HTMap and High Throughput Computing Notebooks

European HTCondor Workshop 2019

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Goal: Bring distributed High Throughput Computing into the scientific Python environment

HTMap

Using Python Map

```
# Describe work
def double(x):
    return 2 * x

# Do work
doubled = map(double,range(10))

# Use results!
print(list(doubled))
# [0, 2, 4, 6, 8, 10, 12, 14, 16, 18]
```

Using Python Map

☹

What if this function takes minutes/hours ?

What if you had hundreds or thousands of inputs ?

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# [0, 2, 4, 6, 8, 10, 12, 14, 16, 18]
```

Using HTMap

```
import htmap

# Describe work
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Using HTMap

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```

This is an iterable object with methods to handle asynchronous properties

Using HTMap Tags

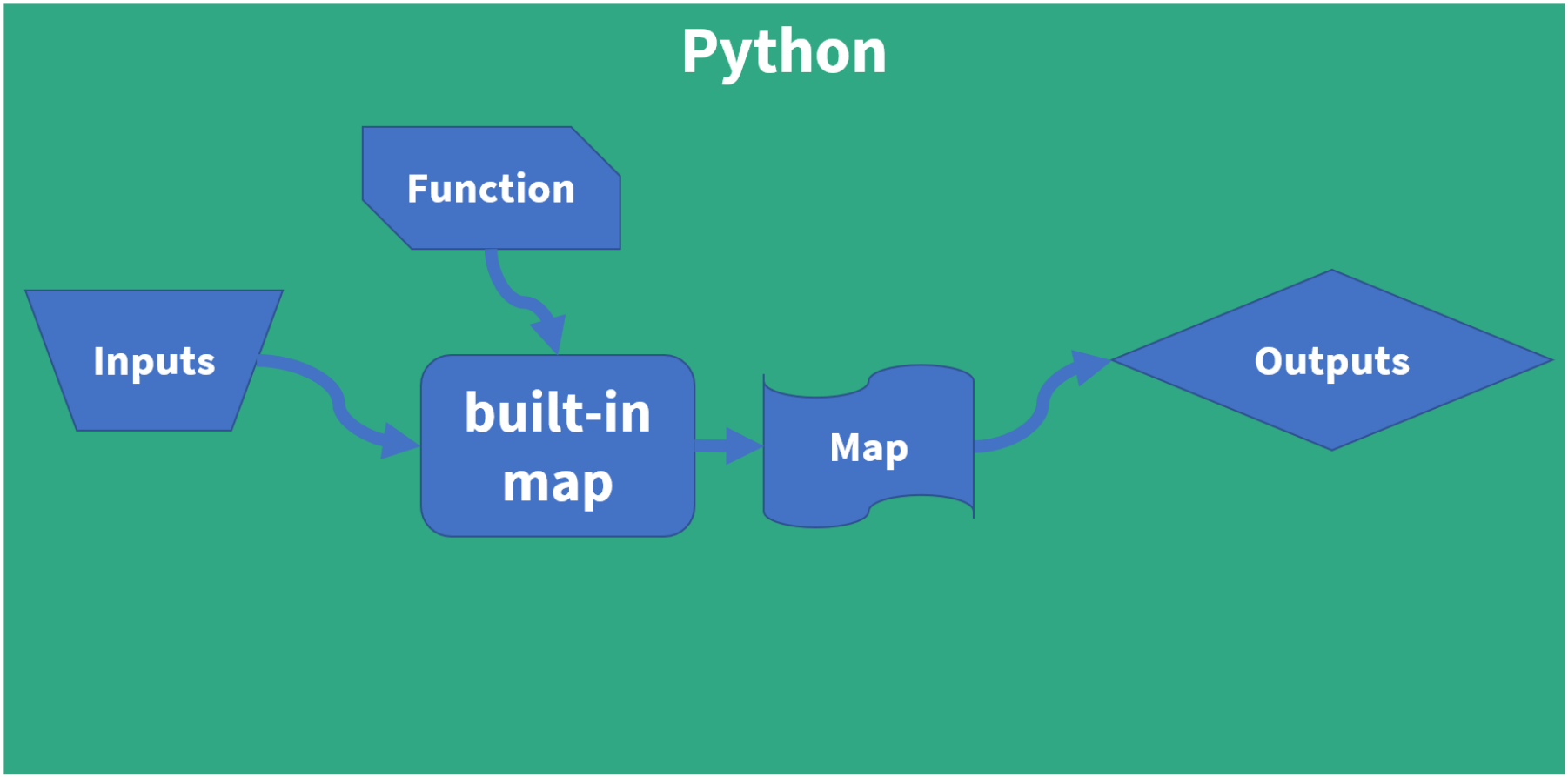
```
import htmap

# Describe work
def double(x):
    return 2 * x

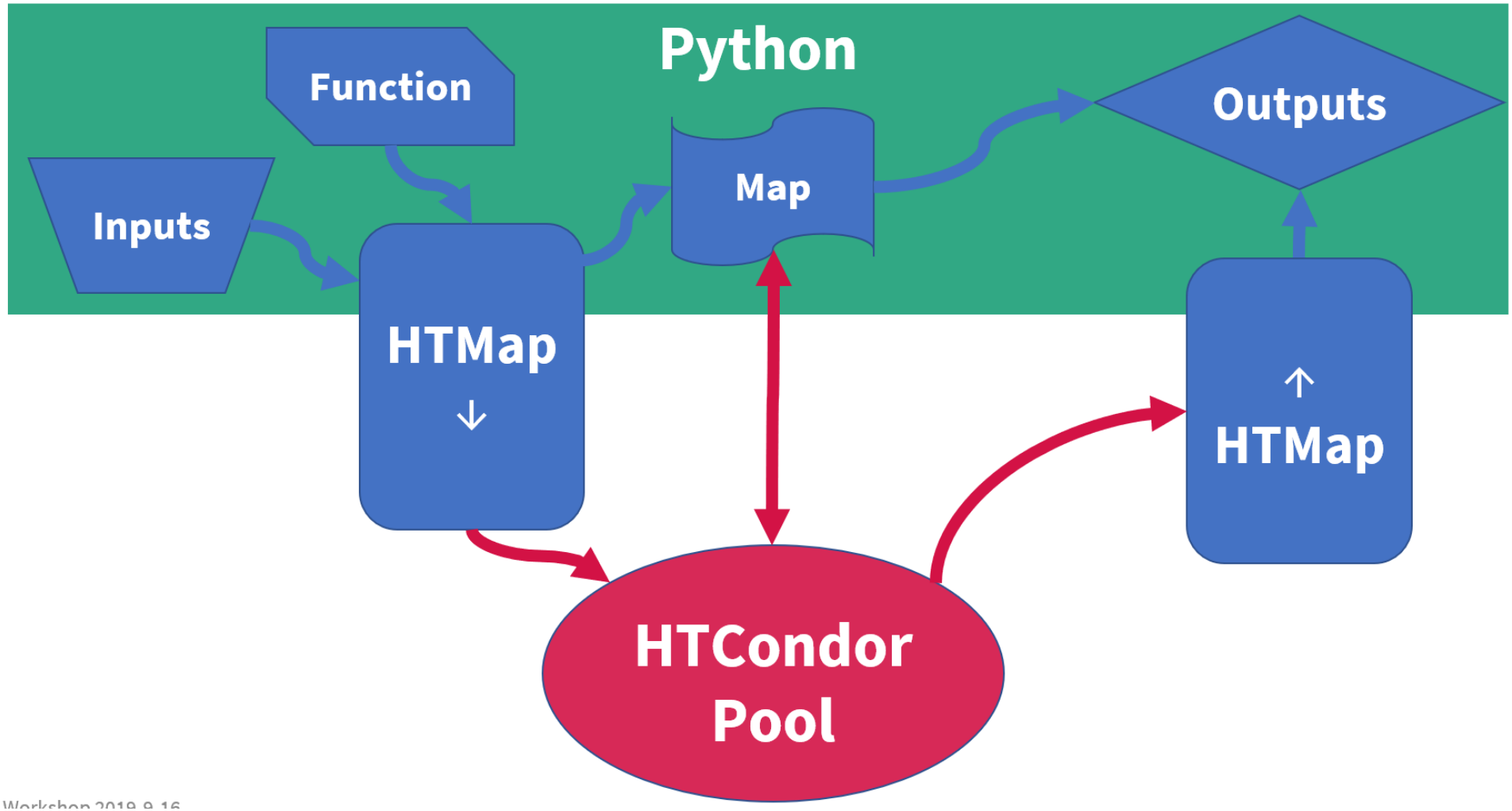
# Do work
doubled = htmap.map(double,range(10), tag="Simulation1")

# Use results!
print(list(doubled))
# [0, 2, 4, 6, 8, 10, 12, 14, 16, 18]
```

