

Singularity

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Basics of singularity

How to create a customized singularity image

How to use a custome image in jupyterhub

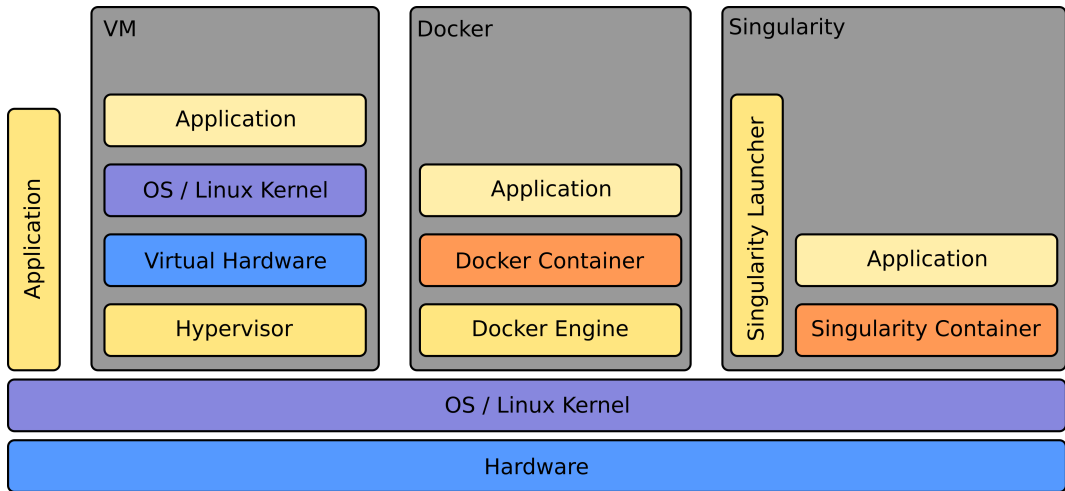
Singularity is a container solution.

Singularity supports HPC systems.

Singularity natively supports InfiniBand, Lustre, and resource managers (e.g. SLURM, SGE, etc.).

Singularity has built-in support for MPI and can access GPU resources.

Virtualization vs. Containerization



basic commands

```
singularity pull  
singularity exec  
singularity shell  
singularity run  
singularity build
```

basic examples

```
(skylake) [VSC-4]$ module load singularity/3.8.5-gcc-12.2.0-kdm7usg  
(zen3) [VSC-5]$ module load singularity/3.8.3-gcc-11.2.0-k6oedzn
```

```
(skylake/zen3) [VSC-4/5]$ singularity pull docker://ubuntu:latest  
(skylake/zen3) [VSC-4/5]$ singularity pull docker://centos:latest  
(skylake/zen3) [VSC-4/5]$ singularity pull docker://python:latest
```

basic examples

```
(skylake/zen3) [VSC-4/5]$ singularity exec ubuntu_latest.sif cat /etc/lsb-  
(skylake/zen3) [VSC-4/5]$ singularity exec centos_latest.sif cat /etc/redha
```


basic examples

```
(skylake/zen3) [VSC-4/5]$ singularity shell ubuntu_latest.sif
Singularity> cat /etc/lsb-release
DISTRIB_ID=Ubuntu
DISTRIB_RELEASE=20.04
DISTRIB_CODENAME=focal
DISTRIB_DESCRIPTION="Ubuntu 20.04.3 LTS"
```

basic examples

```
$ cat hello.py
import sys
print("Hello World: The Python version is %s.%s.%s" % sys.version_info[:3])
```

```
(skylake/zen3) [VSC-4/5]$ python3 hello.py
Hello World: The Python version is 3.9.5
```

```
(skylake/zen3) [VSC-4/5]$ singularity exec python_latest.sif python ./hello.py
Hello World: The Python version is 3.11.0
```

basic examples

```
(skylake/zen3) [VSC-4/5]$ singularity shell python_latest.sif
```

```
Singularity> python ./hello.py
```

```
Hello World: The Python version is 3.11.0
```

```
Singularity> cat /etc/os-release
```

```
(skylake/zen3) [VSC-4/5]$ singularity run python_latest.sif
```

```
Python 3.10.0 (default, Oct 26 2021, 22:20:53) [GCC 10.2.1 20210110] on lin
```

```
Type "help", "copyright", "credits" or "license" for more information.
```

```
>>>
```

