SLES 15 SP4

Replicable Python Environments with JupyterLab

SUSE Linux Enterprise Server 15 SP4

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Summary

This document illustrates how to install and run JupyterLab, the web-based interactive development environment from Project Jupyter, on SUSE Linux Enterprise.

Contents

1 Introduction

1.1 Motivation

The Python (https://www.python.org/) programming ecosystem is popular for its simplicity, extensibility, cross-platform availability, and its large open source community of active developers and users. Developers in many domains benefit from and contribute to the large and growing Python ecosystem of open source tools and libraries. This has resulted in a rapid state of continuous development for the language and for the domains where Python is used.

The modern Python developer's environment can be highly complex, leveraging a wealth of libraries, each with its own development life cycle and dependencies. Such complexity makes it difficult to faithfully replicate and share a development environment for collaboration, testing, and deployment. This is especially relevant in scientific computing, including the modern field of machine learning, where experimental replication is critical for validation but minor variations in the complex weave of library dependencies could invalidate test results or lead to unexpected behaviors in production.

1.2 Scope

This guide helps you take a first step to overcoming the challenge of creating and sharing replicable Python development environments.

Specifically, you get a brief introduction to the following concepts, systems, tools, and applications:

- SUSE Linux Enterprise Server (https://www.suse.com/products/server/), the adaptable, reliable, and secure platform that enables you to go from development to production with confidence.
- Python (https://www.python.org/) programming ecosystem.
- Python Package Index (PyPI) (https://pypi.org/), the Python software repository.
- Lightweight virtual environments with `venv` (https://docs.python.org/3/library/venv.html).
- Python package management with `pip` (https://pip.pypa.io/en/stable/).
- Interactive, computational notebooks with Project Jupyter (https://jupyter.org/)

Note

Many of the steps herein may be followed with little or no modification on the corresponding version of openSUSE Leap.

1.3 Audience

This guide is intended for researchers, engineers, developers, operations teams, and others interested in implementing replicable, ML development environments, featuring Python and computational documents with JupyterLab. The reader should have basic Linux command line skills.

2 Prerequisites

For this guide, you need:

- SUSE Linux Enterprise Server 15 SP4 (SLES 15 SP4)
  - If you do not already have SLES 15 SP4 installed on your system (bare metal or virtual machine), instructions can be found here: https://documentation.suse.com/sles/15-SP4/html/SLES-all/book-deployment.html
  - Make sure your SLES 15 SP4 installation is up-to-date by running `zypper patch`, `zypper update`, or by using YaST online update (https://documentation.suse.com/sles/15-SP4/html/SLES-all/cha-onlineupdate-you.html).
- Python 3
  Python 3.6 is included with SLES 15 SP4 by default. It is a stable version, tested against the libraries and tools that are part of the operating system. This version is usually adequate for many use cases, but may not be new enough to support some workloads.
  This guide uses Python 3.10, which you install in the next section.
- Internet access
  You need Internet access to download additional libraries and applications used in this guide.

3 Setting up your Python environment

Some disciplines, like machine learning, are in fast development and often have strict version dependencies. Installing dependent packages to support one project may thus break another project. Developers need a way to create isolated environments where they can install the packages they need without impacting other projects or system operations.

3.1 Addressing Python versions

Your application may have a hard dependency for a specific version of the Python interpreter itself. You can install a newer version of Python on your system. In fact, you can have multiple versions of Python. But care must be taken not to break dependencies for system tools or other applications.

At the time of this writing, Python 3.6 is the default version installed with SLES 15 SP4. And Python 3.10 is included in the standard repositories.

You should use the Python packages in the official SUSE repositories when possible. These packages have undergone extensive testing and are supported by SUSE. If you must use another version, you can build and install it from source code or use an implementation from a trusted provider (such as Anaconda (https://www.anaconda.com/)).

Tip

SUSE mitigates the risk of Python version conflicts with explicit naming, ensuring that respective versions installed from the official repositories have unique file and directory names. For example, you will find the default Python interpreter is the executable file, `/usr/bin/python3.6`, but, if you have Python 3.10 installed, its interpreter is the file, `/usr/bin/python3.10`.