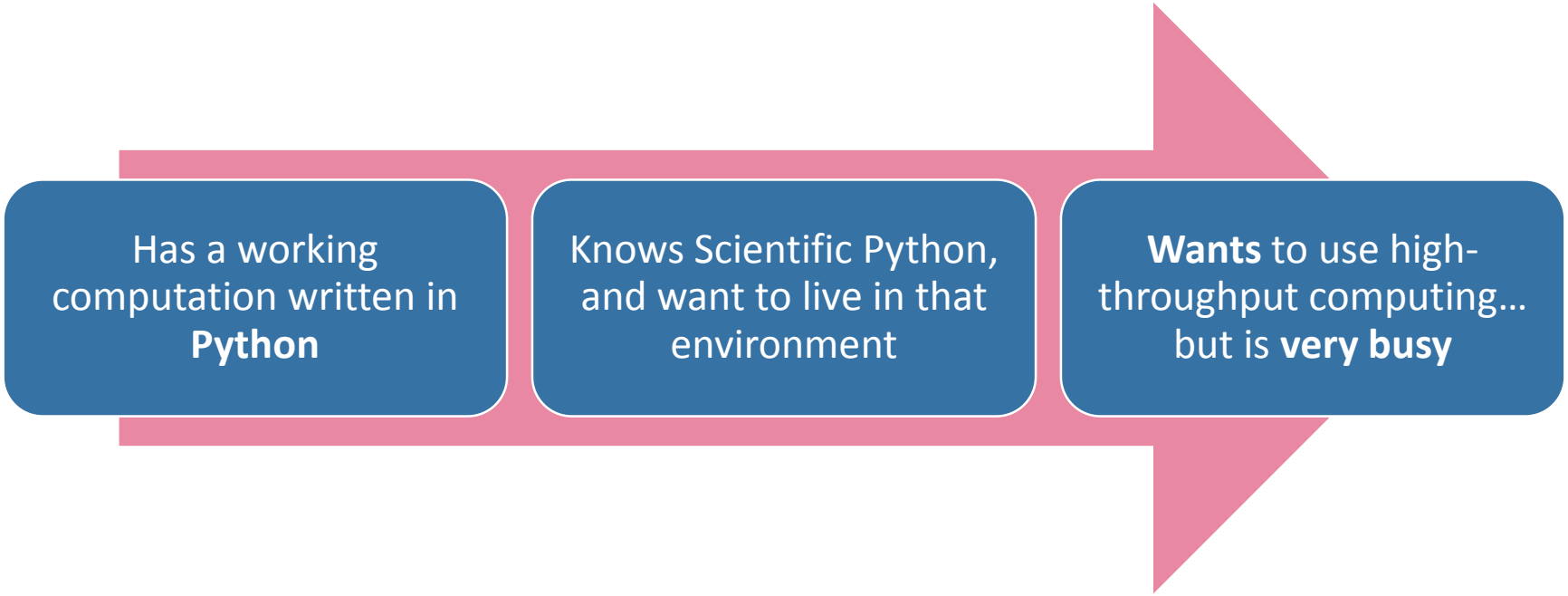
Python Map



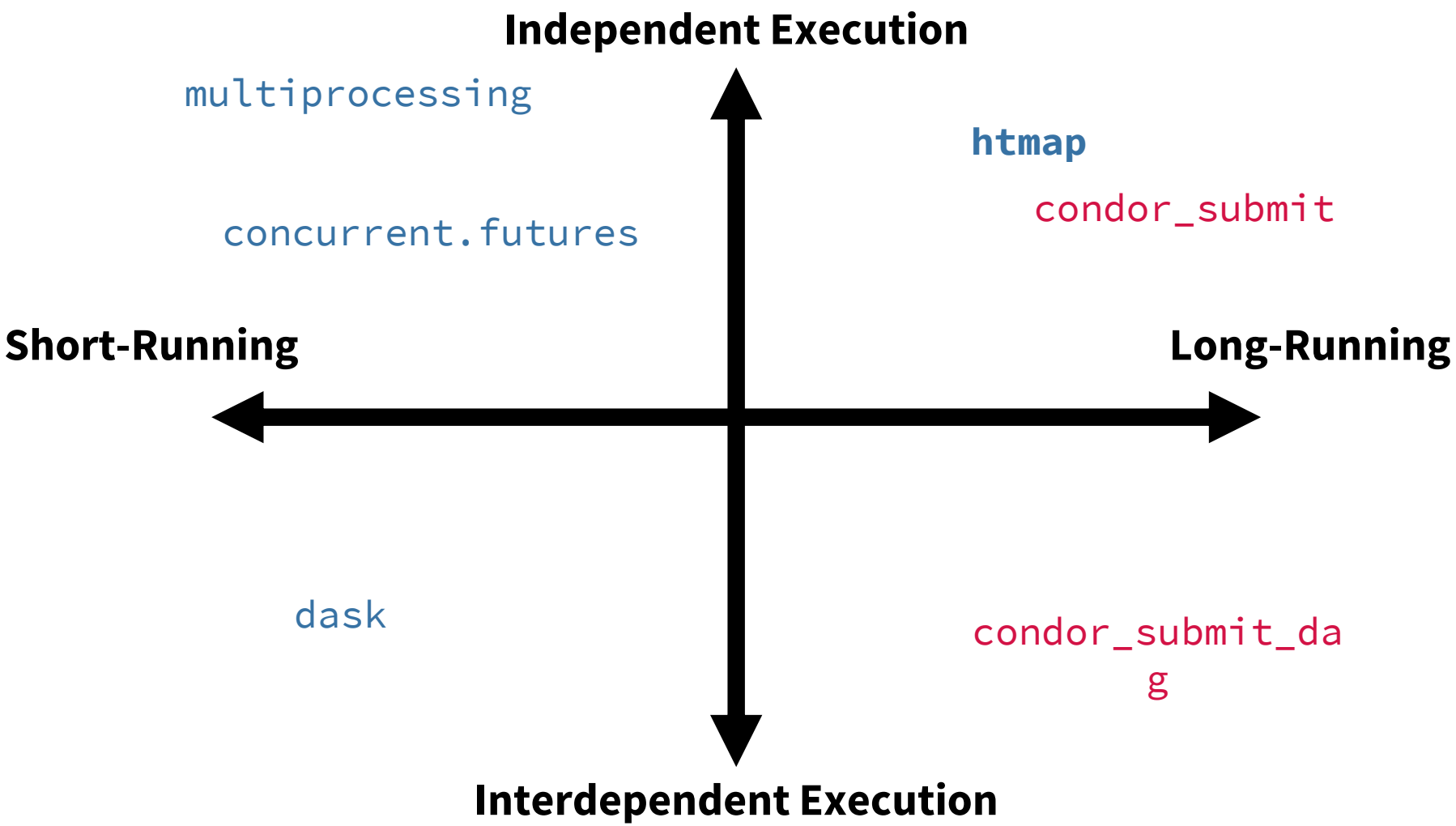
HTMap


Python
Function
Inputs
Map
Outputs
HTMap
↓
↑
HTMap
HTCondor
Pool

Who is HTMap ideal for?



Who is HTMap **NOT** ideal for?


