Simplifying Scientific Python Package Installation and Usage

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IDEAS-BP Webinar
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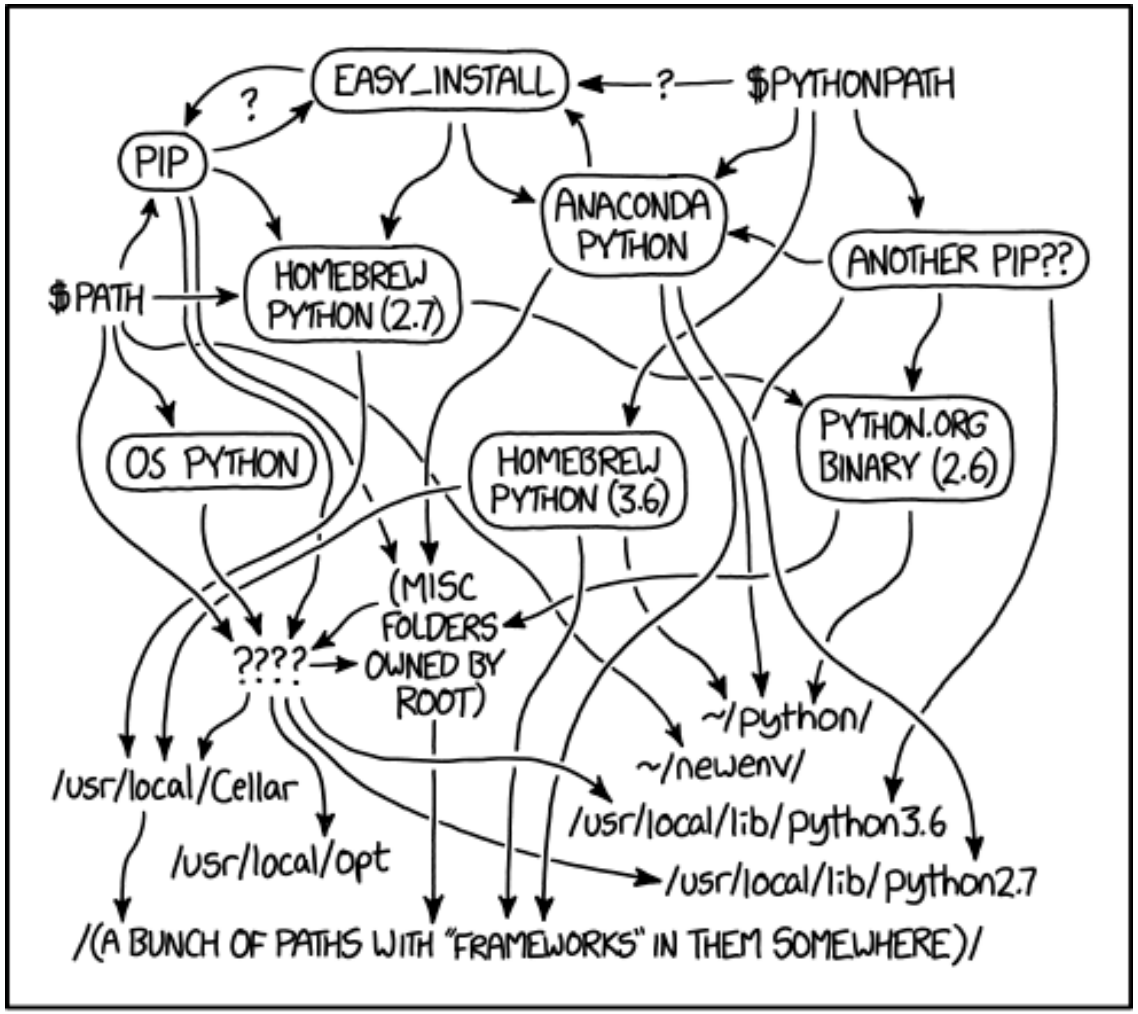
Motivation



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

Source: https://xkcd.com/1987/

- How can I install tensorflow/pytorch?
- Why can't I use tensorflow in Jupyter?
- Why is my Jupyter session not loading?
- Why is "sudo pip install" asking for password?
- Why can't I import the libraries I installed?
- How can I share my environment with a colleague?
- Various conda related issues …

Contributions

Managing and using virtual environments are challenging for novice users

Simplify and streamline installation of Python packages

- **Simplify** management of virtual environments
- **Collect** best practices and configurations from sites
- **Flexible** activation via modules

