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○

# I declare an environment!

Reproducibility with and  
*without* Docker

Dr. Sarah Kaiser (she/they)

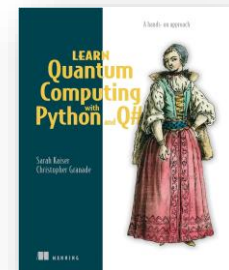
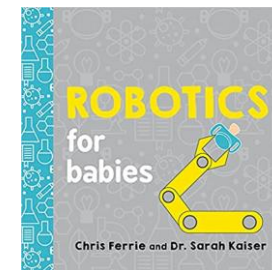
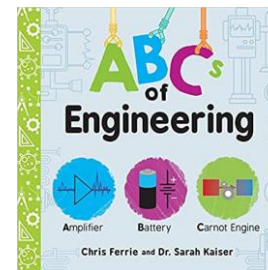
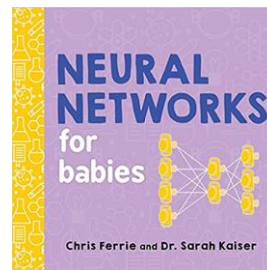
Sr. Developer Advocate @ Microsoft





# Hiya! 🖐️

- 📡 Experimental Physicist by training
- 🐕 Chewie kibble delivery
- 📖 Author of books for all ages
- 🗡️ Plays anything Final Fantasy
- 🚢 Usually floating near Seattle

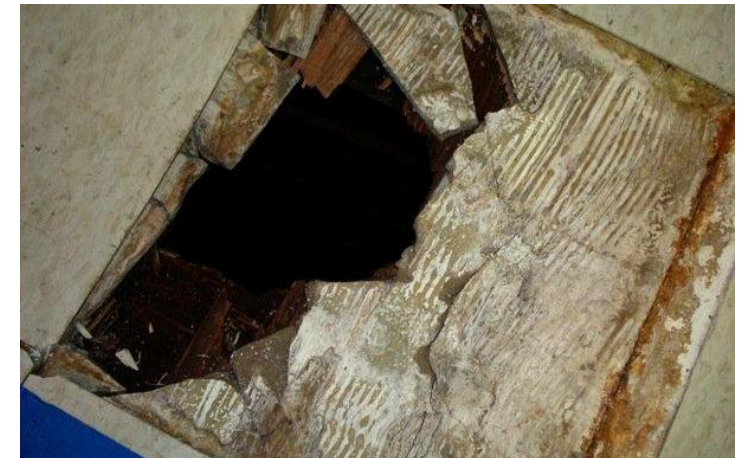
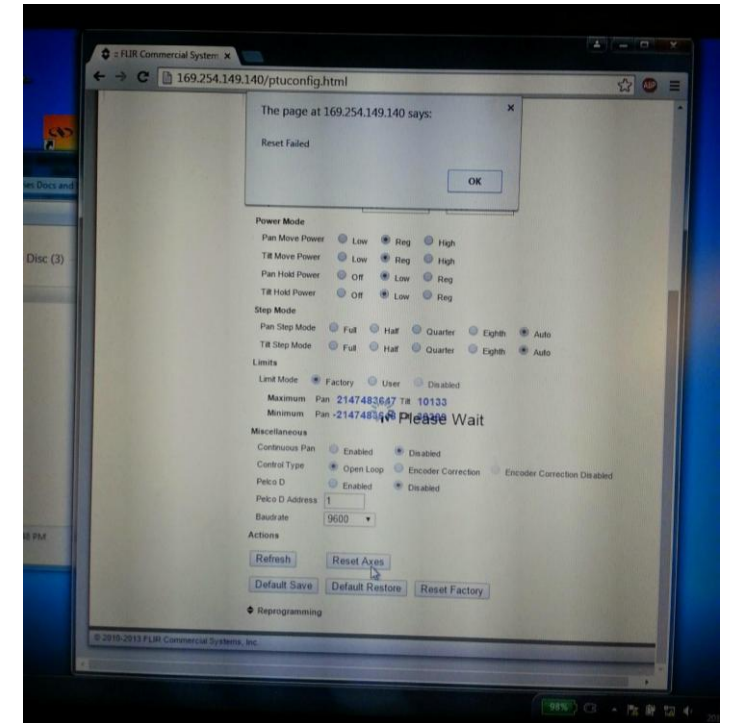