Independent Execution
multiprocessing
htmap
condor_submit
concurrent.futures
Short-Running
Long-Running
dask
condor_submit_dag
Interdependent Execution

Jupyter Notebook

- Open source browser-based application to create and share *interactive documents* that contain
  - Live code
    - Python, R, Julia, Scala, Bash, …
  - Equations
  - Visualizations
  - Narrative Text
- Also has a console window and file mover

jupyter Lorenz Differential Equations (autosaved)

File Edit View Insert Cell Kernel Help Python 3

Code Cell Toolbar: None

Exploring the Lorenz System

In this Notebook we explore the Lorenz system of differential equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

This is one of the classic systems in non-linear differential equations. It exhibits a range of complex behaviors as the parameters (σ, β, ρ) are varied, including what are known as *chaotic solutions*. The system was originally developed as a simplified mathematical model for atmospheric convection in 1963.

In [7]:
```
interact(Lorenz, N=fixed(10), angle=(0.,360.),
         σ=(0.0,50.0),β=(0.,5), ρ=(0.0,50.0))
```

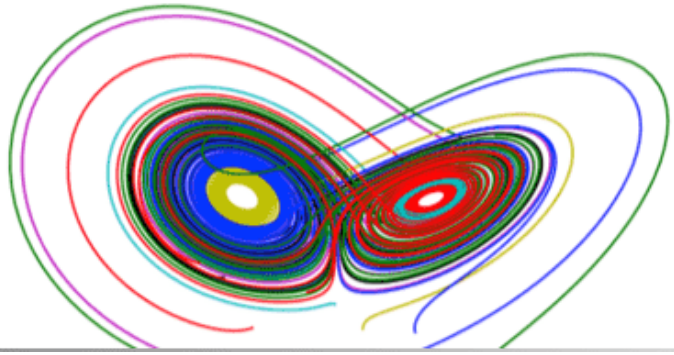
angle 308.2

max_time 12

σ 10

β 2.6

ρ 28



jupyter Welcome to P

File Edit View Insert Cell

jupyter

Welcome to the

This Notebook Server wa

WARNING

Don't rely on this serv

Your server is hosted thar

Run some Python

To run the code below:

1. Click on the cell to se
2. Press SHIFT+ENTER

A full tutorial for using the

In [ ]:
```
%matplotlib inline

import pandas as pd
import numpy as np
import matplotlib
```

Can start a Jupyter instance on your laptop

- Install Jupyter via Anaconda or PIP, e.g.

```
% pip install jupyter
```

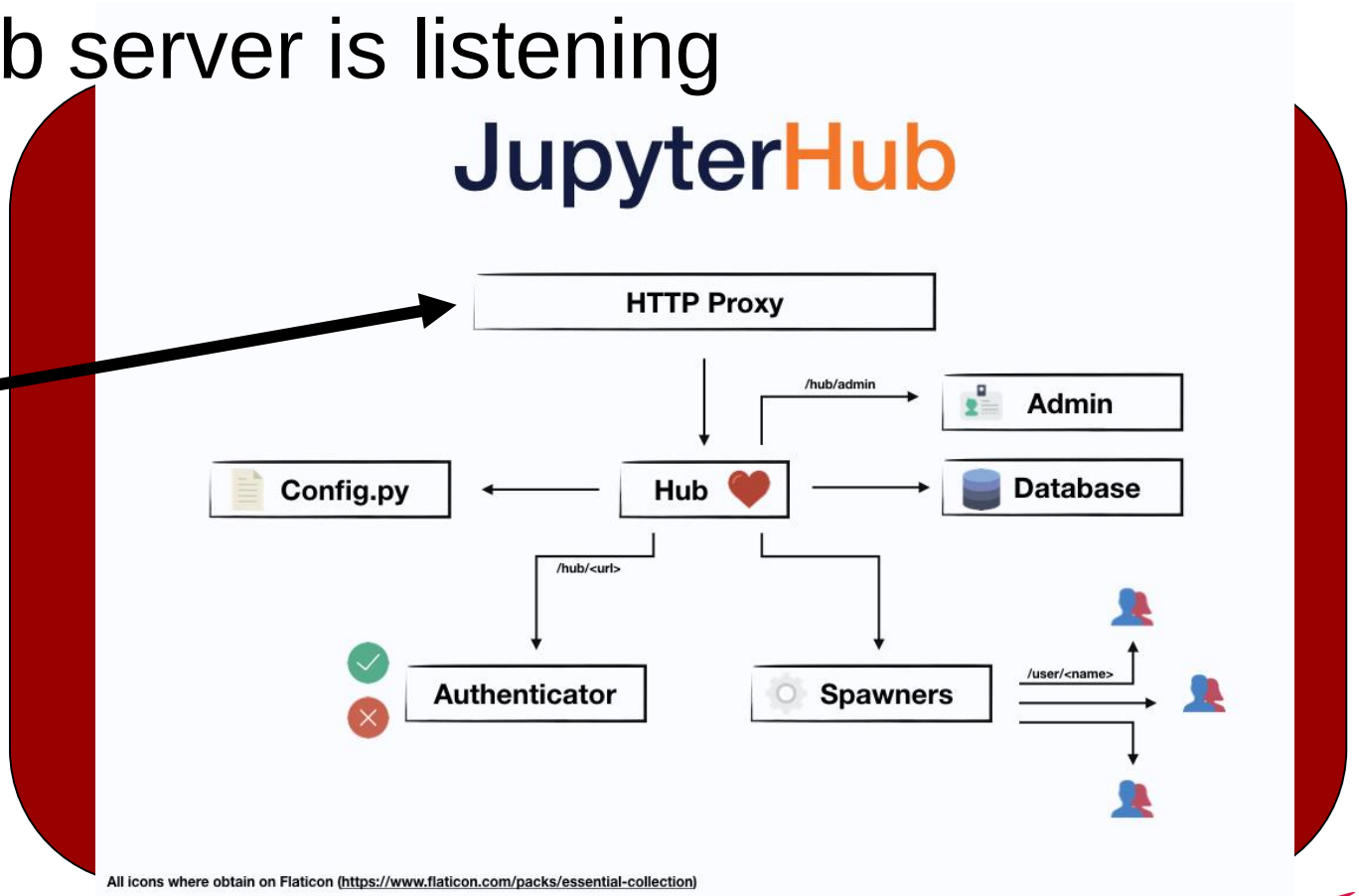
- And fire it up

```
% jupyter notebook
```

