Next Steps in Python:
Virtual Environments

Aaron Geller

(with help from Scotty Coughlin)

Research Computing and Data Services

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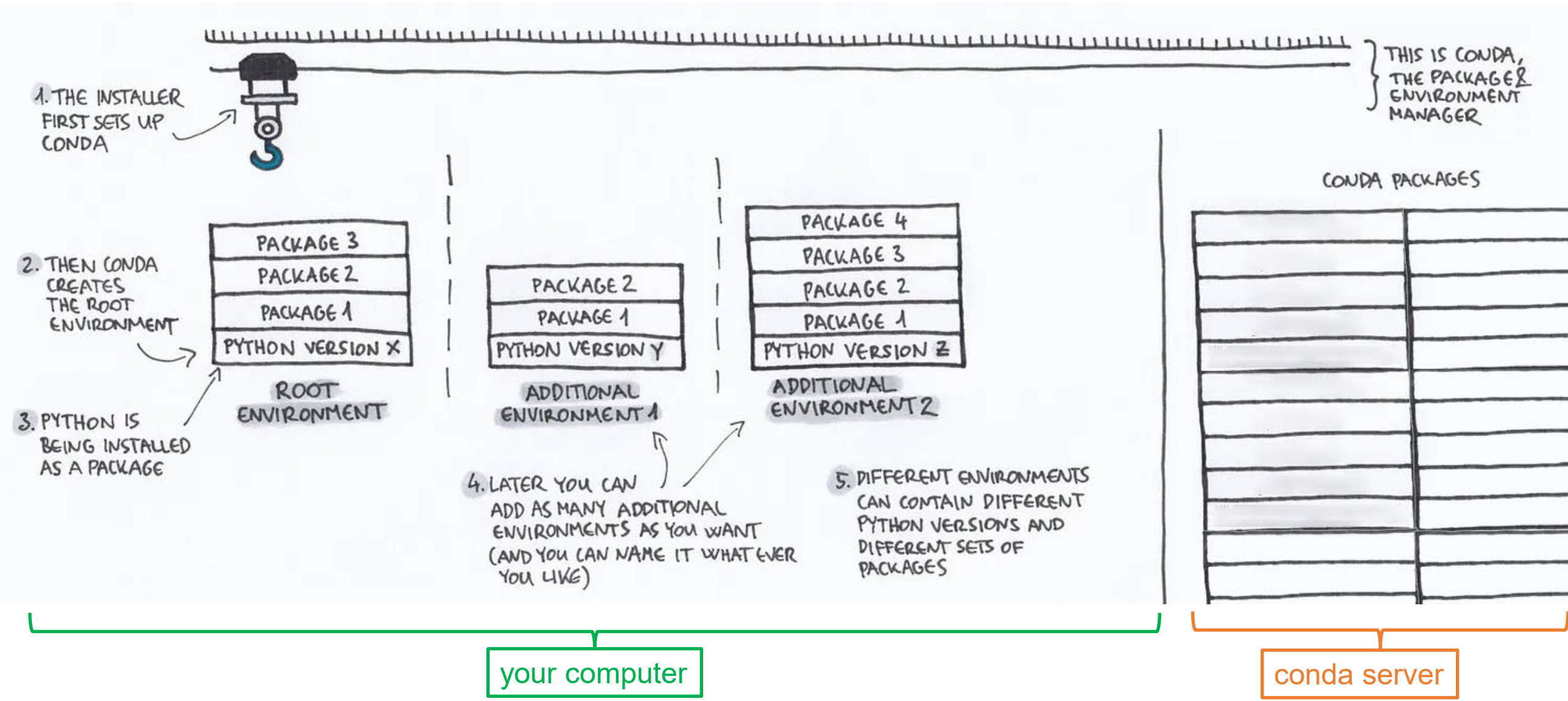
What is a virtual environment?

And why should you use them?

Have you ever…

- Had an issue where installing one Python package caused another previously working Python package to stop working?
- Needed to install a Python package on a system in which you do not have administrative privileges?
- Had trouble sharing or reproducing the environment in which you ran code successfully with other researchers?
- Had issues installing a Python package?

Virtual environments (e.g. conda) can help!



Credit: https://angus.readthedocs.io/ with my own edits

Virtual environments can solve this …

Had an issue where installing one Python package caused another previously working Python package to stop working.

by …

resolving dependencies for all packages and notifying you of any conflicts between packages (before causing errors in existing installations).