# Computers do the darndest things

---

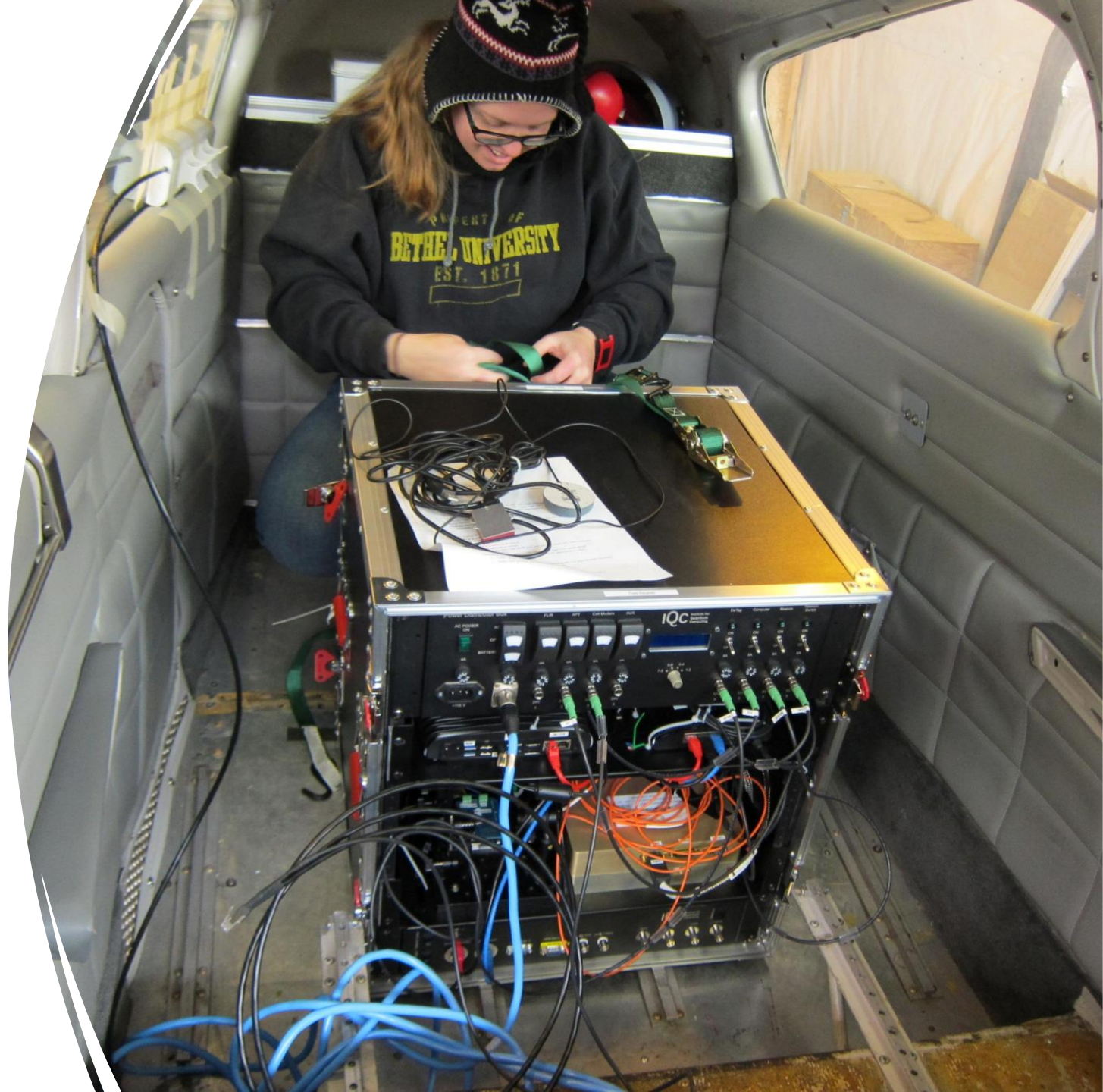
- Install updates
- Get lost
- Get arrested
- Fall out of orbit
- Get sat on
- Catch on fire



What is the best way  
to make sure my \_\_\_\_  
works tomorrow?