- This command will start a small embedded web server on your laptop; point your browser at http://localhost:8888 and go.

Can start a Jupyter instance on a remote server

- Point your browser at a URL where a JupyterHub server is listening



All icons where obtain on Flaticon (https://www.flaticon.com/packs/essential-collection)

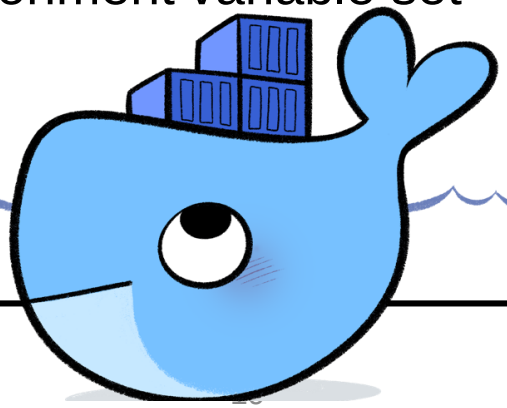
Goal: Bring distributed High Throughput Computing into the scientific Python environment

Allow users to easily *develop/test* using a small/responsive pool (eg their laptop!), and then easily *run* using all the cores in an HTCondor cluster

High Throughput Computing Notebook

Docker container with

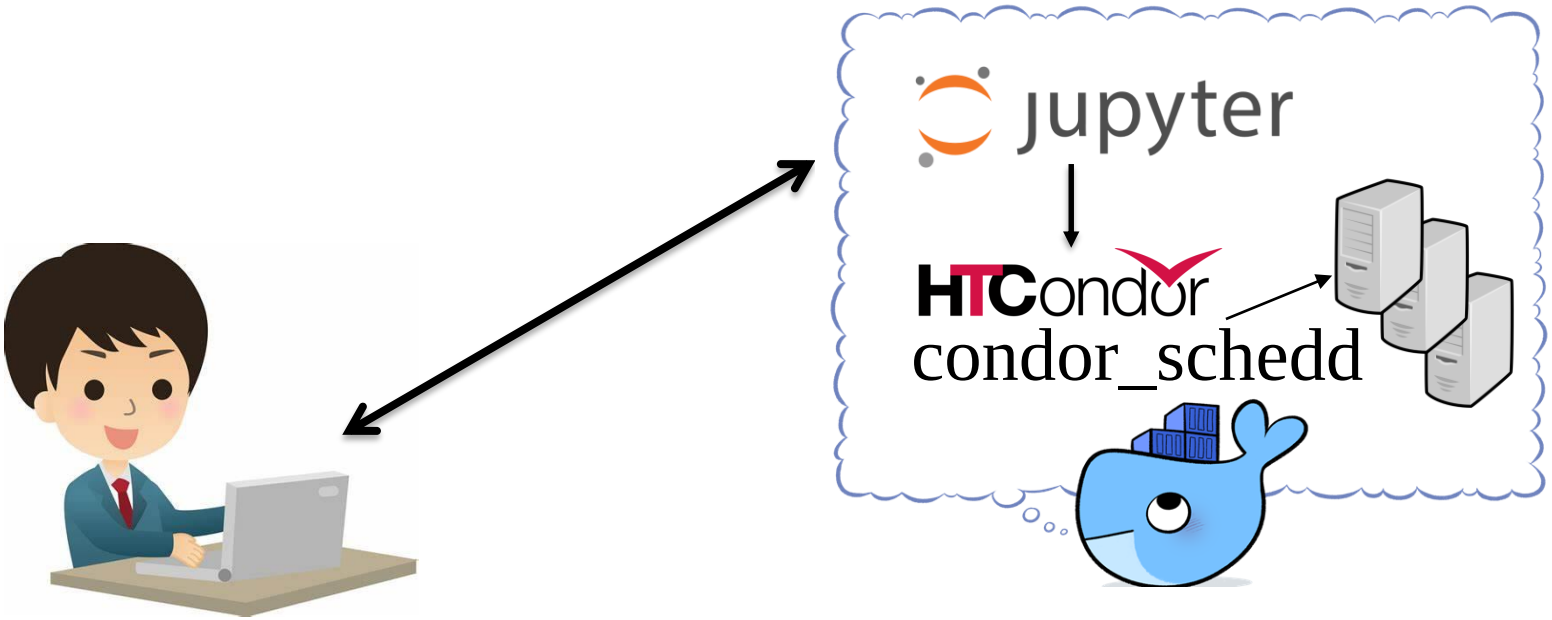
- Python 3
- Jupyter
- Popular Python science packages
- HTCondor Python bindings
- HTMap
- Personal HTCondor pool
  - Started if no _condor_SCHEDD_HOST environment variable set