Empower interactive Python users

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Challenges

1	Non-root installation isolated from base Python
2	Package documentation assuming root access
3	Complex dependencies, often on system libraries
4	Frequent package updates
5	Incompatible or missing dependencies
6	Updating packages later can break existing environment
7	Need to share installations with colleagues
8	Need to use custom packages in Jupyter notebooks
9	Filesystem and IO issues for parallel computing
10	Security policy compliance

Review of HPC Python docs

Public documentations

- National Labs
- University HPC centers
- International HPC centers

Common themes

- Use virtual environments (Conda, venv, virtualenv)
- Install from source
- Do not install in $HOME
- Python with MPI needs care
- Complex workflows need simplification
  - Install mpi4py
  - Create Jupyter Kernel

Dissimilarities

- Varying degrees of details
- Opinions about binary packages/Conda

Common use-cases

How do I install a Python package
How do I use an installed Python package in my code
How do I install and use a Python package in Jupyter notebooks
How do I list the Python environments that I have created
How do I delete a Python environment that I have created
How do I list the packages that I have installed
How do I update a package that I have installed
How do I share my environment with a colleague
How do I recreate an existing environment

Tasks for managing Python packages

Colored arrows indicate steps for a specific workflow

Need for simplification and automation

Many best-practices can be achieved with configuration files	• pip.conf • condarc
Some workflows require automation	• Create Jupyter Kernel • Install mpi4py, h5py etc.
Set sensible default values	• Default location of environments • Default package cache • Default threading • Do not use user site-packages
Create a central resource for best practices/scripts/configurations	• https://hpc-python-solutions.readthedocs.io/en/latest/motivation/main.html

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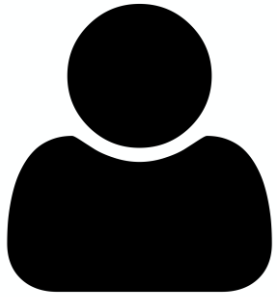
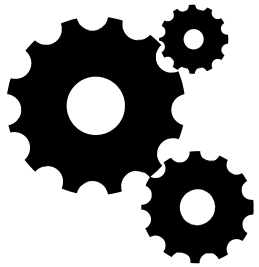
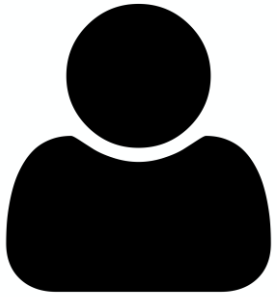
`conda-env-mod`: Install Python packages



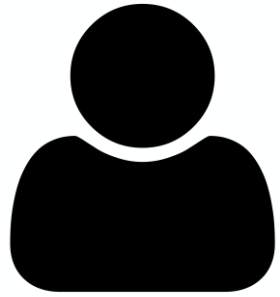
create myenv



- conda create
- create module
- create kernel



module load



- pip install
- conda install

Demo

Supported operations

create	Name Prefix YAML specifiction
export	YAML specification
module	Lmod Tcl
kernel	
list	
delete	

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Benefits of environment modules

Environment modules are powerful tools

Programmatic way to set up runtime environment
Users can start with a clean environment and load modules on demand
Modules take care of setting appropriate variables (PATH, PYTHONPATH, etc.)

HPC center staff can incorporate best-practices into modules

Track dependencies on system modules

Detailed help messages

Other benefits

Avoid conda init and conda activate
No more polluting your bashrc

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Other benefits

Sharing Python installations within a cluster

One person manages the environment
Others load a module/kernel to use it

Sites can customize module file/kernel templates

Allows stacked environments

Environment with stable packages (module X)
Environment with experimental packages (module Y)
Load modules X and Y
Caveat: Need compatible Python version

Python package developers can easily share environments

environment.yaml
modules files
Jupyter kernel

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Success stories

- Deep Learning package installation
  - 11 applications (multiple versions)
  - 3 Python versions
  - CPU and GPU version
- Shared Python environment for teaching
  - Instructor uses conda-env-mod to install packages
  - Students load modules and Jupyter Kernels
  - 12+ course, 1500+ students (between 2019-20)
  - Data Science, Atmospheric Science, Molecular Chemistry, Library Science
- Shared Python environment for research groups
  - New feature requests

Conclusion

Broad impacts

- Capture best practices for scientific Python application installation
- Engage the scientific Python community for better packaging
- Improve scientific productivity, reduce user errors
- Help interactive Python use
  - JupyterHub
  - Gateway/Open OnDemand

Download

- https://github.com/amaji/conda-env-mod

Best practices document

- https://hpc-python-solutions.readthedocs.io/

Contributions are welcome!

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- Mailing List: https://bssw.io/pages/receive-our-email-digest
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Questions

Thank You

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