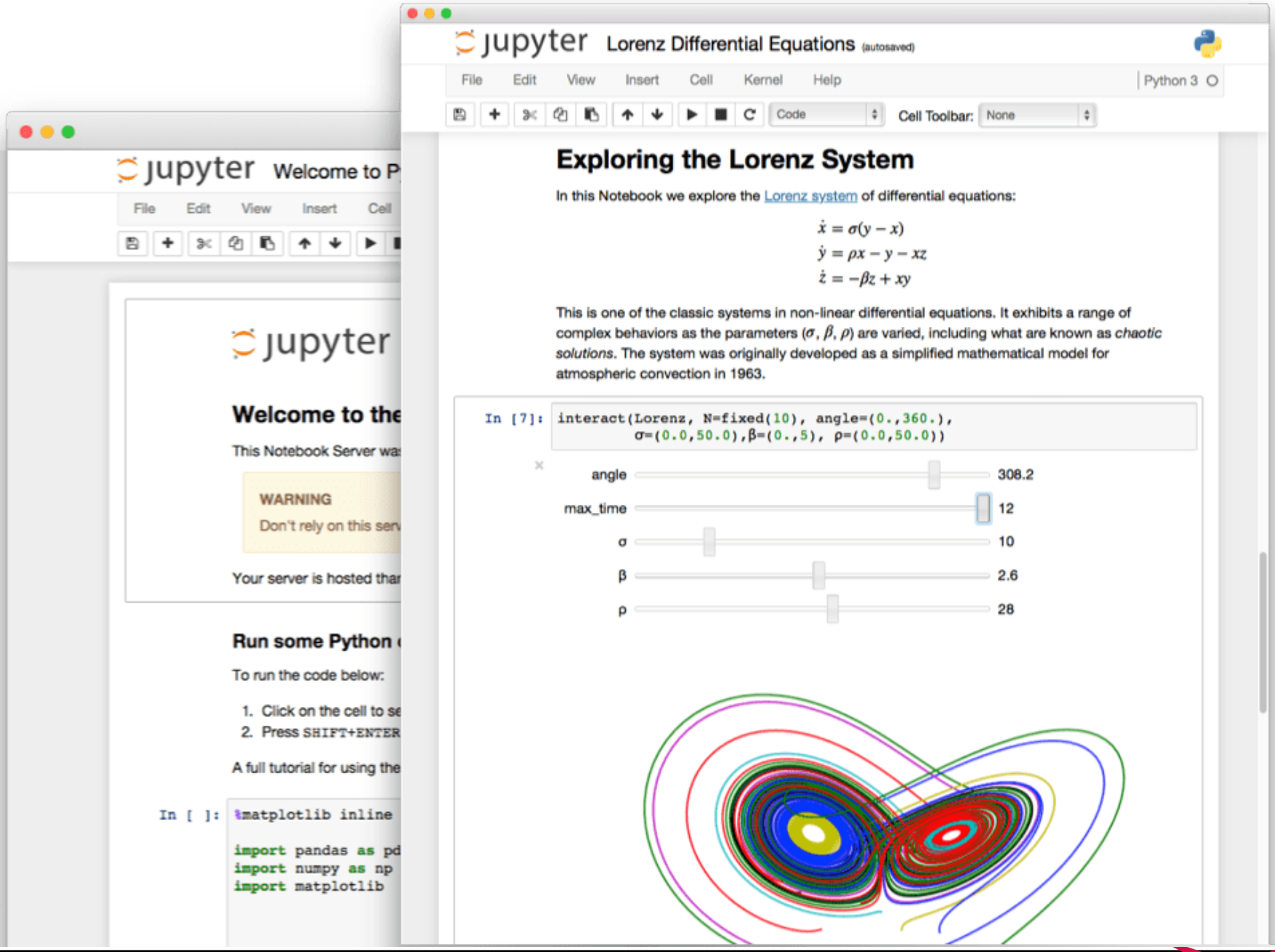
High Throughput Computing Notebooks

HTCondor Week 2019

Todd Tannenbaum
Center for High Throughput Computing

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
```

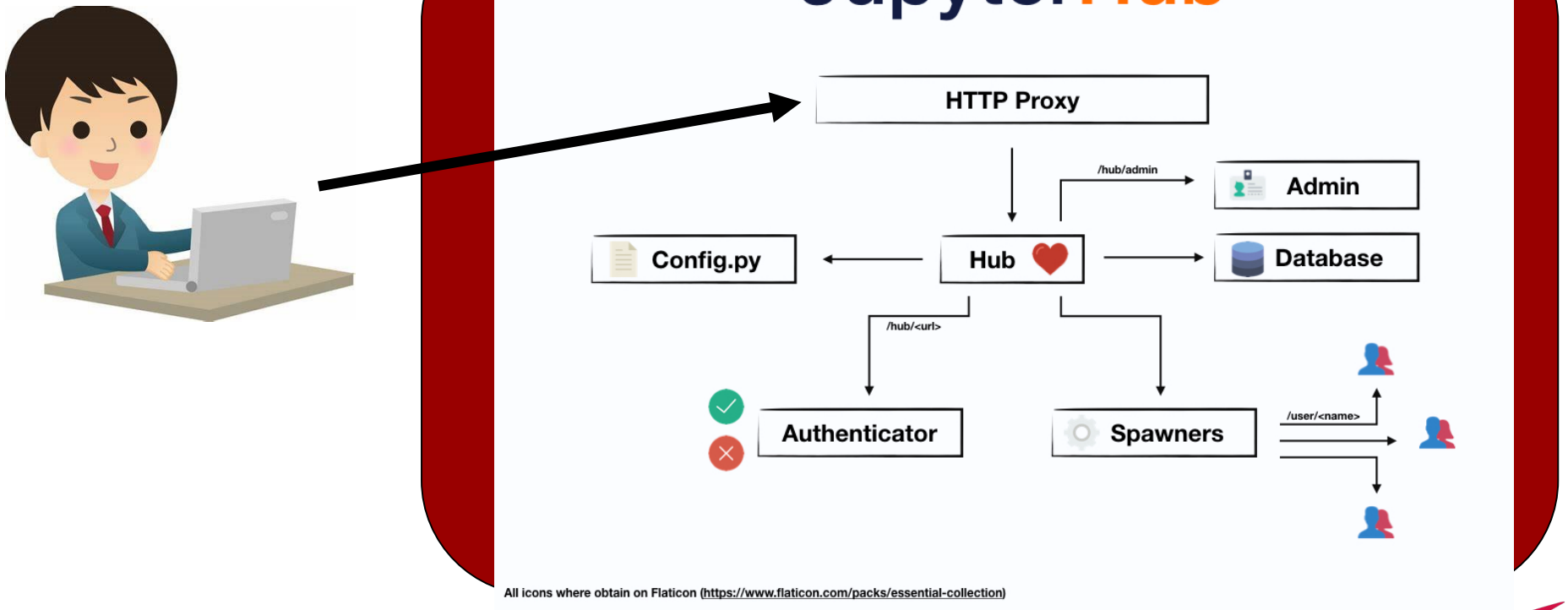
- And fire it up

```
% 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



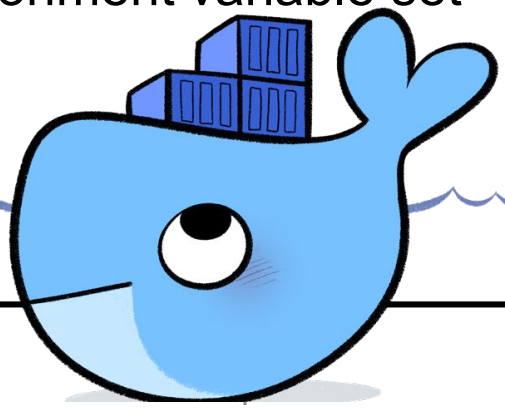
Goal: Bring distributed High Throughput Computing into the scientific Python environment