High Throughput Computing Notebook

- Run it on your laptop
  - Container will start up a personal HTCondor pool, and then Jupyter
  - HTMap uses the personal pool
- Run it on a server that has both JupyterHub and a HTCondor Schedd connected to your site's pool
  - Container will start Jupyter
  - HTMap uses the entire site pool

Run htc-notebook on your laptop with a personal pool



- Container will start up a personal HTCondor pool, and then Jupyter
- HTMap uses the personal pool

Run htc-notebook on a *remote server* with a *personal pool*

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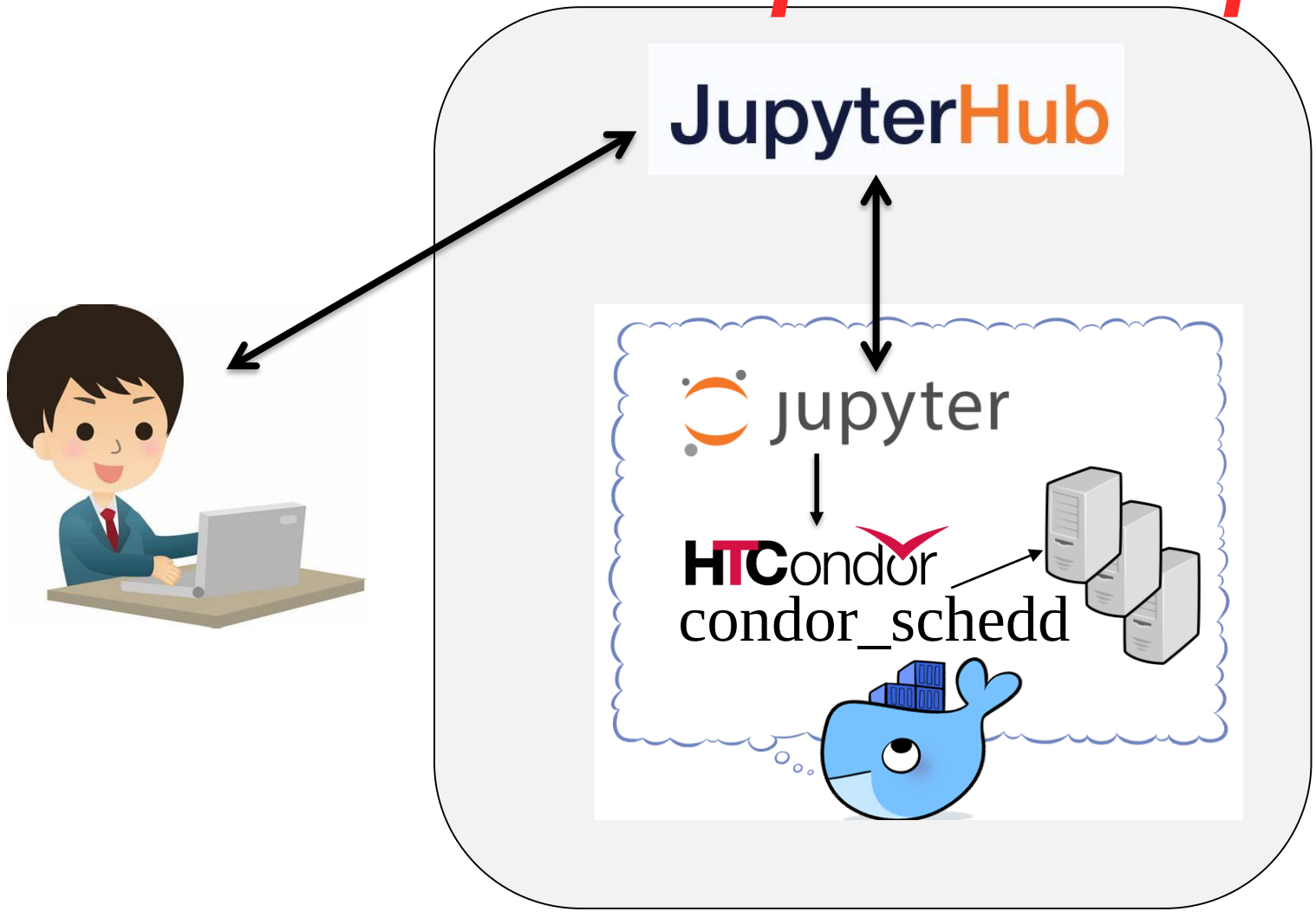
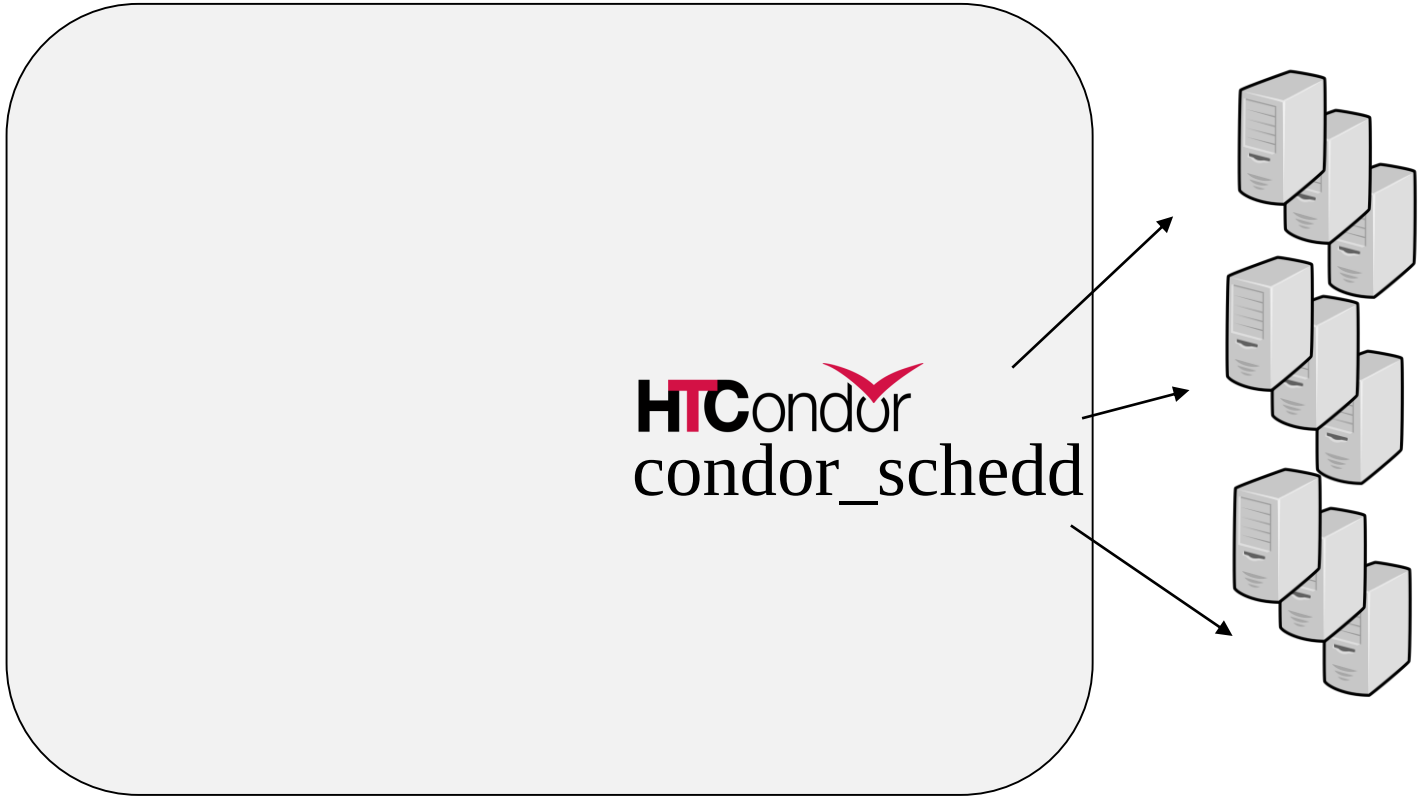
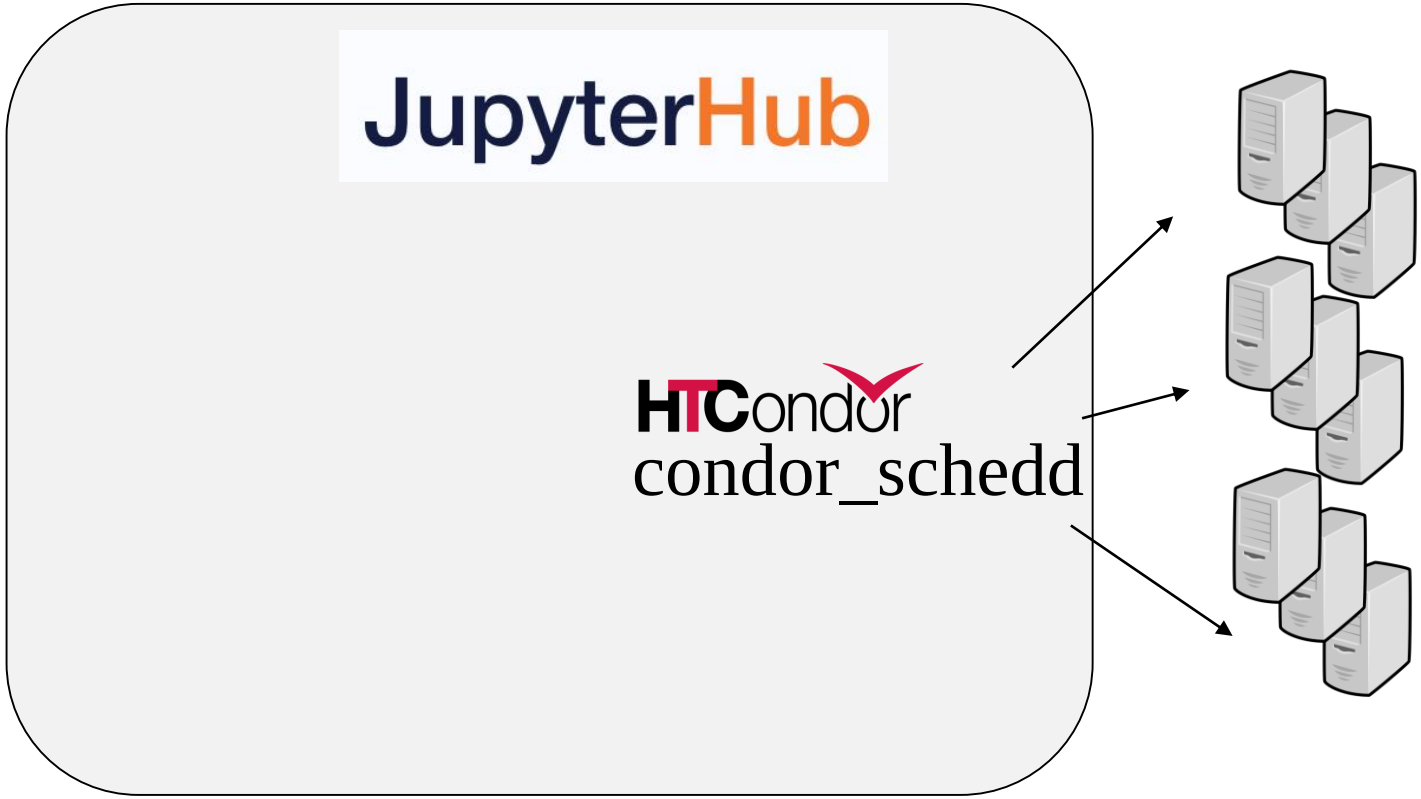