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Project, lab, house, car, etc.





# tl;dr

1. Good reproducible environments need **declarative** and **imperative** specs.
2. A combination of Docker and Nix can make reproducible Python projects easier!

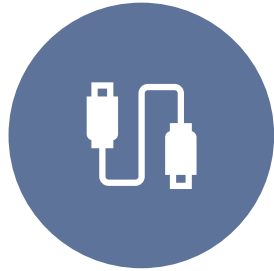


# Reproducible...

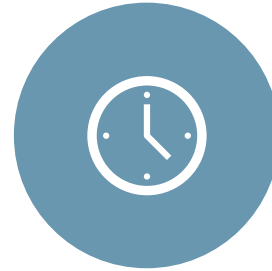
---



for who?



on what  
device?



when?



with what  
resources?

# ...Environments!

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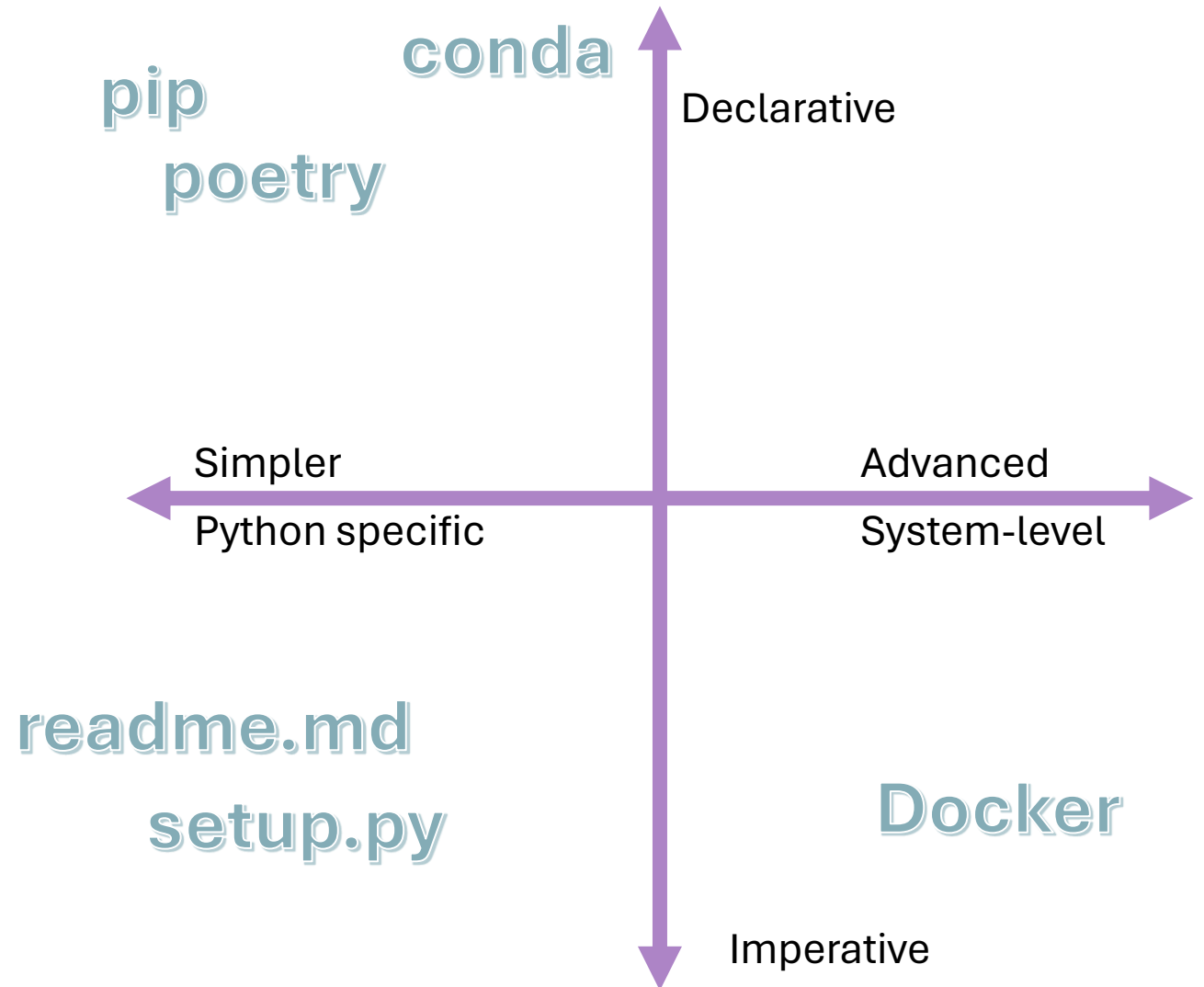


