PURDUE UNIVERSITY | Information Technology RESEARCH COMPUTING

# Managing Jupyter Kernels on ITaP Community Clusters

*ITaP Research Computing Virtual Workshop Series*

June 12, 2020

An intermediate level discussion of how the Jupyter system (JupyterHub, Jupyter Notebook, etc.) function at an application level on a distributed computing cluster. The workshop explains how Jupyter Kernels function and how to extend them.

Other topics related to Jupyter are open for discussion.
A brief listing of possible topics is included at the end for reference.

**Geoffrey Lentner**
Senior Research Data Scientist
ITaP Research Computing

# *Prerequisites*

- Basic Linux/Unix command-line knowledge.
- Basic understanding of Computing Clusters.
- Familiarity with Python

## *Content*

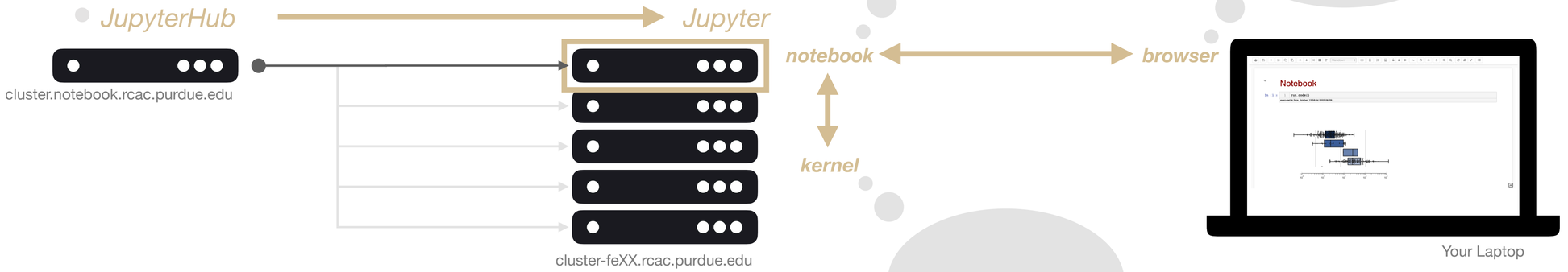
- What is Jupyter
- Where does Jupyter Look for Kernels
- How do Kernels Work
- Anatomy of a Jupyter Kernel
- Extending and Customizing a Kernel
- Other Topics

# What is Jupyter

***JupyterHub*** only does ***login*** and ***redirection***. It will start a Jupyter Notebook server on your behalf on one of the front-ends and redirect you.

The ***notebook server*** is fundamentally a web server that responds to requests from your browser and communicates with the ***kernel*** process its babysitting.

The browser is doing all of the ***user interface***. When you execute a code cell it sends a request to the notebook server.




The ***kernel*** process is merely the interpreter running in a ***headless*** state (Python, R, etc…).

***Jupyter[Hub] is a Python application***. It behaves, responds, and can be debugged as such. To understand problems that arise in the Jupyter ecosystem you need to ***identify at which layer*** the issue is occurring.

# *Where Does Jupyter Look for Kernels*

A kernel is ***installed*** when it is ***discoverable*** by Jupyter in one of these locations.

```
~ jane@cluster-fe03
❯ tree /opt/anaconda3
.
├── bin/
│   ├── ...
│   ├── jupyter*
│   └── jupyterhub*
├── etc/
├── include/
├── lib/
├── var/
└── share/
    └── jupyter/
        └── kernels/
            ├── bash/
            │   ├── ...
            │   └── kernel.json
            ├── ir/
            │   ├── ...
            │   └── kernel.json
            └── python3/
                ├── ...
                └── kernel.json
```

```
~ jane@cluster-fe03
❯ tree ~/.local
.
├── bin/
├── etc/
├── include/
├── lib/
├── var/
└── share/
    └── jupyter/
        └── kernels/
            └── my_env/
                ├── ...
                └── kernel.json
```

The *kernel.json* file specifies both ***how to launch*** the program and its ***environment***.

Jupyter looks for kernels in the ***system location it neighbors*** and in a fixed location in your ***home directory***.

# How Do Kernels Work

```
~ jane@cluster-fe03
❯ tree ~/.local
.
├── bin/
├── etc/
├── include/
├── lib/
├── var/
└── share/
    └── jupyter/
        └── kernels/
            └── my_env/
                ├── ...
                └── kernel.json
```

The *kernel.json* file specifies both ***how to launch*** the program and its ***environment***.

```
~ jane@cluster-fe03
❯ $CONDA_ENVS_PATH/my_env/python -m ipykernel_launcher -f my_session.json
...


~ jane@cluster-fe03
❯ cat my_session.json
{
  "shell_port": 36368,
  "iopub_port": 37524,
  "stdin_port": 46088,
  "control_port": 49141,
  "hb_port": 48572,
  "ip": "127.0.0.1",
  "key": "bc624cbf-5be3e02b2dbf13507a005a45",
  "transport": "tcp",
  "signature_scheme": "hmac-sha256",
  "kernel_name": ""
}
```

Jupyter is merely ***one of many*** clients that can manage an interactive Python session running in a ***headless state***.

A kernel can be implemented in most languages (dozens are). Python is pretty easy to setup, only requiring a launch point. Others (e.g., R) can be more tricky and require detailed configuration.

***Python can install its own kernel***.
If you have your environment activated and IPython installed *in that environment*:

```
(my_env) $ ipython kernel install --user --name my_env --display-name “Python 3.7 (my_env)”
```

# Anatomy of a Jupyter Kernel

```
~ jane@cluster-fe03
❯ cat ~/.local/share/jupyter/kernels/my_env/kernel.json
{
    "argv": [
        "/home/jane/.conda/envs/cent7/5.3.1-py37/my_env/bin/python",
        "-m",
        "ipykernel_launcher",
        "-f",
        "{connection_file}"
    ],
    "display_name": "Python 3.7 (my_env)",
    "language": "python"
}
```

The “argv” section is literally the command-line arguments that will be ***invoked on your behalf***.

# Extending and Customizing a Kernel

```
~ jane@cluster-fe03
❯ cat ~/.local/share/jupyter/kernels/my_env/kernel.json
{
    "argv": [
        "/home/jane/.conda/envs/cent7/5.3.1-py37/my_env/bin/python",
        "-m",
        "ipykernel_launcher",
        "-f",
        "{connection_file}"
    ],
    "display_name": "Python 3.7 (my_env)”,
    "language": "python",
    "env": {
        "PROJ_HOME": “/home/jane/.conda/envs/cent7/5.3.1-py37/my_env/share/proj"
    }
}
```

The “argv” section is literally the command-line arguments that will be ***invoked on your behalf***.

The “env” section is not present by default. You can ***add this section*** to define ***environment variables*** that you need for the libraries in the environment.

Many libraries require environment variables defined to function properly. When you install libraries with Anaconda these variables will be present after you activate the environment.

***Jupyter doesn’t know anything about Anaconda.***

# *Thank You*

# *Other Topics*

- Non-Python Kernels
- Integrating Modules with Jupyter Notebooks
- Distributing Computing from Jupyter Notebooks
- Notebook Extensions
- Customizing Notebooks with HTML/CSS/Javascript
- Debugging Jupyter, Notebooks, and Kernels
- OnDemand and Jupyter
- Running your own Jupyter from Backend Nodes
- Git and Jupyter
- JupyterLab
- Notebook Size and Visualization Libraries

ITaP Community Cluster Specifics
Technical Specifics
Features and Extensions