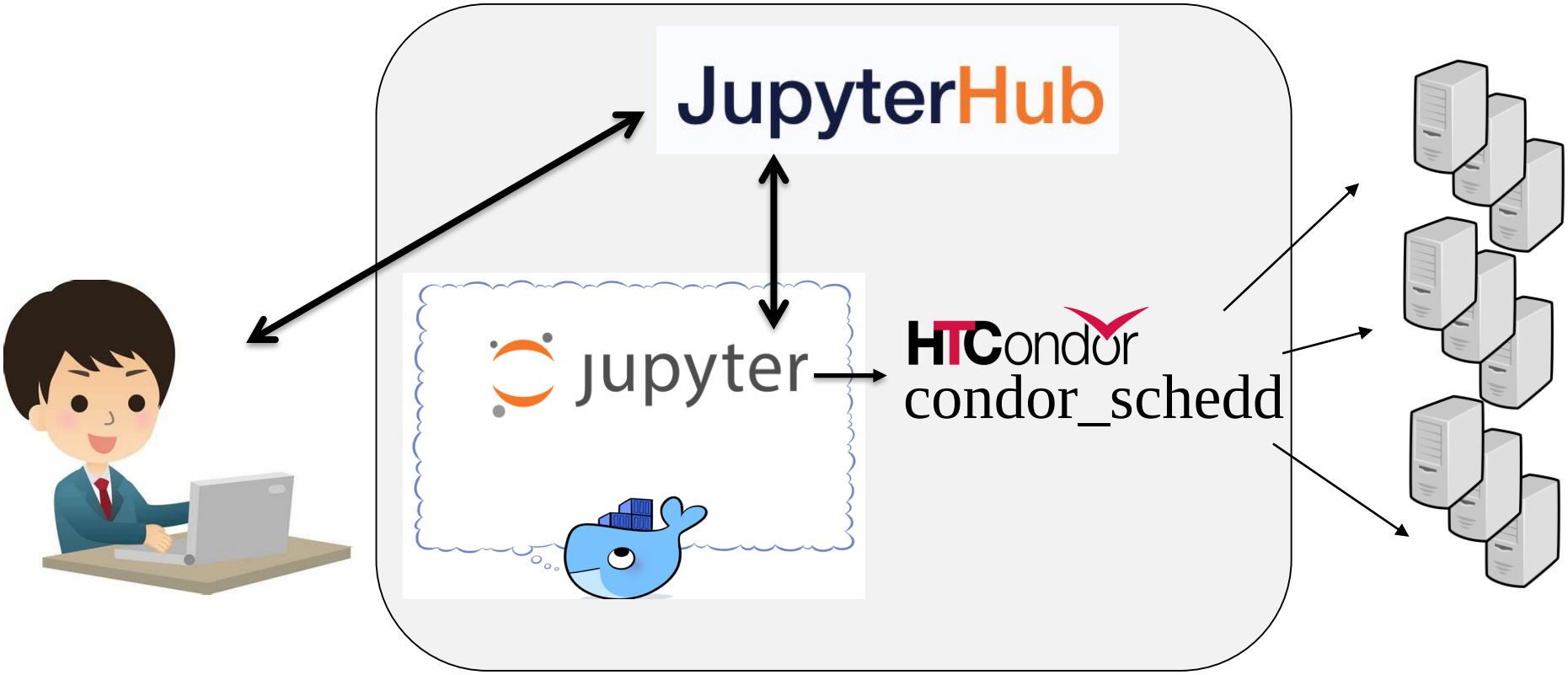
Run on a remote server *using entire site pool*



Run on a remote server *using entire site pool*



Run on a remote server *using entire site pool*



- Docker Hub (images) / GitHub Repos (src)

https://hub.docker.com/u/htcondor

https://github.com/htcondor/htc-notebook

- Run it on your laptop

```
docker run -p 8888:8888 htcondor/htc-base-notebook
```

```
(then open your web browser as instructed)
```

- Pick a software environment!
  - htcondor/htc-scipy-notebook
  - htcondor/htc-tensorflow-notebook
  - htcondor/htc-r-notebook
  - htcondor/htc-pyspark-notebook
  - htcondor/htc-datascience-notebook

Thank You

Interested? Talk to us!

https://github.com/htcondor/htmap
https://github.com/htcondor/htc-notebook