Virtual environments can solve this …

Needed to install a Python package on a system in which you do not have administrative privileges.

by …

allowing you to install packages without using `sudo` or having administrative privileges.

Virtual environments can solve this …

Had trouble sharing or reproducing the environment in which you ran code successfully with other researchers.

by …

allowing you to export your environment as a YAML file which you can send to someone else so they can reproduce your environment.

Virtual environments can solve this …

Had issues installing a Python package.

by …

pre-compiling and validating that all the dependencies of the application in question work for your Operating System (for packages available through conda/mamba).

Do not mess with your system Python!

- Avoid `sudo pip install XXX`
- If you break the system Python it will be hard to recover.
- Instead, a virtual environment provides you with an isolated location/directory on your computer, where nothing bad will happen if you mess it up. (As a last resort, you can always delete that directory, reinstall Python+conda, and start fresh.)

Creating virtual environments via conda/mamba

Two different ways

(Ana)conda

- There are a few ways to create Python virtual environments. We will focus on using `conda`/`mamba`.
- Regardless of the install method, the main components include
  - The executable `conda` or `mamba` (on your computer)
  - Folder/directory containing all your environments and packages (on your computer)
  - “Channels” with pre-tested packages (on a separate server)

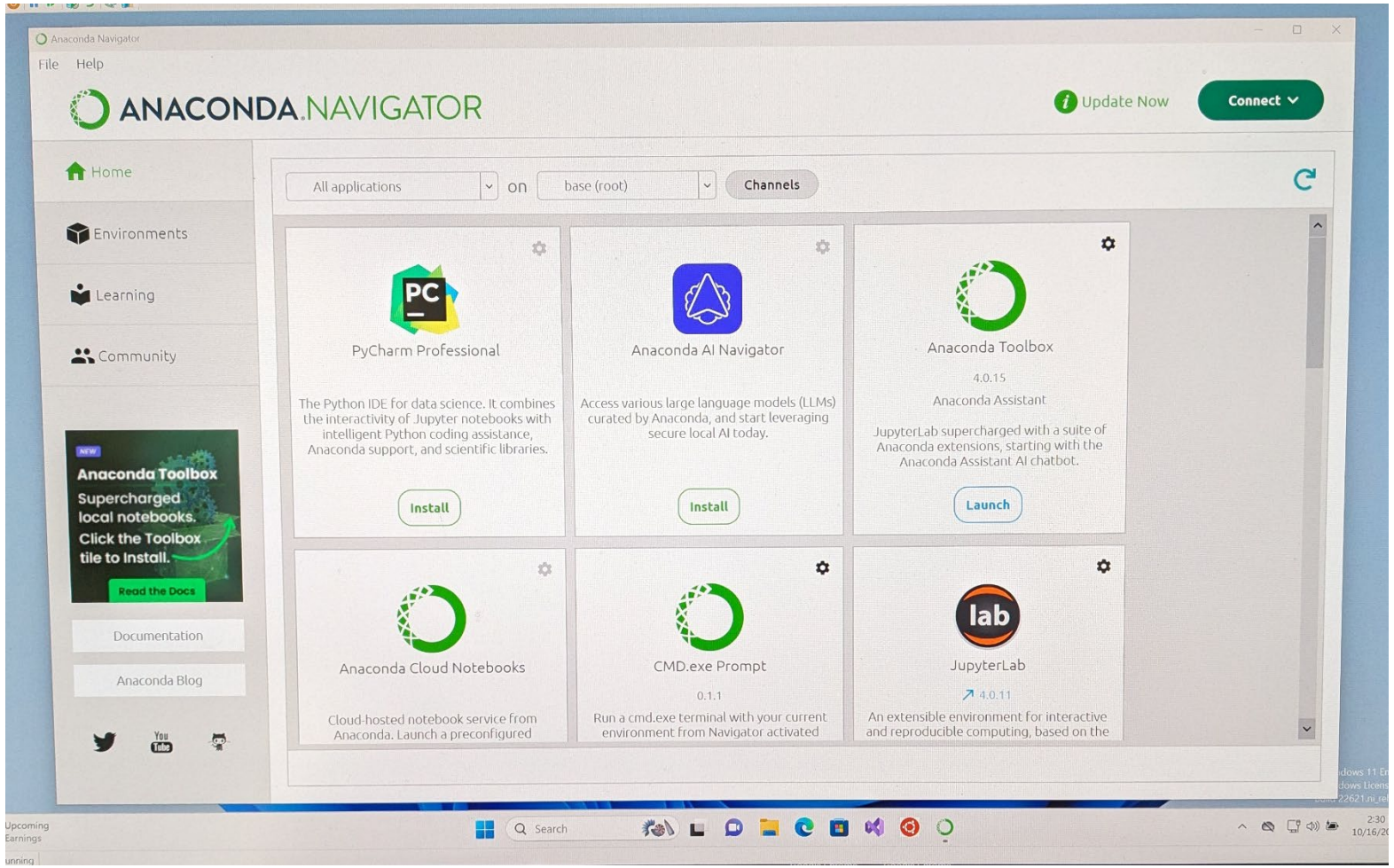
Anaconda Distribution using the Navigator

