Table of Contents

| Python FAQ | 1 |
|---|----|
| Workshop: using Python at IAC | 2 |
| General | 3 |
| Warning: do not automatically activate an environment in .bashrc | |
| Also check the docs on JupyterHub! | |
| Should I use Python? | |
| Tutorials | |
| Which version should I use? python 2 or python 3? | |
| What's the recommended way to use python at IAC? | |
| What about other solutions? | |
| What are Best Practices when using python? | 4 |
| Why is it important to work with a fixed environment? | |
| Using Conda (on Linux) | 5 |
| What is conda? | 5 |
| What is mamba? | 5 |
| What is a conda environment? | 5 |
| What is a conda package? | 5 |
| How do I use conda? | |
| What environments are available? | 6 |
| I am missing a package - what can I do? | 7 |
| How can I install a single package? | 7 |
| How can I create my own environment? | 7 |
| Create a new environment | |
| Clone and tweak an existing environment | |
| Background information about the differences between pip, conda and anaconda | 8 |
| How can I create an executable python script when using a conda environment? | |
| Run spyder remotely | |
| Spyder 3 shows strange symbols | |
| user packages no longer available in conda environment and JupyerHub Why was this change introduced? | |
| I'am missing my self-installed packages, what can I do? | |
| What has changed? | |
| Packages | 10 |
| xarray | 10 |
| matplotlib | |
| DEPRECATED - NO LONGER RELEVANT | |
| How to run jupyter notebook on a server? | 11 |
| Access notebook from your personal computer | 11 |

Python FAQ

Workshop: using Python at IAC

Slides of the Using Python at IAC workshop (11.12.2019)

General

Warning: do not automatically activate an environment in .bashrc

- Automatically activating an environment in (e.g. source activate iacpy3_2019) in your .bashrc can break your login
- If you cannot login and suspect it is because of this issue
 - ♦ open alternative (non-graphical) shell with CTRL + ALT + F1
 - ♦ edit your .bashrc and remove the line with source activate environment

Also check the docs on JupyterHub!

JupyterHub

Should I use Python?

• Absolutely.

Tutorials

- Python Scientific Lecture Notes: http://scipy-lectures.github.io
- Scientific Python Lectures: https://github.com/jrjohansson/scientific-python-lectures
- Book for Beginners "Dive Into Python": http://www.diveintopython.net

Which version should I use? python 2 or python 3?

- You should use python 3 for every new project.
- Note: Python 2 has reached its end-of-life in 2019. It no longer receives bugfixes. Most projects (numpy, matplotlib, ...) stoped supporting python 2!

What's the recommended way to use python at IAC?

• We recommend to use conda to manage packages and environments. See below.

What about other solutions?

• Python installed on the machines?

It is discouraged to use the python installation on the machines. Package versions can change unexpectedly which may lead to code incompatibilities. This solution is not viable for long-term reproducibility.

• Virtual environments?

Conda is superior to virtual environments because it also handles non-python dependencies (such as the netCDF library) and can therefore offer a more stable environment.

What are Best Practices when using python?

• For each project you should decide on a conda environment and note which one you use. You could for example create a startup file that you call every time you work on the project:

```
#!/bin/bash
module load conda/2022
source activate iacpy3_2022
```

- This file has to be made executable (chmod +x startup) and needs to be invoked as source startup.
- See this gist for a more complete example

Why is it important to work with a fixed environment?

• Python packages undergo a rapid development and may become incompatible with your script. If you want to re-run your analysis in at a later stage you want to have the same versions for the packages you used. Therefore it is important that you know which environment you used.

Using Conda (on Linux)

What is conda?

• conda is a program that manages (python) packages and environments. It allows to use a centralized installation while still providing user flexibility in term of package installation.

What is mamba?

• mamba is a faster drop-in replacement for conda - it allows for much faster dependency solving. You can replace almost every conda command by mamba command

What is a conda environment?

• From the conda documentation: A conda environment is a directory that contains a specific collection of conda packages that you have installed. For example, you may have one environment with NumPy 1.7 and its dependencies, and another environment with NumPy 1.6 for legacy testing. If you change one environment, your other environments are not affected. You can easily activate or deactivate environments, which is how you switch between them. You can also share your environment with someone by giving them a copy of your environment.yaml file.

What is a conda package?

- A conda package is a compressed tarball file that contains system-level libraries, Python or other modules, executable programs and other components. Conda keeps track of the dependencies between packages and platforms. Thus, it can not only handle python packages but also other dependencies (e.g. the netCDF c library).
- See also conda documentation

How do I use conda?

• Load the module

module load conda

• View all environments

conda env list

• Work in an environment

source activate iacpy3_2024

• Warning: do not do this in your .bashrc, instead define an alias (see below)

• List installed python packages

```
conda list
• jupyter -> use JupyterHub)
• Start spyder
```

spyder • Use ipython ipython

• For a simpler and quicker usage, you can create an alias in your ~/.bashrc:

```
alias iacpy24='module load conda; source activate iacpy3_2024'
```

What environments are available?