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

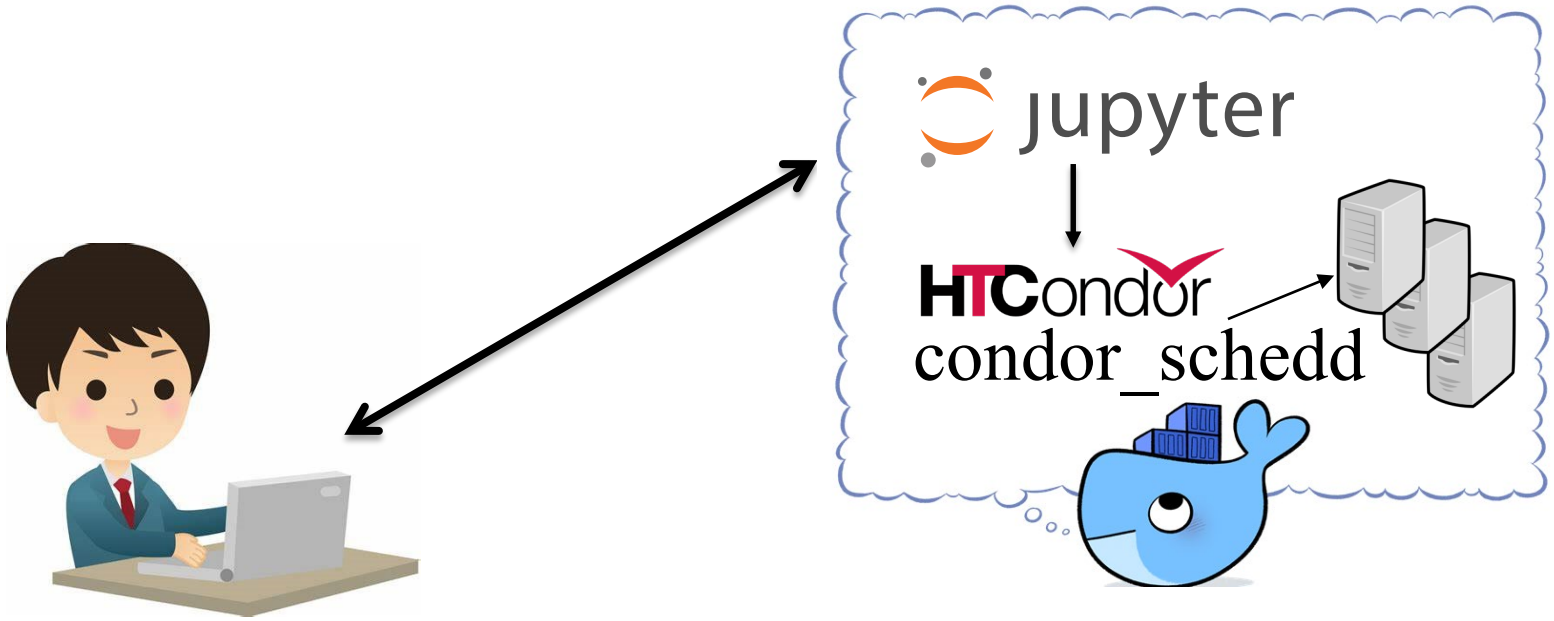
- Python 3
- Jupyter
- Popular Python science packages
- HTCondor Python bindings
- HTMap
- Personal HTCondor pool
  - Started if no _condor_SCHEDD_HOST environment variable set