VSC-4:

```
#!/bin/bash
#
#SBATCH -J myjob
#SBATCH -o output.%j
#SBATCH -p skylake_0096
#SBATCH -N 1

module load singularity/3.8.5-gcc-12.2.0-kdm7usg
singularity exec docker://python:latest python ./hello.py
```

VSC-5:

```
#!/bin/bash
#
#SBATCH -J myjob
#SBATCH -o output.%j
#SBATCH -p skylake_0096
```

Singularity image for jupyterhub

Examples can be found in

```
/home/fs70824/training/examples/14_singularity/jupyterhub
```

Minimal notebook with developer tools:

```
# cat jupyter-minimal.def
BootStrap: docker
From: jupyter/minimal-notebook:latest

%post
apt update
apt -y upgrade
apt -y install environment-modules gcc gfortran g++
/opt/conda/bin/pip install batchspawner
```

On a workstation with root permission:

```
singularity build jupyter-minimal.sif jupyter-minimal.def
```

Minimal notebook with python modules:

```
# cat jupyter-pytorch.def
Bootstrap: docker
From: jupyter/minimal-notebook:latest

%post
/opt/conda/bin/pip install torch numpy matplotlib batchspawner
```

On a workstation with root permission:

```
singularity build jupyter-pytorch.sif jupyter-pytorch.def
```

Server Options

Select profile to use:

VSC-4 (Singularity Image) for Training

Select IDE to start with:

☒ JupyterLab

☐ Jupyter Notebook

Choose image type:

☐ Use predefined image

☒ Use custom image

Provide your own custom singularity image

/home/fs70824/trainee78/VSC-Jupyterhub/singularity-examples/jupyter-minimal.sif

Please note: The image has to be placed on a share reachable from the cluster nodes

Number of (hyperthreading) cores

2 cores

4 cores

8 cores

12 cores

24 cores

48 cores

Memory needed

8GB

16GB

32GB

64GB

Maximum running time

4 hours

12 hours

24 hours

3 days

Start

Server Options

Select profile to use:

VSC-4 (Singularity Image) for Training

Select IDE to start with:

☒ JupyterLab

☐ Jupyter Notebook

Choose image type:

☐ Use predefined image

☒ Use custom image

Provide your own custom singularity image

/home/fs70824/trainee78/VSC-Jupyterhub/singularity-examples/jupyter-pytorch.sif

Please note: The image has to be placed on a share reachable from the cluster nodes

Number of (hyperthreading) cores

2 cores

4 cores

8 cores

12 cores

24 cores

48 cores

Memory needed

8GB

16GB

32GB

64GB

Maximum running time

4 hours

12 hours

24 hours

3 days

Start

Singularity image for jupyterhub

The screenshot displays the JupyterLab Launcher interface. On the left is a sidebar with a file browser. The top menu bar includes File, Edit, View, Run, Kernel, Tabs, Settings, and Help. The file browser shows a search bar and a list of files in the directory `/ ... / fs70824 / trainee78 /`.

Name	Last Modified
VSC-Jupyter...	18 minutes ago
slurm-168...	3 minutes ago
slurm-168...	seconds ago
Untitled.ip...	12 minutes ago
Untitled1.i...	5 minutes ago
Untitled2.i...	4 minutes ago
Untitled3.i...	4 minutes ago

The main workspace area is titled "Launcher" and shows the path `home/fs70824/trainee78`. It contains three sections:

- Notebook**: A section with a Python 3 (ipykernel) icon.
- Console**: A section with a Python 3 (ipykernel) icon.
- Other**: A section with five icons: Terminal, Text File, Markdown File, Python File, and Show Contextual Help.

Singularity image for jupyterhub

The screenshot displays the JupyterLab interface within a Singularity container. The top menu bar includes File, Edit, View, Run, Kernel, Tabs, Settings, and Help. The left sidebar features a file browser with a search bar and a table of files.

