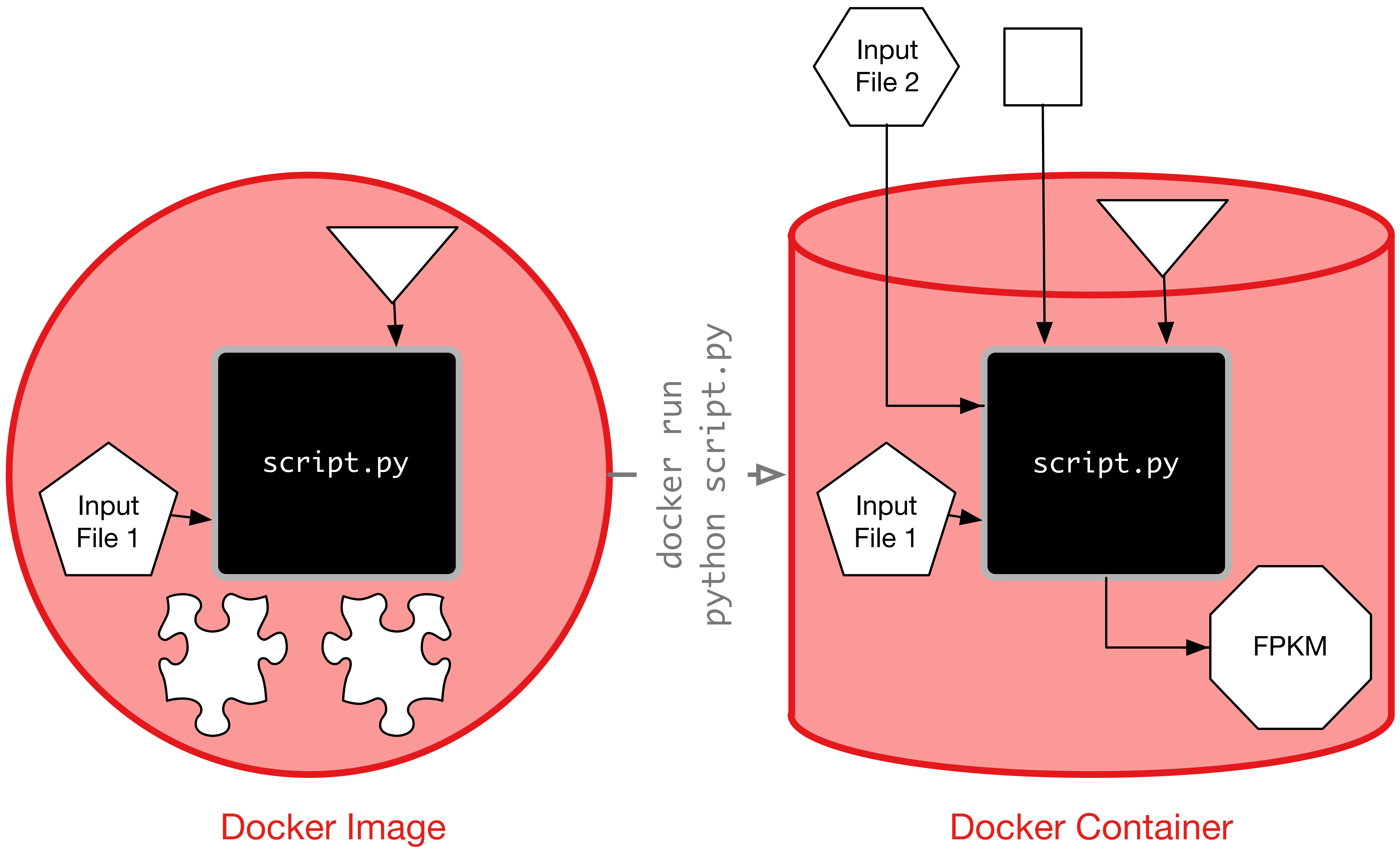
- Provides uniform environment for executing tool
- Libraries, tool incorporated into docker image
    - Some (small) datasets can also be built into docker image

