MANAGING JUPYTER KERNELS ON RCAC CLUSTERS

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About Me

Data Scientist, Astrophysicist, Research Software Engineer

Things I do at the Rosen Center for Advanced Computing (RCAC)

- System Support
- Scientific Software
- Consulting
- Training and Teaching

- Outreach and Engagement
- Innovation



Things we assume you already know

- Linux command-line basics (Unix 101 and Unix 102)
- Cluster basics (<u>Clusters 101</u>)
- Python basics (not critical)



Overview

Topics covered

- What is Jupyter
- What is a kernel and where does Jupyter look for them
- Anatomy of a kernel and how to customize them
- Extra topics



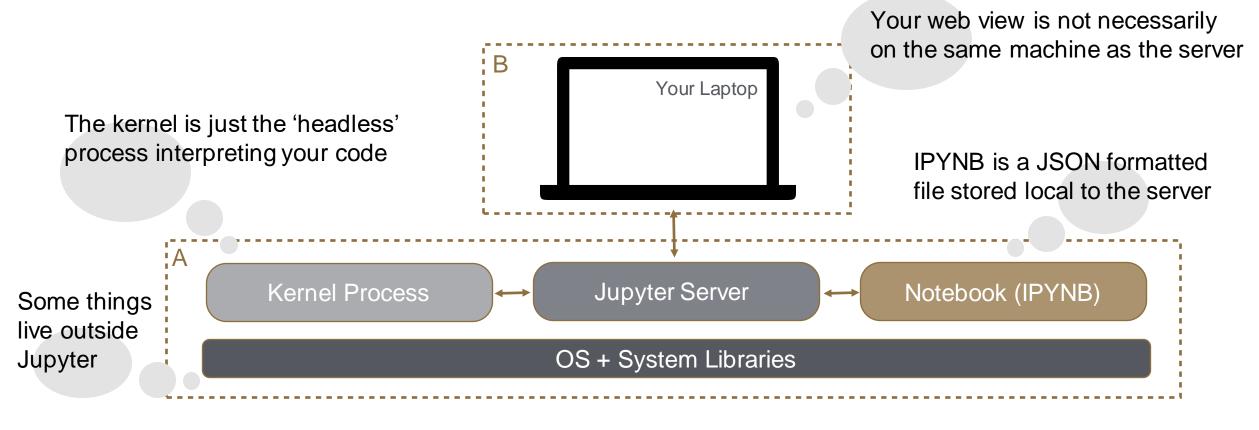
What is Jupyter

What are the components that make up the Jupyter ecosystem?



What is Jupyter

Elements of the Jupyter system





What is a Kernel

The runtime environment specification that underpins Jupyter notebooks.



What is a kernel?

A Jupyter "kernel" can refer to two things

- The "kernel spec" or **configuration file**
- The **runtime** environment it refers to (e.g., Anaconda)



What is a kernel?

Where does Jupyter look for kernels?

jane@login00.cluster [~] \$ tree ~/.local	
<pre> bin/ etc/ include/ lib/ var/ share/ jupyter/ kernels/ kernel.json</pre>	
	_

- System: /usr/local/share/jupyter/kernels
- User: ~/.local/share/jupyter/kernels
- Local: ../share/jupyter/kernels

Within the same installation **prefix** as Jupyter itself





Anatomy of a Kernel

What's inside a kernel specification?



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What's inside a kernel specification

Take a look inside the kernel.json file

jane@login00.cluster [~] \$ cat ~/.local/share/jupyter/kernels/py39-foo/kernel.json

"argv":[

"/home/jane/.conda/envs/cent7/2020.11-py38/py39-foo/bin/python", "-m",

"ipykernel_launcher",

"-f",

"{connection_file}"

"display_name":"Python 3.9 (Foo)", "language":"python" The **"argv**" section is literally the command-line arguments that will be *invoked on your behalf*.



What's inside a kernel specification

Take a look inside the kernel.json file

jane@login00.cluster [~] \$ cat ~/.local/share/jupyter/kernels/py39-foo/kernel.json
{
 "argv": [
 "/home/jane/.conda/envs/cent7/2020.11-py38/py39-foo/bin/python",
 "-m",
 "ipykernel_launcher",
 "-f",
 "{connection_file}"
],
 "display_name": "Python 3.9 (Foo)",
 "language": "python",
 "env": {
 "PROJ_HOME": "/home/jane/.conda/envs/cent7/5.3.1-py37/my_env/share/proj"
 }
}

You can do things like customize environment variables within the kernel specification



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Special Topics

What other things can you do with Jupyter? Alternative configurations? How to trouble shoot when things goes wrong?



Troubleshooting

How to find issues when Jupyter/kernels aren't working

jane@login00.cluster [~] \$ module load jupyterhub jane@login00.cluster [~] \$ jupyter notebook --port 8787 --no-browser .

Errors from Jupyter itself as well as anything to do with the running kernel will appear in the logs



Other Topics

We can discuss many other things

- Non-Python kernels
- Integrating Modules with Jupyter Notebooks
- Distributed Computing within notebooks
- Notebook extensions
- Debugging Jupyter, Notebooks, Kernels

- OnDemand and Jupyter
- Running custom Jupyter on compute nodes
- Git and Jupyter
- Jupyter Lab
- Notebook size and visualizations



THANK YOU

Please reach out to <u>rcac-help@purdue.edu</u> for questions.