Pro:

- Easy installation
- No command-line needed
- Point and click

Con:

- Slower to load, lots of bloat
- Confusing changes to TOS recently
- Cannot be used for commercial purposes at Northwestern



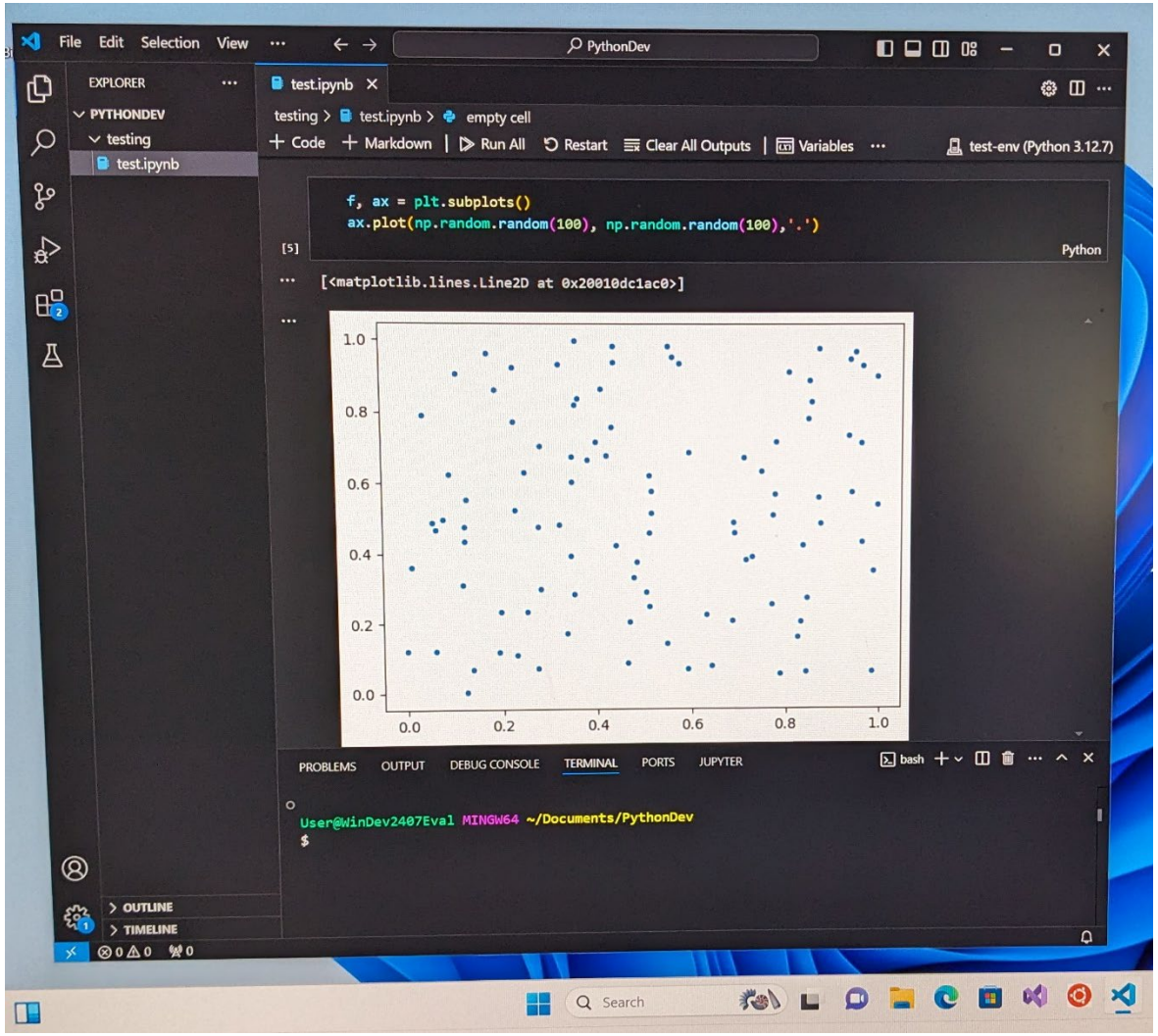
Open source version using VS Code and miniforge