Docker: Making an image



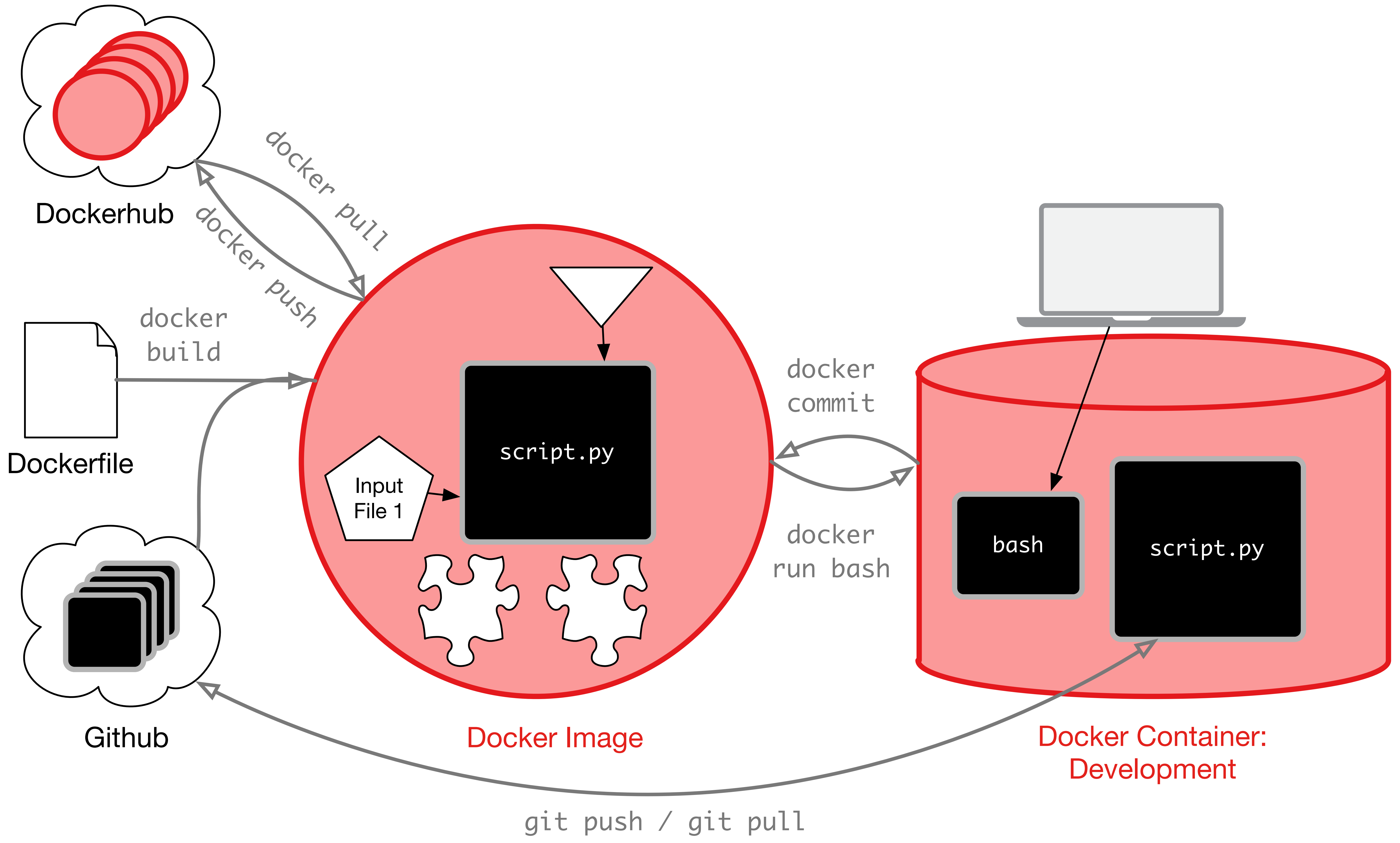
- Docker image typically built from Dockerfile
  - Installs OS, all libraries
  - Pulls tool code from Github
- Docker images can be stored on Dockerhub
  - Push and pull images as needed