1. Install Python 3.10 or the latest version available in the official repositories.

```
sudo zypper install python310
```

Tip

You can list the available Python 3 packages with `sudo zypper search -d "Python 3 Interpreter"` or `sudo zypper search python3`.

2. Verify installation.

```
/usr/bin/python3.10 --version
```

or, with `/usr/bin/` in your path:

```
python3.10 --version
```

Warning

The default Python is still symbolically linked to `/usr/bin/python3`. Do not change this symbolic link, as this could break system tools that rely on the default version.

Tip

Tools like pyenv (https://github.com/pyenv/pyenv) can help simplify installation and management of multiple Python environments, but this is out of scope for this document.

3.2 Creating a Python virtual environment

The Python `venv` module (https://docs.python.org/3/tutorial/venv.html) provides a mechanism for creating lightweight "virtual environments" and gives us a tool for isolating software dependencies. See the Python Enhancement Proposal 405 - Python Virtual Environments (https://peps.python.org/pep-0405/) for more details on the `venv` module.

Creating a Python virtual environment is easy. Run the following commands as your user (root access is not required):

1. Create a virtual environment, named 'myproj'.

```
python3.10 -m venv $HOME/myproj
```

This creates a new `myproj/` subdirectory in your home directory and populates it with files, subdirectories, and symbolic links to enable the virtual environment to use the Python interpreter you specify with this command.

2. Change to the new directory.

```
cd $HOME/myproj
```

3. Activate the new virtual environment.

```
source ./bin/activate
```

The `activate` script cannot be run on its own and must be "sourced" to update current environment variables in support of the isolated environment.

Tip

When your virtual environment is active, your command prompt is prefixed with the environment name. In the present example, you should see '(myproj)' before your normal prompt.

4. Deactivate your active virtual environment.

```
deactivate
```

When you are done working in this virtual environment, you can use the `deactivate` command to reset all the environment changes (including your prompt). This does not delete the virtual environment. To reactivate it, simply source the activate script again.

You can use the Python `venv` module to create as many virtual environments as you need, each in its own working directory.

Note

If you no longer need a virtual environment and want to delete it, simply:

1. deactivate the environment.
2. delete its directory.

4 Managing Python packages

The SUSE Linux Enterprise Server repositories include many Python packages, tested against the included version of Python. These can be installed system-wide and are fine for many development projects. Sometimes your project may require a different version of one of these packages or a package not available in the standard repositories. In these cases, you may choose to use the Python Package Index (PyPI) (https://pypi.org/). This is a public repository of open source licensed packages made available by a community of developers from around the world.

There are many ways to install Python packages from PyPI, but the preferred method is with `pip` (https://pypi.org/project/pip/). `pip` is a powerful tool for managing Python packages from PyPI, but it can also install from a Git repository or from local distribution files.

Many Python packages are dependent on other packages. But manually identifying and installing all dependencies can be grueling, especially when each package may have additional dependencies of its own. Fortunately, `pip` automatically performs dependency resolution to ensure installation of all required packages and alerts you if resolution fails. See the `pip` documentation (https://pip.pypa.io/en/stable/) for details.

Note

Your Python virtual environment has its own *pip* executable and symbolic links to the Python interpreter you used to create it. These are located in the *bin/* subdirectory of your working directory. After activating your virtual environment, use `python --version` and `pip --version` to verify the versions of these commands.

4.1 Performing basic package management

With the following commands, you will perform some basic operations with the `pip` package installer.

1. Activate your virtual environment.

```
cd $HOME/myproj
source ./bin/activate
```

2. Upgrade `pip` itself to the latest version.

```
pip install --upgrade pip
```

3. Install a specific version of the `numpy` (https://pypi.org/project/numpy/1.18.5/) package.

```
pip install numpy==1.18.5
```

Tip

Be sure to use two equal signs ('==') between the package name and the desired version.