Pro:

- VS Code is a very powerful general-purpose IDE
- No restrictions on use
- Great integration with GitHub

Con:

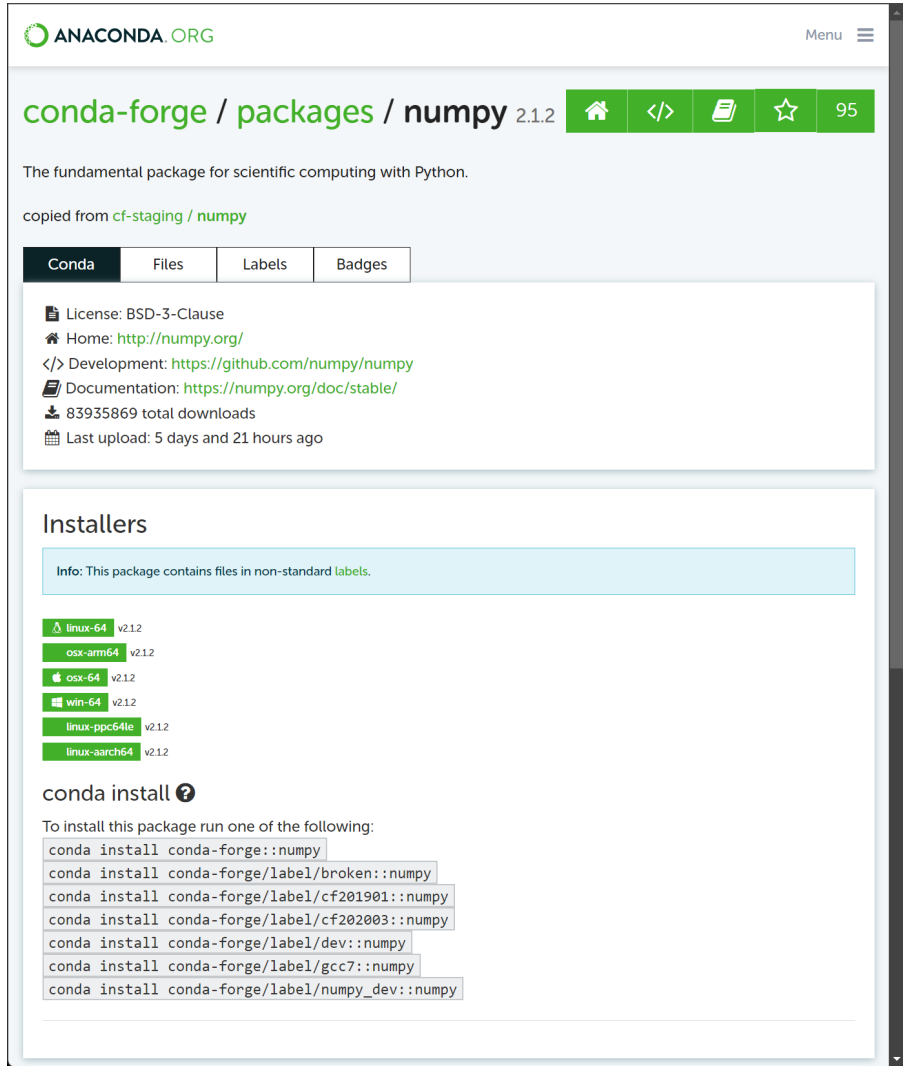
- Need to use some command-line (to create envs)
- More installation steps (I installed VS Code, Git Bash and miniforge)
- Steeper learning curve than Anaconda Navigator