**Declarative:** Describe the desired final state as completely as possible



**Imperative:** Provide a list of steps or actions

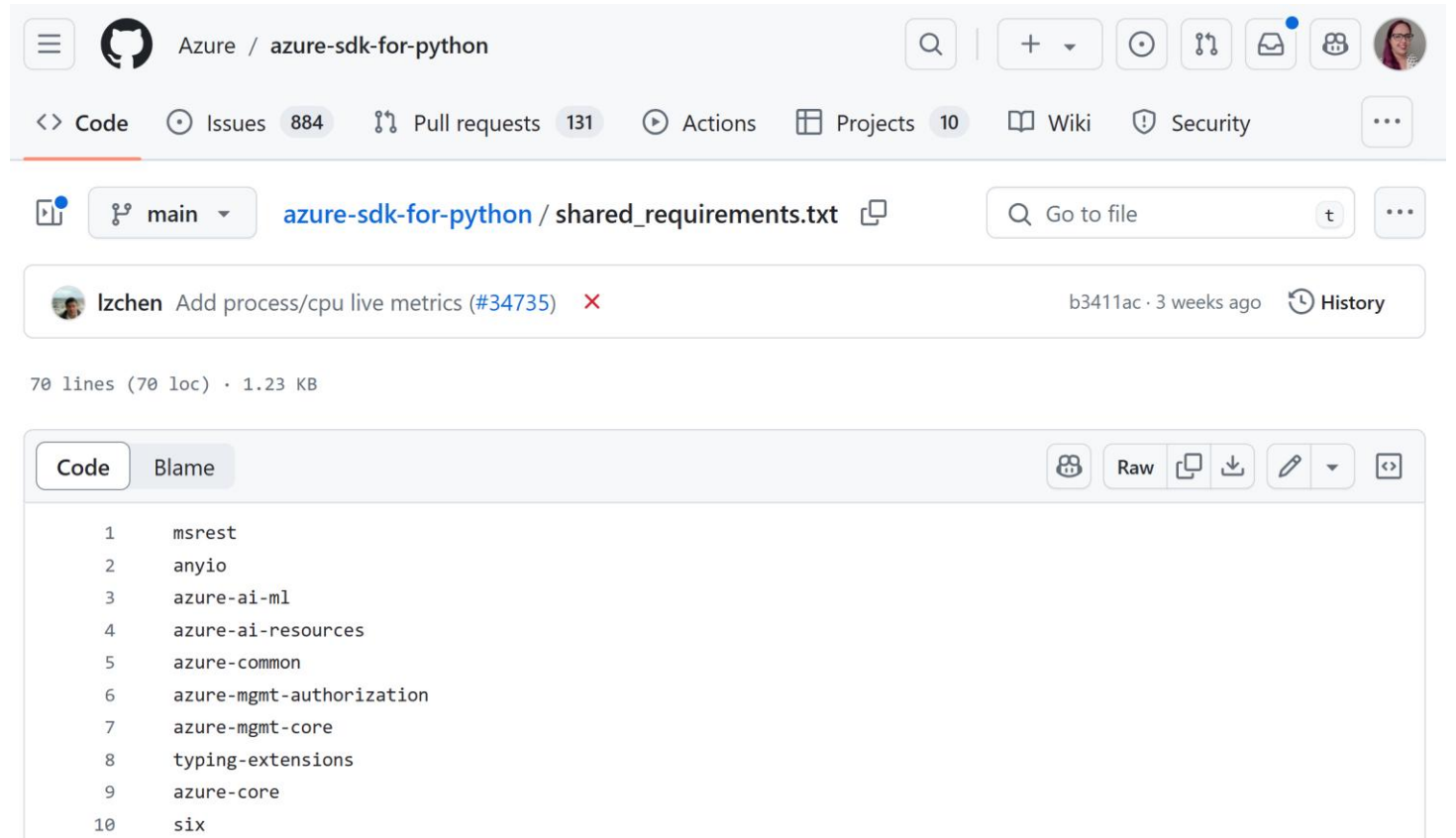
# What kinds of tools do people use?