4. Upgrade to the latest compatible version of `numpy`.

```
pip install --upgrade numpy
```

Note

You may not actually get the *latest* version of a package. Instead, you get the latest version that is compatible with your Python environment.

5. Uninstall `numpy`.

```
pip uninstall numpy
```

6. Install multiple packages (`numpy`, `pandas`, and `matplotlib`) together.

```
pip install numpy pandas matplotlib
```

```
Collecting numpy
  Using cached numpy-1.19.5-cp36-cp36m-manylinux2010_x86_64.whl (14.8 MB)
Collecting pandas
  Using cached pandas-1.1.5-cp36-cp36m-manylinux1_x86_64.whl (9.5 MB)
Collecting matplotlib
  Using cached matplotlib-3.3.4-cp36-cp36m-manylinux1_x86_64.whl (11.5 MB)
Collecting pytz>=2017.2
  Using cached pytz-2022.2.1-py2.py3-none-any.whl (500 kB)
Collecting python-dateutil>=2.7.3
  Using cached python_dateutil-2.8.2-py2.py3-none-any.whl (247 kB)
Collecting pyparsing!=2.0.4,!=2.1.2,!=2.1.6,>=2.0.3
  Using cached pyparsing-3.0.9-py3-none-any.whl (98 kB)
Collecting cycler>=0.10
  Using cached cycler-0.11.0-py3-none-any.whl (6.4 kB)
Collecting pillow>=6.2.0
  Using cached Pillow-8.4.0-cp36-cp36m-
manylinux_2_17_x86_64.manylinux2014_x86_64.whl (3.1 MB)
```

```
Collecting kiwisolver>=1.0.1
  Using cached kiwisolver-1.3.1-cp36-cp36m-manylinux1_x86_64.whl (1.1 MB)
Collecting six>=1.5
  Using cached six-1.16.0-py2.py3-none-any.whl (11 kB)
Installing collected packages: six, pytz, python-dateutil, pyparsing, pillow, numpy,
 kiwisolver, cycler, pandas, matplotlib
Successfully installed cycler-0.11.0 kiwisolver-1.3.1 matplotlib-3.3.4 numpy-1.19.5
 pandas-1.1.5 pillow-8.4.0 pyparsing-3.0.9 python-dateutil-2.8.2 pytz-2022.2.1
 six-1.16.0
```

Note

Because some additional packages are required by those requested, `pip` automatically downloads and installs them.

4.2 Creating replicable experiments

Repeatability is key to many disciplines, but particularly in the sciences. Ensuring that your Python environment can be recreated the same way with the same packages and the same versions of those packages can be a challenge.

Fortunately, with the `pip freeze` command, you can generate a package requirements file, containing a list of the packages and versions that should be installed. See https://pip.pypa.io/en/stable/cli/pip_freeze/ for more information.

Create a requirements file for your Python virtual environment by following these steps:

1. Activate your virtual environment (if not already active).
2. Generate a requirements file with `pip freeze`.

```
pip freeze > requirements.txt
```

3. Take a look at the requirements file.

```
cat requirements.txt
```

```
cycler==0.11.0
kiwisolver==1.3.1
matplotlib==3.3.4
numpy==1.19.5
pandas==1.1.5
Pillow==8.4.0
```

```
pyparsing==3.0.9
python-dateutil==2.8.2
pytz==2022.2.1
six==1.16.0
```

When you have a requirements file, you can share it with another developer or use it yourself to make sure a new environment contains all the same packages.

1. If you are in an active virtual environment, deactivate it and leave that working directory.

```
deactivate
cd ..
```

2. Create a new Python virtual environment.

```
python3 -m venv myproj2
```

3. Enter the working directory and activate the new environment.

```
cd myproj2
source ./bin/activate
```

4. Upgrade `pip`.

```
pip install --upgrade pip
```

5. Install packages with the requirements file.

```
pip install -r ../myproj/requirements.txt
```

6. Verify correct packages are installed.

```
pip freeze
```

```
cycler==0.11.0
kiwisolver==1.3.1
matplotlib==3.3.4
numpy==1.19.5
pandas==1.1.5
Pillow==8.4.0
pyparsing==3.0.9
python-dateutil==2.8.2
pytz==2022.2.1
six==1.16.0
```

Tip

`pip freeze` excludes `pip` and a few other packages. To see a complete list of packages, use `pip list`.