Name	Last Modified
VSC-Jupyter...	19 minutes ago
slurm-168...	4 minutes ago
slurm-168...	in a few seconds
Untitled.ip...	13 minutes ago
Untitled1.i...	6 minutes ago
Untitled2.i...	5 minutes ago
Untitled3.i...	5 minutes ago
• Untitled4.i...	seconds ago

The main area shows a code editor with the following code:

```
[1]: import numpy
[2]: import matplotlib
[3]: import torch
[ ]:
```

Advantage: no need to rebuild the container everytime you want to install a new package.

Required steps:

- ▶ Create a venv
- ▶ Make the venv available in jupyterlab

Create a new venv:

```
(skylake) [VSC-4]$ module load miniconda3/4.12.0-intel-2021.5.0-kwofrye  
(skylake) [VSC-4]$ conda create -n newenv python=3.10  
Collecting package metadata: done  
Solving environment: done
```

```
## Package Plan ##
```

```
environment location: /home/fs60000/jz/.conda/envs/newenv
```

```
added / updated specs:  
- python=3.10
```

The following packages will be downloaded:

```
(skylake) [VSC-4]$ conda init bash
(s skylake) [VSC-4]$ bash
(base)(skylake) [VSC-4]$ conda activate newenv
(newenv)(skylake) [VSC-4]$ which python3
~/ .conda/envs/newenv/bin/python3
(newenv)(skylake) [VSC-4]$ python3 --version
Python 3.10.0
```

Conda virtual env in jupyterhub

Add Virtual Environment to Jupyter Notebook:

```
```shell
```

```
(newenv)(skylake) [VSC-4]$ pip install --user ipykernel
```

```
(newenv)(skylake) [VSC-4]$ cat /home/fs60000/jz/.local/share/jupyter/kernels/
{
 "argv": [
 "/home/fs60000/jz/.conda/envs/newenv/bin/python",
 "-m",
 "ipykernel_launcher",
 "-f",
 "{connection_file}"
],
 "display_name": "newenv",
 "language": "python",
 "metadata": {
 "debugger": true
 }
}
```

```
(newenv)(skylake) [VSC-4]$ jupyter kernelspec list
```

```
Available kernels:
```

myenv	/home/fs60000/jz/.local/share/jupyter/kernels/myenv
newenv	/home/fs60000/jz/.local/share/jupyter/kernels/newenv
python3	/home/fs60000/jz/.local/share/jupyter/kernels/python3



# Conda virtual env in jupyterhub

The screenshot displays the JupyterLab interface. On the left is a file browser sidebar with a search bar and a list of files and directories. The main area is titled 'Launcher' and shows the path 'home/fs60000/jz'. It is divided into three sections: 'Notebook', 'Console', and 'Other'. Each section contains buttons for different environments or actions.

**File Browser Sidebar:**

Name	Last Modified
slurm-168...	3 days ago
slurm-168...	3 days ago
slurm-168...	3 days ago
slurm-168...	a day ago
slurm-168...	28 minutes ago
slurm-168...	in a few seconds
SPEC-201...	2 years ago
SPECFP_V...	8 months ago
SPECFP_V...	8 months ago
specfp201...	2 years ago
specfp201...	2 years ago
Untitled.ip...	2 months ago
untitled.md	6 days ago
untitled.py	6 days ago
untitled.txt	6 days ago
Untitled1.i...	2 months ago
Untitled10...	6 days ago
Untitled11.i...	6 days ago
Untitled12...	6 days ago
Untitled13...	6 days ago
Untitled14...	6 days ago
Untitled15...	6 days ago
Untitled16...	3 days ago
Untitled17.i...	3 days ago

**Launcher Section: home/fs60000/jz**

- Notebook:** Contains three buttons with the Python logo: 'Python 3 (ipykernel)', 'myenv', and 'newenv'.
- Console:** Contains three buttons with the Python logo: 'Python 3 (ipykernel)', 'myenv', and 'newenv'.
- Other:** Contains five buttons: 'Terminal' (with a terminal icon), 'Text File' (with a list icon), 'Markdown File' (with a purple 'M' icon), 'Python File' (with the Python logo), and 'Show Contextual Help' (with a help icon).

Try:

```
(newenv)(skylake) [VSC-4]$ pip install numpy
```