Docker: Containers



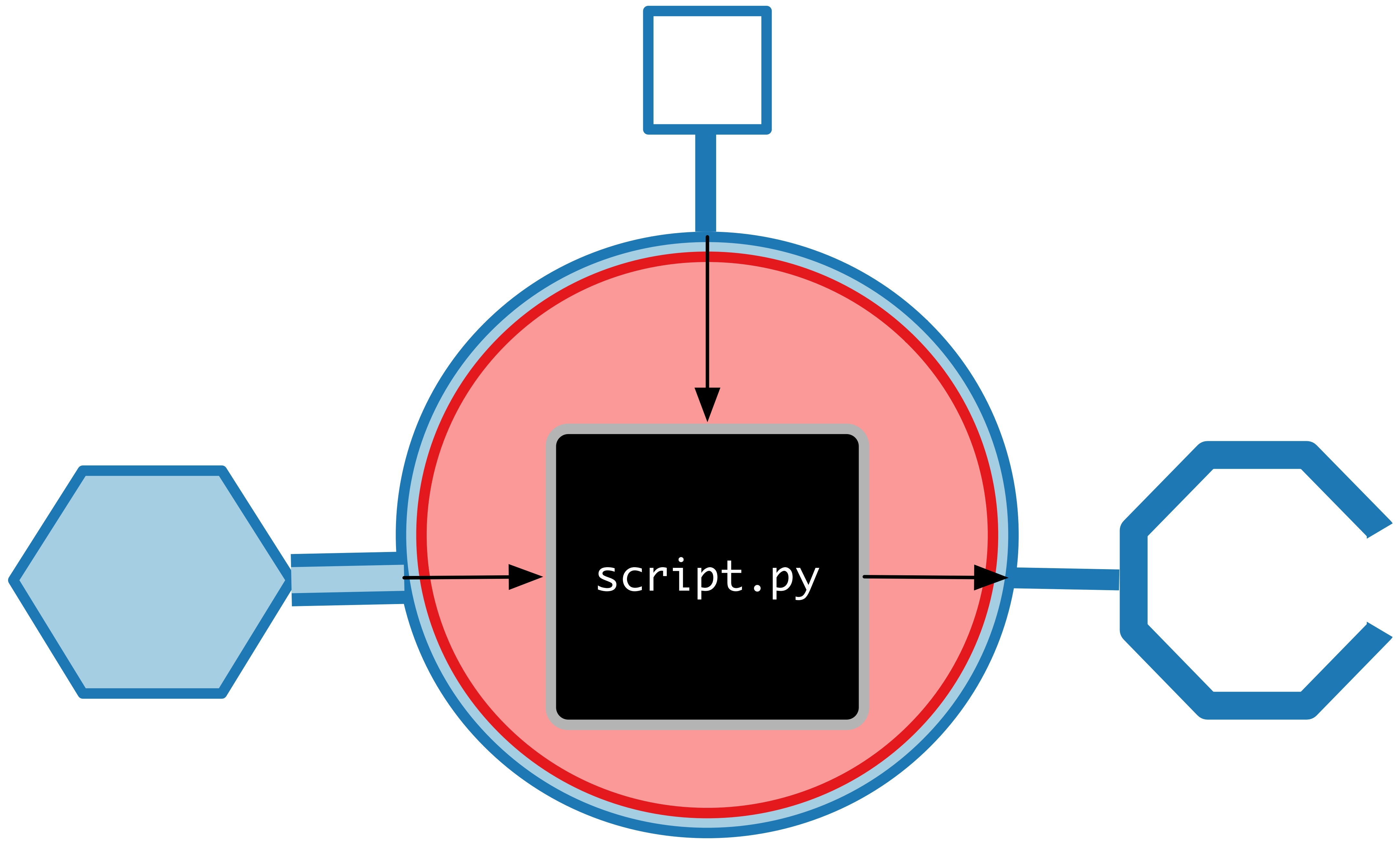
- Docker image is *recipe* for creating Docker container
    - Container has allocated memory, disk space
- Typically, container executes tool script and runs to completion

Docker: Development



- Alternative is to run bash in container - good for development
    - Can execute `python script.py` in same environment as running container
    - Like SSH to container
- Docker commit will incorporate changes to local image
    - Good for testing, but incorporate changes to Dockerfile eventually