5 Project Jupyter and JupyterLab

Project Jupyter (https://jupyter.org/) was born out of the IPython Project (https://ipython.org/) in 2014 as it evolved to support interactive data science and scientific computing across more programming languages.

Under the Jupyter umbrella are:

- Jupyter Notebook: the original Web application that allows data scientists to create and share computational documents, called notebooks.
- JupyterLab: the latest generation of Jupyter Notebook with a modular design to allow users to customize the interface to support workflows in data science, scientific computing, computational journalism, and machine learning.
- JupyterHub: the multiuser version of Jupyter Notebook that enables companies, classrooms, and research labs to deliver computational environments and resources to users while managing them centrally.
- Voilà: a tool that transforms Jupyter notebooks into secure, stand-alone Web applications.

Note

The Jupyter team maintains the IPython project and includes the IPython kernel (IPyKernel) by default to enable interactive Python in JupyterLab. A variety of community maintained kernels are available to enable use of other programming languages, such as R (https://irkernel.github.io/), Julia (https://github.com/JuliaLang/IJulia.jl), and many others (https://github.com/jupyter/jupyter/wiki/Jupyter-kernels).

5.1 Getting JupyterLab up and running

JupyterLab is a Web application, so you need a Web browser to access it.

1. Install JupyterLab.

   JupyterLab is easy to install right from PyPI. In your active virtual environment, issue the command:

   ```
   pip install jupyterlab
   ```

2. Update your requirements file so JupyterLab will be included.

   ```
   pip freeze > requirements.txt
   ```

   Tip

   Update your requirements file each time you install packages.

3. Launch JupyterLab.

   Once JupyterLab is installed, launch it with the command:

   ```
   jupyter-lab
   ```

   In your terminal window, you see something like the following:

   ```
   [I 2022-08-22 13:14:26.394 ServerApp] Jupyter Server 1.13.1 is running at:
   [I 2022-08-22 13:14:26.394 ServerApp] http://localhost:8888/lab?
   token=4baab78a6959bbc8b9992572b8faf7d2416741c2d00768f7
   [I 2022-08-22 13:14:26.394 ServerApp]  or http://127.0.0.1:8888/lab?
   token=4baab78a6959bbc8b9992572b8faf7d2416741c2d00768f7
   [I 2022-08-22 13:14:26.394 ServerApp] Use Control-C to stop this server and shut
    down all kernels (twice to skip confirmation).
   [C 2022-08-22 13:14:26.398 ServerApp]

       To access the server, open this file in a browser:
           file:///home/suse/.local/share/jupyter/runtime/jpserver-31811-open.html
       Or copy and paste one of these URLs:
           http://localhost:8888/lab?
   token=4baab78a6959bbc8b9992572b8faf7d2416741c2d00768f7
        or http://127.0.0.1:8888/lab?
   token=4baab78a6959bbc8b9992572b8faf7d2416741c2d00768f7
   ```

4. Access the JupyterLab user interface (UI).

   JupyterLab will attempt to open your default Web browser to the UI. If this fails, you can manually open your browser to one of the URLs provided in your terminal window.

Note

JupyterLab uses an access token to authenticate you to the Web UI. This token is unique to each instance of the environment.

Tip

If your environment is on a remote, headless host, you can use SSH port forwarding to gain access.

1. Log in to the remote host with a local port forward.

   ```
   ssh -L8888:localhost:8888 USER@REMOTE-IP
   ```

   where USER is your user name on the remote host and REMOTE-IP is its IP address or domain name.

2. Activate your virtual environment.

3. Launch JupyterLab.

4. Open your local Web browser to the URL (with your access token) specified in the command terminal.

5. Shut down JupyterLab.

   Shutting down JupyterLab means stopping running extensions, kernels, terminals, and the UI.