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

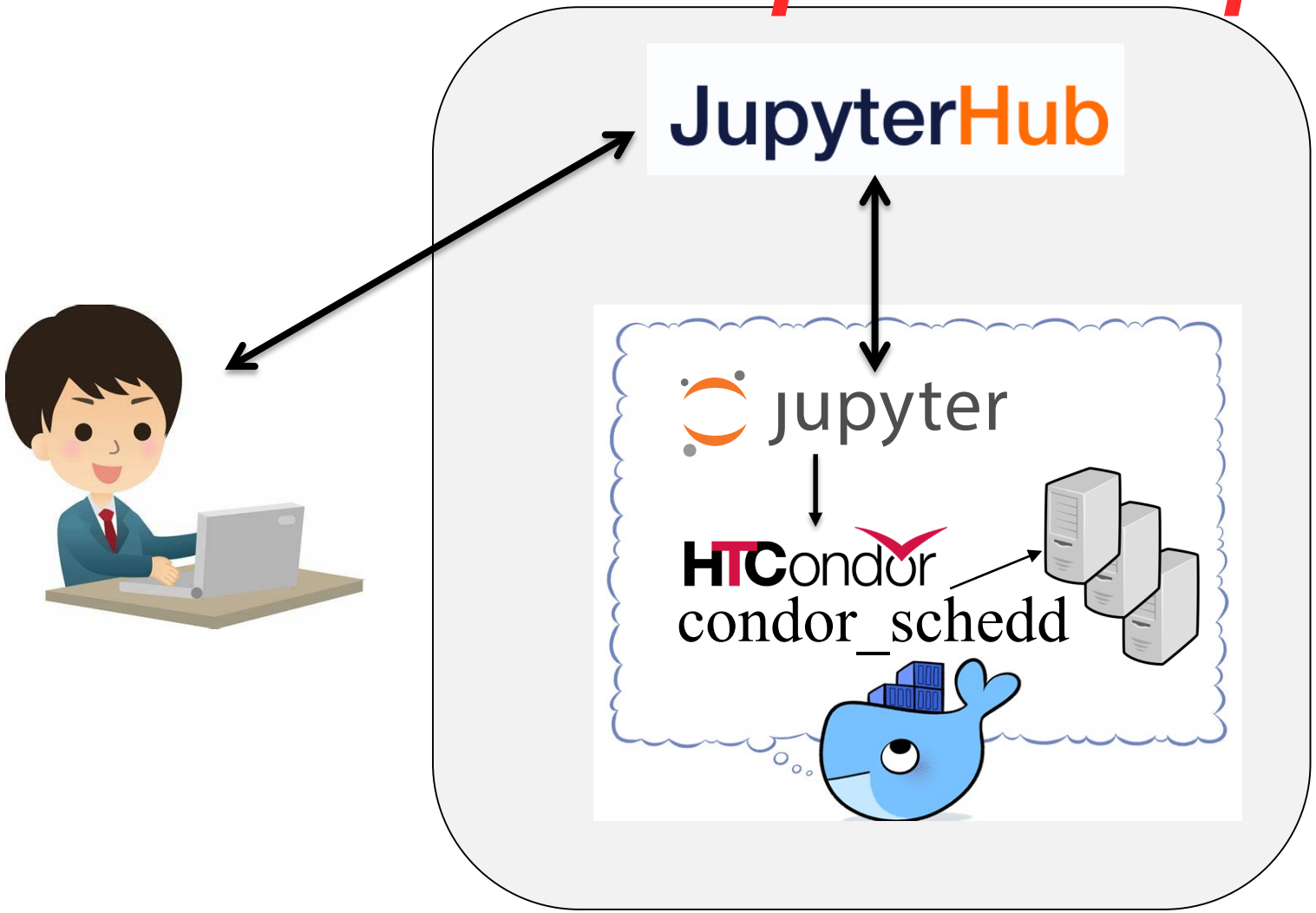
Run htc-notebook on your laptop with a personal pool



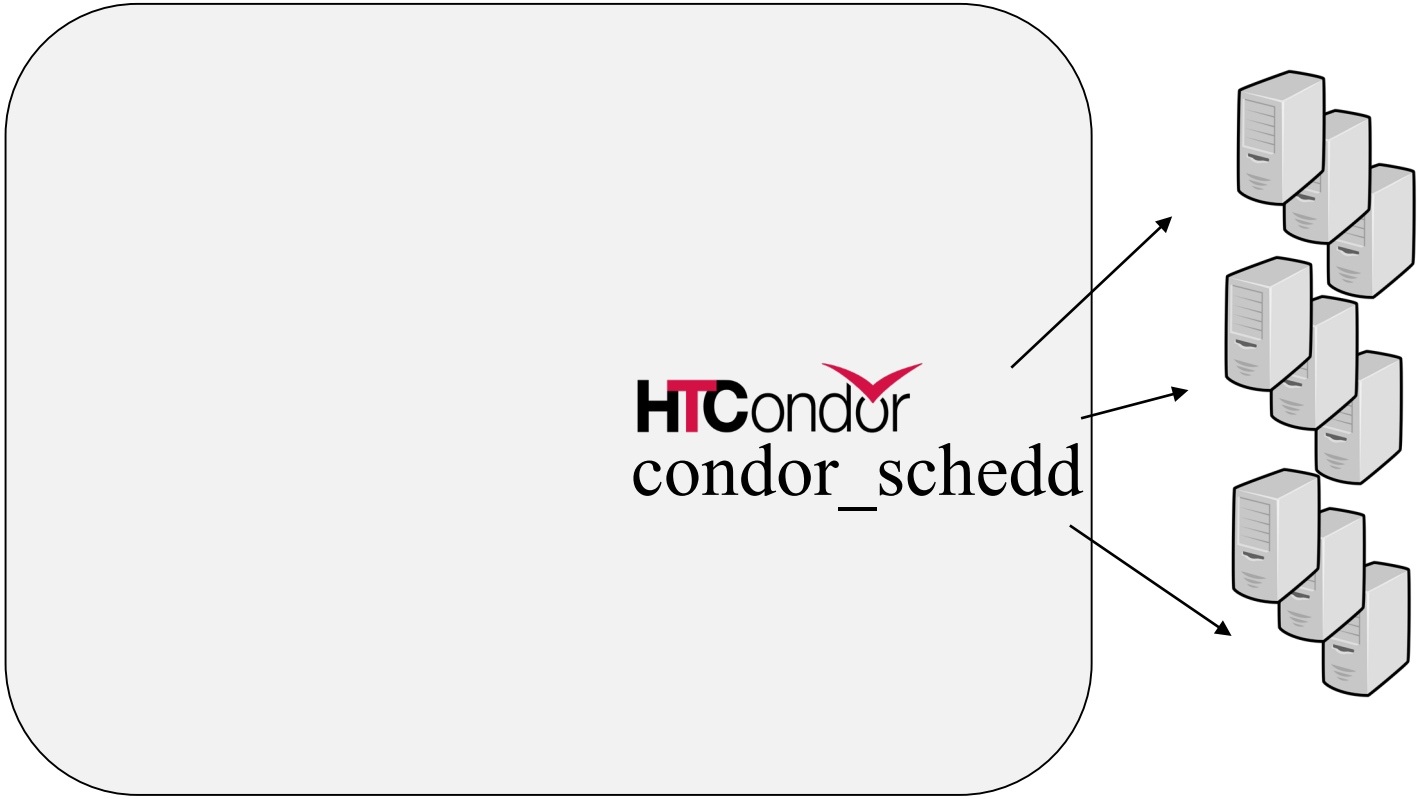
- Container will start up a personal HTCondor pool, and then Jupyter
- HTMap uses the personal pool