- You can also make all environments available with module load conda
- 2024 environments

```
module load conda/2024
conda env list
```

- iacpy3_2024: based on iacpy3_2023, uses python 3.11; updated all packages on 16.04.2024; Note that a number of packages have been removed from the environment contact iac-linux@env.ethz.ch if you are missing something.
- 2023 environments

```
module load conda/2023
conda env list
```

♦ iacpy3_2023: based on iacpy3_2022, uses python 3.11; updated all packages on 08.08.2023; Note that a number of packages have been removed from the environment - contact iac-linux@env.ethz.ch if you are missing something.

Older environments

• 2022 environments

```
module load conda/2022
conda env list
```

- iacpy3_2022: based on iacpy3_2021, uses python 3.9; updated all packages on 16.03.2022;
- 2021 environments

```
module load conda/2021
conda env list
```

- iacpy3_2021: based on iacpy3_2020, uses python 3.9; updated all packages on 22.04.2021;
- 2020 environments

```
module load conda/2020
conda env list
```

- iacpy3_2020: based on iacpy3_2019, uses python 3.7; updated all packages on 15.04.2020;
- 2019 environments

```
module load conda/2019
conda env list
```

- iacpy3_2019: based on iacpy3_2018, uses python 3.7; updated all packages on 08.04.2019;
- iacpy_cmip6_ng environment used to create the cmip6 new generation archive, please use iacpy3_2019
- 2018 environments

```
module load conda/2018
conda env list
```

- ♦ iacpy3_2018: based on dypy, uses python 3.6; updated all packages on 03.04.2018;
- ♦ iacpy2_2018: based on dypy, but uses python 2.7; updated all packages on 03.04.2018
- 2017 environments

```
module load conda/2017
conda env list
```

- ◆ dypy: python3.5 environment with dypy (for LAGRANTO) and suitable for most users
- **cis_env**: python3.5 environment with cis tools in version 1.5.4
- **pyferret_env**: python3.5 environment with pyferret in version 7.0
- pyn_env: python2.7 environment with PyNgl and PyNio in version 1.5
- module load miniconda3 is equivalent to module load conda

I am missing a package - what can I do?

• Write to iac-linux@env.ethz.ch - we can generally add single packages to the existing environments. If you are impatient, see below.

How can I install a single package?

• You will need to create your own environment (see below), and then add the package with

mamba install <package>

How can I create my own environment?

• conda allows to manage environments without being root!

Create a new environment

• You can create your own environment. E.g.:

mamba create -n myenv scipy

• NB: don't forget to include ipython in your new environment

Clone and tweak an existing environment

• If you want to have more control on your environment but still exiting one as a base, you can do the following:

```
mamba create -n analysis_2019 --clone iacpy3_2019
```

• You can now add packages to the new environment:

```
source activate analysis_2019
mamba install <package>
# - OR -
pip install <package> # installation with mamba is preferred!
```

Background information about the differences between pip, conda and anaconda

• Blogpost by Jake Vanderplas

How can I create an executable python script when using a conda environment?

• To run a python script directly from the command line (./script.py) you need to add the following at the top of your script

#!/usr/bin/env python

- However, the environment needs to be loaded, before it is executed.
- Of course the file needs to be executable (chmod +x scripy.py)

Run spyder remotely

- Please don't run spyder on fog or fog2. These are login nodes that don't have many ressources.
- ssh to any of the servers to run your analyis, e.g.:

```
ssh -X <username>@fog.ethz.ch
ssh -X litho
module load conda
source activate iacpy3_2023
spyder
```

• If you don't want to log in twice (-> fog -> server), see tipps above (Run a notebook on a server)

Spyder 3 shows strange symbols

- Something goes wrong with the font in spyder3. The workaround is to use the symbols of spyder2.
- In spyder3 go to Tools > General (Appearance) > Icon Theme: Change to Spyder 2 and restart spyder.

user packages no longer available in conda environment and JupyerHub

• Packages installed with pip install <package> --user (site packages) are no longer available in personal conda environments.

• This should not effect most users.

Why was this change introduced?

- Conda environments should be self-contained and reproducible. Site packages 'pollute' the clean workspace (i.e. there could be packages in an environment that were never installed into it).
- You don't need --user to install packages with conda+pip.
 - Most often you will be able to install packages directly with conda (conda install
 <package>)
 - When using conda+pip it is not necessary to install packages with --user; you can do this with pip install <package>

I'am missing my self-installed packages, what can I do?

• Recommended: You should re-install the packages into your environment:

```
module load conda
source activate <environment>
pip install <package>
```

- NB: Make sure that pip is included in the environment before installing extra packages into it.
- If you installed site packages into an existing environment (one managed by IAC-IT), you will have to clone this environment, see instructions above.
- Not recommended: You can get the old behaviour back by adding the following line to your ~/.bashrc (for bash):

```
module load conda # as before
unset PYTHONNOUSERSITE
```

What has changed?

