



Containers and Notebooks

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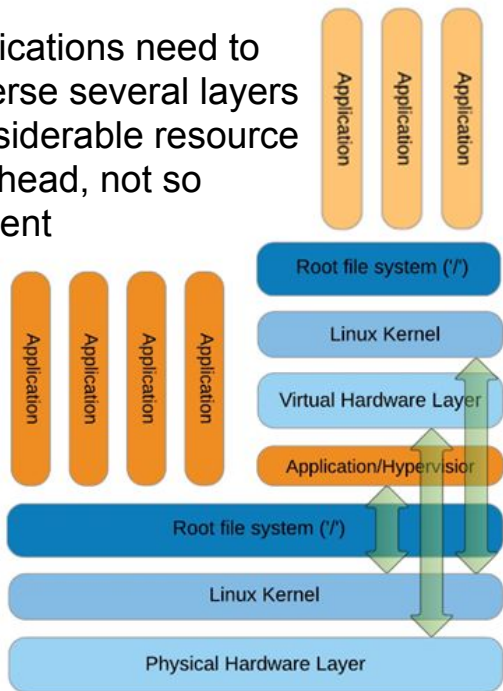
Motivation

- Containers:
 - Software dependencies all in one package
 - Dive right into analysis without painful installation procedures
 - Portable, can run on different machine architectures

- Jupyter Notebooks:
 - Code development, documentation, execution, and plot presentation all-in-one
 - Fast interactive access to remote computing resources and data
 - Shareable, so people know exactly what you did and how

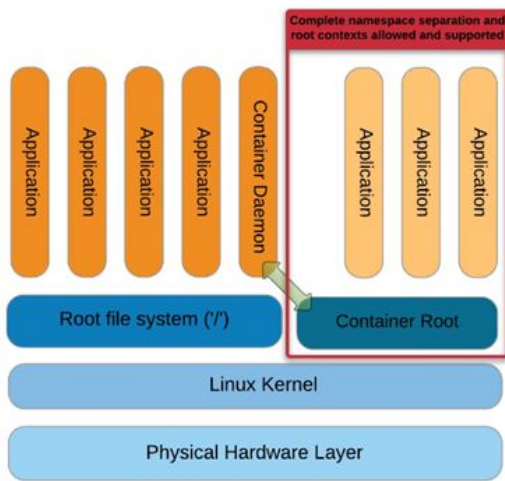
Virtualization

- Applications need to traverse several layers
- Considerable resource overhead, not so efficient



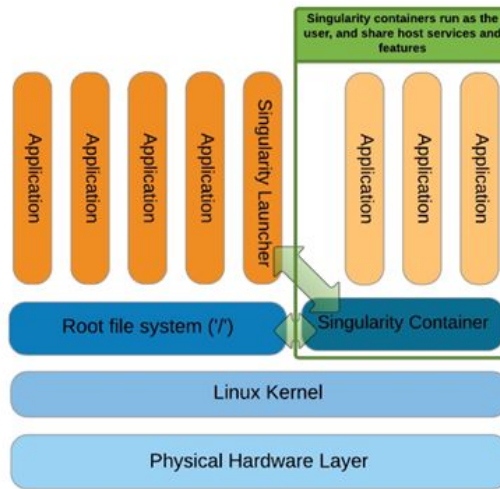
General VM
eg ESXi

- Needs root access
- Problematic with HPC



General Container
eg Docker

- This workshop
- Designed for HPC
 - Support for GPUs



HPC Container
Singularity

Container Workflow

- Install packages you need
 - This part requires root access

- Collection of images to build from exists!
 - E.g. [here](#)

This workshop

- Container already built for you to use
- Distributed to all the AWS instances



Interactive Development

```
sudo singularity build --sandbox tmpdir/ Singularity
```

```
sudo singularity build --writable container.img Singularity
```

BUILD ENVIRONMENT

Build from Recipe

```
sudo singularity build container.img Singularity
```

Build from Singularity

```
sudo singularity build container.img shub://vsoch/hello-world
```

Build from Docker

```
sudo singularity build container.img docker://ubuntu
```

Container Execution

```
singularity run container.img  
singularity shell container.img  
singularity exec container.img ...
```

Reproducible Sharing

```
singularity pull shub://...  
singularity pull docker://... *
```

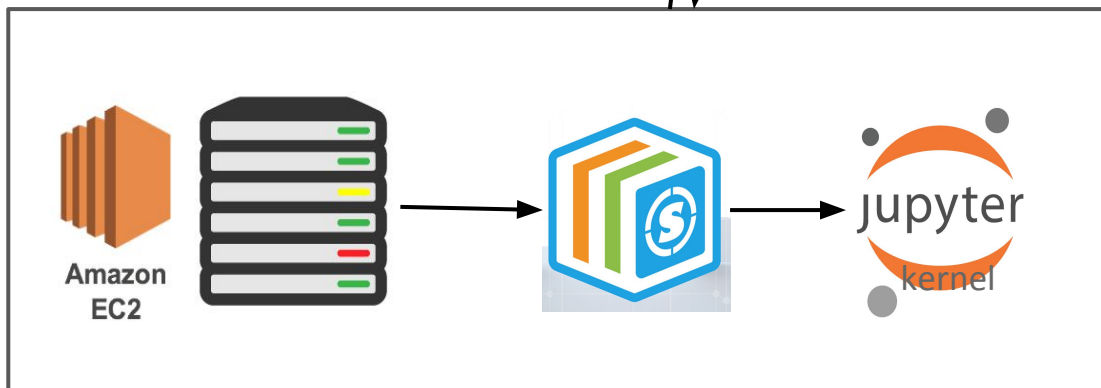
PRODUCTION ENVIRONMENT

Jupyter Notebook

- Web-based GUI interface to IPython interactive shell
 - Like ROOT CINT, but built on industry-standard analysis, plotting, etc. libraries
- Quick run-through of pre-workshop tutorial to get a Jupyter notebook running
- Go through [live demonstration of features](#)
 - Development
 - Execution
 - Visualization
 - [Online notebook viewer](#)
- Huge community with lots of resources for learning ([ex.](#))



ssh tunnel (or open port)



GitHub Organization

- <https://github.com/WatChMaL>
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