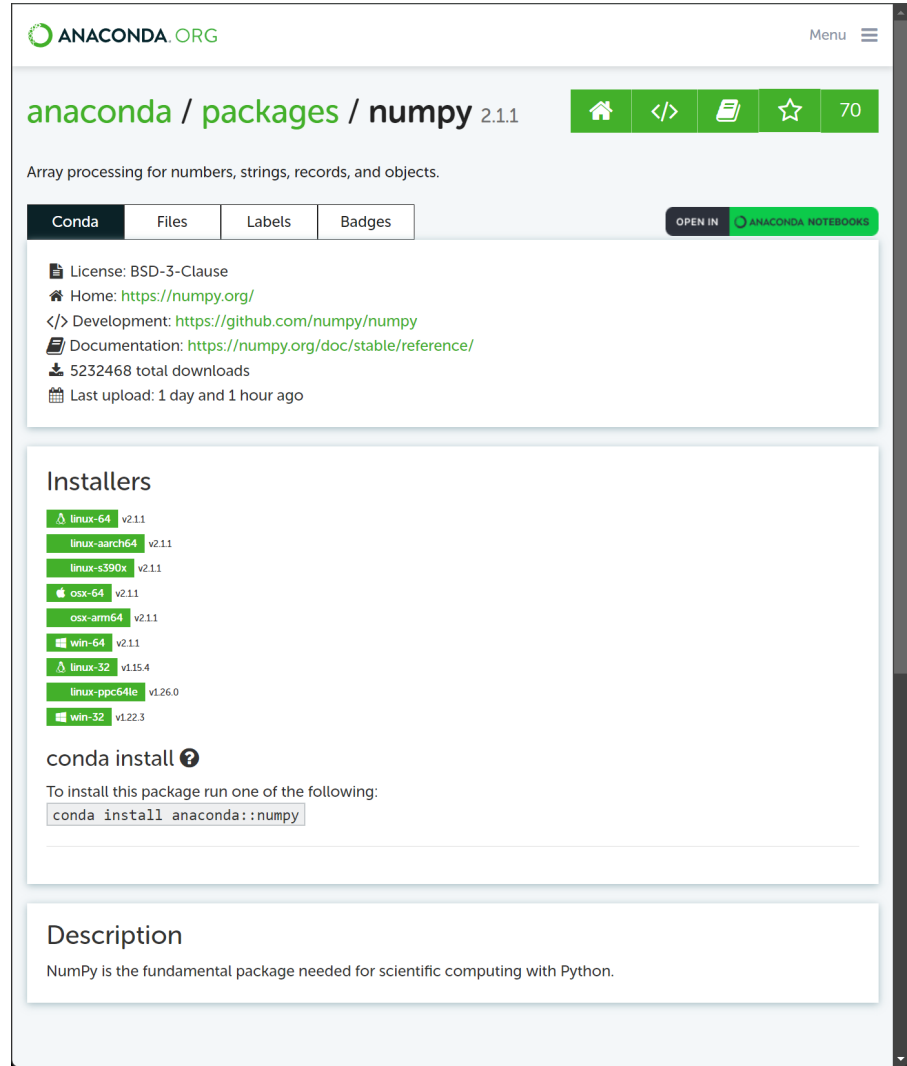
Channels

- servers containing pre-tested packages that work well together
- Many options

conda-forge : community driven



default/anaconda : “proprietary”



Common commands (if using command line)

`$ mamba create`	Create a new environment (requires other arguments, e.g. name)
`$ mamba install`	Install a package within an environment (add package name)
`$ mamba activate`	Activate/enter an environment (add environment name)
`$ mamba search`	Search for a particular package (add package name)
`$ mamba list`	List all packages installed in the active environment

(You can replace `mamba` with `conda` and get the same result; `mamba` is usually faster.)

Link to the conda cheat sheet

Exercises

Your turn!

Create two environments and test some code

1. Create two environments:

```
conda create --name numpy1-test python=3.12 numpy=1.26.4 jupyter

conda create --name numpy2-test python=3.12 numpy=2.1.2 jupyter
```

2. Go to the workshop's GitHub repo, download the two test notebooks, and run them both in both environments. (One should only work in `numpy1-test`, and the other should only work in `numpy2-test`)
3. Experiment with creating your own virtual environment(s) and then running your own code.

Questions?

Thank you!