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

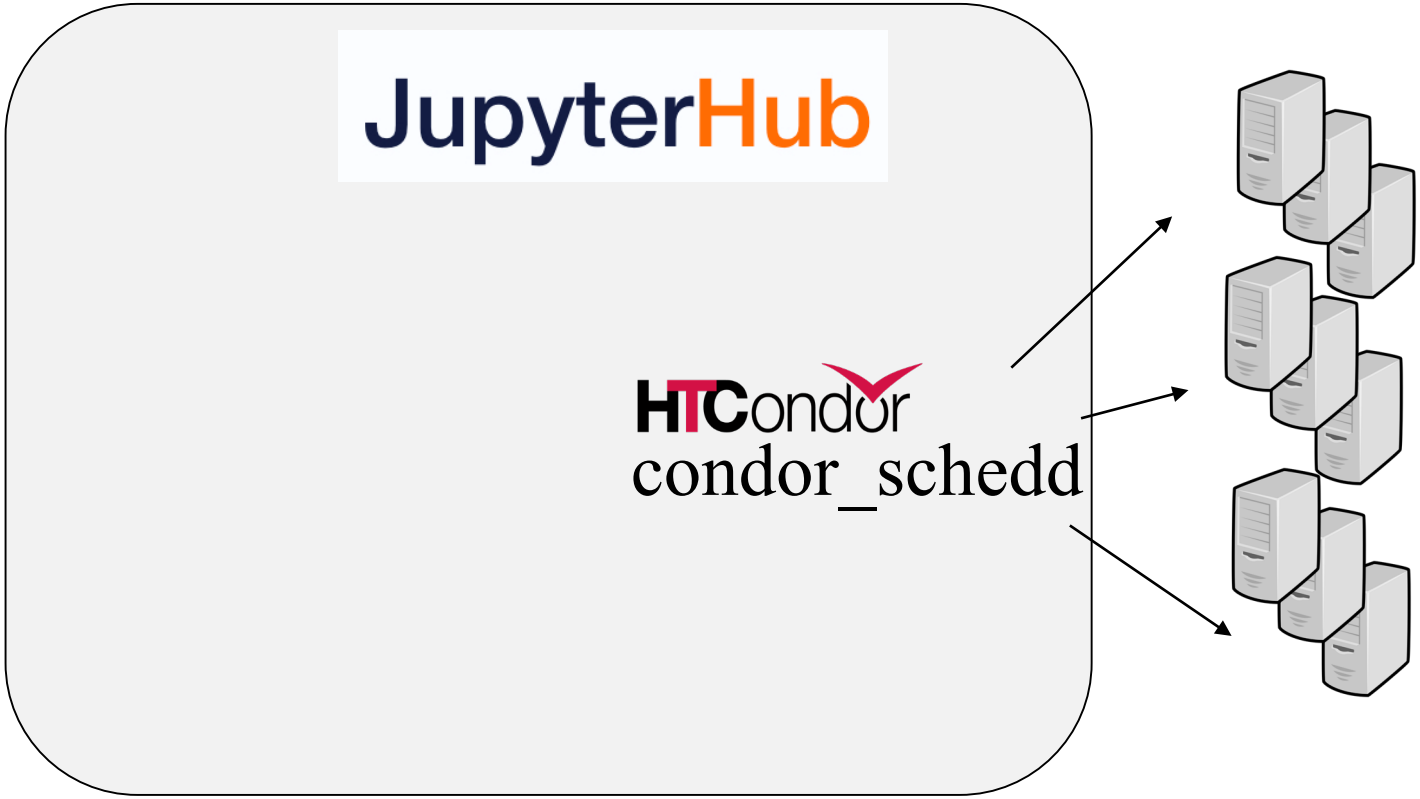
Run htc-notebook on a *remote server* with a *personal pool*