   Shut down JupyterLab directly from the UI by selecting *Shutdown* under the *File* menu.

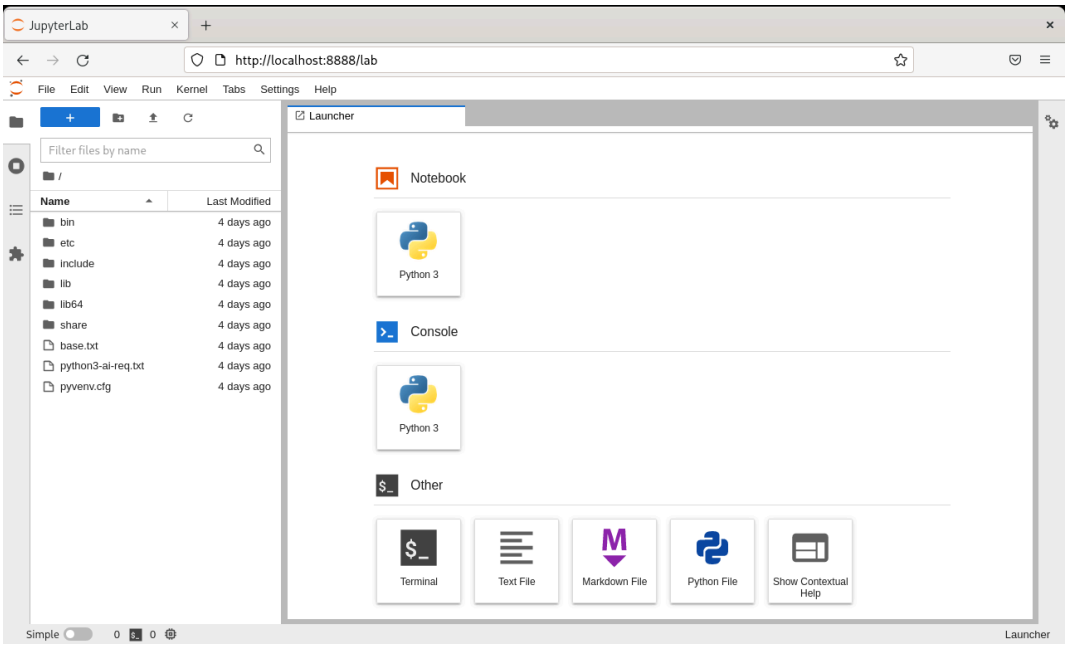
Note

If you select *Logout* from the *File* menu or close your browser, the JupyterLab environment continues to run. You can shut it down from the command terminal by issuing 'CTRL-C'. You will be prompted to confirm that you want to shut down the Jupyter server. Bypass confirmation by issuing 'CTRL-C' twice.

5.2 Exploring JupyterLab

JupyterLab has many of the features of a traditional integrated development environment (IDE), but it focuses on interactive and exploratory computing.

The main JupyterLab interface consists of a menu at the top, a collapsible sidebar on the left, and a main work area in the middle.



The menu provides access to some familiar functions, like file management, editing functions, UI view and settings, and help. It also includes functions specific to working in an interactive computing environment, like running code and managing compute kernels.

The sidebar offers a file browser, process controls, extension management, and more.

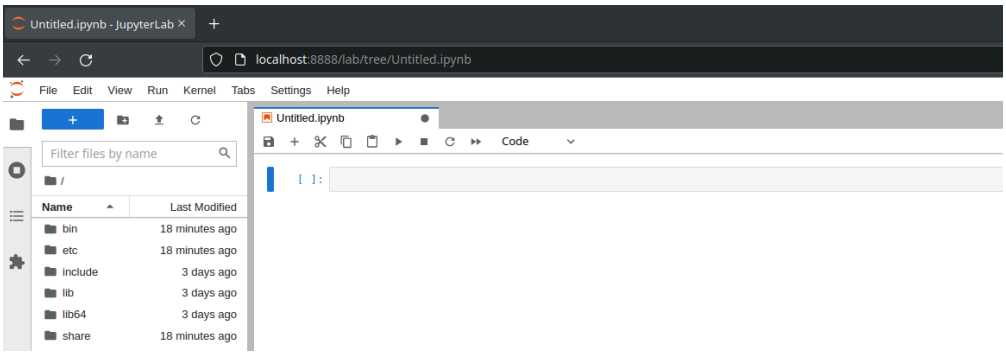
JupyterLab opens with the main work area displaying the *Launcher* tab. From the *Launcher*, you can start a notebook, console, terminal window, and more. These appear as additional tab in the main work area.