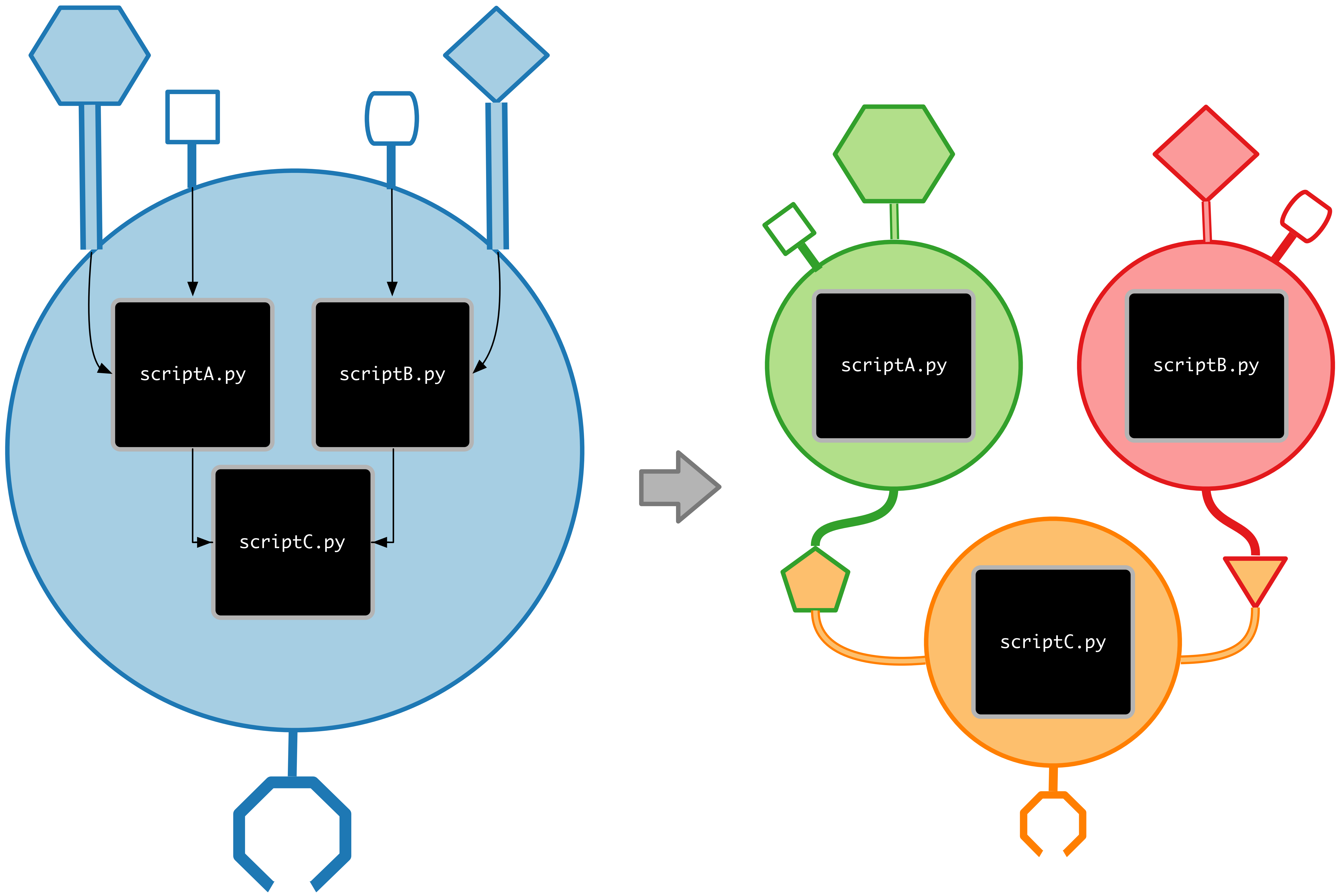
CWL: Tool



CWL Tool

- CWL is a wrapper around Docker image which provides uniform interface to workflow engines
  - Allows parallelization, scheduling, restarting, etc.
- Define input data types, input parameters, output data
- Use Rabix Composer for writing CWL tool wrappers
  - Rabix Executor for running CWL tools

CWL: Workflow



- Complex tools are better broken up into multiple tools linked together into a workflow
- Use Rabix Composer for writing CWL workflows
- Use Rabix Executor for running workflows
  - Other execution engines exist

Rabix Composer Tutorial

- Use Rabix Composer to wrap a sample program in CWL
  - http://docs.rabix.io/tutorial-1-wrapping-samtools-sort
  - Don’t need to log into images.sbgenomics.com
- See TinDaisy: CWL wrapper around SomaticWrapper
  - https://github.com/ding-lab/tin-daisy