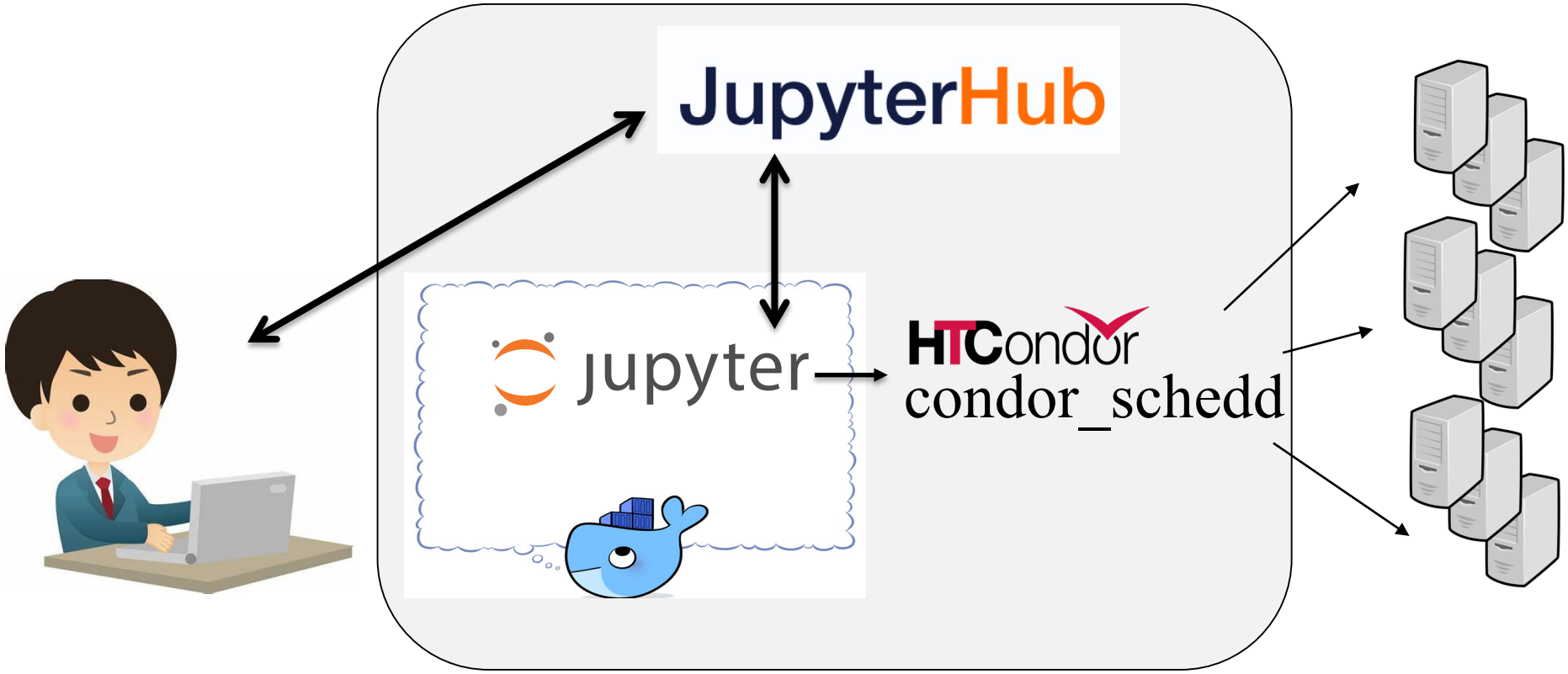
Run on a remote server *using entire site pool*



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!

Docker Hub (images) / GitHub Repos (src)

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

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