Tip

If you accidentally close the *Launcher*, you can open a new one from the *File* menu.

Try creating a notebook.

1. Start a notebook by clicking *Python 3* in the *Notebook* area of the *Launcher*.



2. In the first command cell of your notebook, enter:

```
from sys import version
```

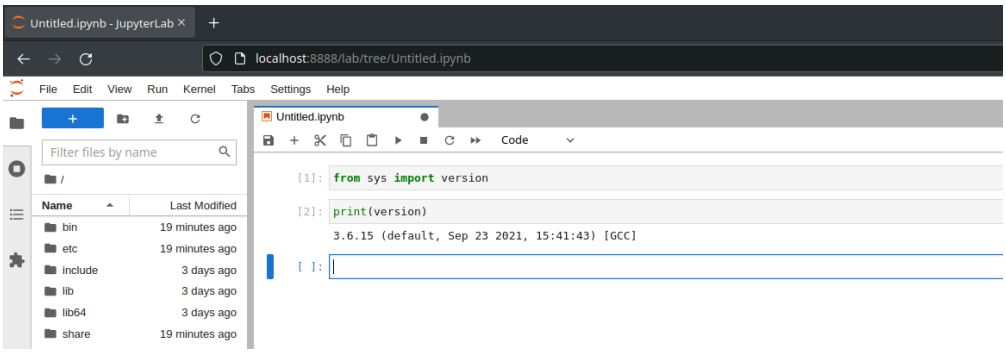
Press 'CTRL-ENTER' at the end of the line to execute it.

Tip

You can enter multiple lines by pressing 'ENTER' at the end of each line. The code will not execute until you press 'CTRL-ENTER'.

3. In the second command cell, enter:

```
print(version)
```



4. Save your notebook by selecting *Save Notebook As…* from the *File* menu.
Enter a name when prompted, such as `mypythonversion.ipynb`.

5. Close your notebook by clicking the 'X' in the notebook tab.

6. Reopen your notebook by double-clicking `mypythonversion.ipynb` in the sidebar file browser.

5.3 Collaborating with JupyterLab

JupyterLab provides a great environment for interactive experimentation, and the notebook format offers an easy mechanism for sharing your code with others. But a Jupyter notebook by itself may not be sufficient, as your colleague's development environment may be different.

When you are ready to share your work, you should include your:

- notebook
- data
- requirements file

With these three items, your colleague can recreate your development environment and run your code against your data.

6 Summary

Whether you are getting started on your Python development journey or already looking to scale to production, start from a capable, adaptable, and supported foundation with SUSE Linux Enterprise Server.

In this guide, you learned to:

- isolate your Python projects in virtual environments.
- manage Python packages.
- simplify replicability and sharing.
- deploy JupyterLab for a self-documenting, interactive development environment.

Take your next steps with JupyterLab and Python with the following resources:

- JupyterLab documentation (https://jupyterlab.readthedocs.io/en/stable/)
- IPython tutorial (https://ipython.readthedocs.io/en/stable/interactive/index.html)
- Introduction to Jupyter and JupyterLab (https://coderefinery.github.io/jupyter/)
- Jupyter wiki (https://github.com/jupyter/jupyter/wiki) - a curated collection of Jupyter/IPython notebooks

- Kaggle (https://www.kaggle.com/) - a data science community with notebooks, datasets, training, and competitions
- Different ways to share a notebook (https://coderefinery.github.io/jupyter/sharing/#different-ways-to-share-a-notebook)

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