• module load conda now does the following: export PYTHONNOUSERSITE=1. This avoids putting the site-packages in the pythonpath, as explained in the documentation.

Packages

xarray

How do I prevent xarray from automatically adding _FillValue to coordinates or variables without NaN?

• Specify encoding when saving to disk (xarray version 10.2)

```
# Saving back to disk with encoding dictionary telling not to use _FillValues for sp
encoding = {'lat' : {'_FillValue' : None}, 'lon' : {'_FillValue' : None}, 'time' : '
xarray.Dataset.to_netcdf('./outfile.nc',format='NetCDF4',encoding=encoding)
```

Why did xarray change the type of an nc attribute to string, causing other software to crash on the resulting nc file?

• Probably there was a special character (e.g. 'ü') in the attribute. Two suggested workarounds. (xarray version 10.2)

```
# Workaround A) use 'NetCDF4_CLASSIC'
xarray.Dataset.to_netcdf('./outfile.nc',format='NetCDF4_CLASSIC')
# Workaround B) change the attribute name
xarray.Dataset.attrs['institution'] = 'IAC ETH Zuerich' # instead of 'IAC ETH Zürich
xarray.Dataset.to_netcdf('./outfile.nc',format='NetCDF4')
```

matplotlib

I don't see a figure when typing plt.show()?

• Per default the plot backend is set to "agg". The "agg" backend is for writing to file and does not show a plot. Type the following to see your backend:

```
import matplotlib as plt
plt.get_backend()
```

There are two ways to achieve this:

• Set the backend in your code:

```
import matplotlib
matplotlib.rcParams['backend'] = "Qt4Agg"
Or define your backend incide your - / config/matplotlib/matplotlibre fi
```

• Or define your backend inside your ~/.config/matplotlib/matplotlibrc file

backend : Qt4Agg

Important If you have a ~/.matplotlib folder, first move it to the new location ~/.config:

mv ~/.matplotlib ~/.config/matplotlib

More information can be found here: http://matplotlib.sourceforge.net/users/customizing.html

DEPRECATED - NO LONGER RELEVANT

How to run jupyter notebook on a server?

• Use JupyterHub instead

- See below how to run a notebook on a server from your personal computer.
- Here we to setup a jupyter notebook running on a server and use it from your computer.
- It will make use of tmux on the server to keep a session running even if you are not logged in anymore.
- For security purpose the jupyter notebook produces a token at start, you need to copy this token (password) to the login screen of the notebook.
- On the server

```
tmux new-session -s 'background jobs'
cd ~
module load conda
source activate <environment>
jupyter notebook --no-browser --port 55000
```

- If the port is already in use jupyter will select the next higher available. Make sure that you use the right port in the next part.
- On your computer:

```
ssh -f -N -L localhost:8888:localhost:55000 SERVER
```

- Open the browser and go to: http://127.0.0.1:8888
- Copy the token given by the jupyter notebook on the server and paste it in the login field.
- This also works to tunnel a notebook from a linux machine to a windows machine
 - ♦ e.g. via (WSL [windows subsystem for linux]), or Start -> cmd
- You can recover the full address including the token on the SERVER by pressing CTRL C once.

Access notebook from your personal computer

- Use JupyterHub instead
- Please don't run jupyter/ python on fog or fog2. These are login nodes that don't have many ressources.

You cannot directly ssh to our servers. Therefore, the above solution does not work from you personal computer. There are two possibilities.

1) Configure fog as a 'jumphost'

• Edit (or create) ~/.ssh/config file as follows (on your personal computer)

Host fog User <username> # your ETH username Hostname fog.ethz.ch Host atmos # change this according to the SERVER you want to use User <username> # your ETH username Hostname atmos.ethz.ch # change this as well • now the following command should work

ssh -f -N -L localhost:8888:localhost:55000 atmos

- if you try to access the server from Windows using putty, make sure that you add the forwarded port to the profile for your session (on the left under "Category" go to "Connection" -> "SSH" -> "Tunnels" and type "8888" into source port, "localhost:55000" into destination, then click "Add")
- do NOT write atmos.ethz.ch, only atmos

2) USE VPN

- Connect to the VPN (see VpnAccess)
- See HomeOfficeLinux for the list of servers you can access

Edit | Attach | Print version | History: %REVISIONS% | Backlinks | Raw View | More topic actions Topic revision: r60 - 15 Jan 2025 - 14:59:13 - MathiasHauser

• . IT

- Log In
- IT Web
- Create New Topic
- Index
- Search
- Changes
- Notifications
- RSS Feed
- Statistics
- Preferences
- Webs
- Public
- System

•

٠

EVEN FOOMICE Copyright © by the contributing authors. All material on this collaboration platform is the property of the contributing authors.

Ideas, requests, problems regarding Wiki? Send feedback