# Simple declarative: requirements.txt

- `pyproject.toml`,  
  `environment.yml`
- May not capture all non-Python requirements
- Can be hard to manage without additional tools



The screenshot shows the GitHub interface for the repository 'Azure / azure-sdk-for-python'. The file 'shared\_requirements.txt' is selected, showing its content. The file is 70 lines long, 70 loc, and 1.23 KB. The content of the file is as follows:

```
1 msrest
2 anyio
3 azure-ai-ml
4 azure-ai-resources
5 azure-common
6 azure-mgmt-authorization
7 azure-mgmt-core
8 typing-extensions
9 azure-core
10 six
```

# Simple imperative: readme.md

- Easy to write
- Hard to maintain
- Need to test, automation testing can help



vscode-jupyter

Public



README



Code of conduct



MIT license



Security



## Working with Python

### Quick Start

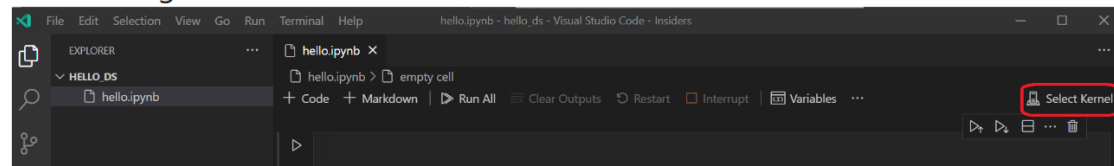
- Step 1. Install [VS Code](#)
- Step 2. Install [Anaconda/Miniconda](#) or another Python environment in which you've installed the Jupyter package
- Since not working with Python, make sure to have a [Jupyter Kernel](#) that corresponds to the language you would like to use installed on your machine.
- Step 3. Install the [Jupyter Extension](#) and the [Python Extension](#)
- Step 4. Open or create a notebook file by opening the Command Palette ( `Ctrl+Shift+P` ) and select `Jupyter: Create New Jupyter Notebook`.

>create notebook

Create: New Jupyter Notebook



- Step 5. Select your kernel by clicking on the kernel picker in the top right of the notebook or by invoking the `Notebook: Select Notebook Kernel` command and start coding!



# Advanced Imperative: Dockerfile

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```
1 FROM mcr.microsoft.com/devcontainers/miniconda:0.202.19-3
2
3 RUN conda install -n base -c conda-forge mamba
4 COPY environment.yml* .devcontainer/noop.txt /tmp/conda-tmp/
5 RUN if [ -f "/tmp/conda-tmp/environment.yml"
    ]; then umask 0002 && /opt/conda/bin/mamba env create -f /tmp/
    conda-tmp/environment.yml; fi && rm -rf /tmp/conda-tmp
6
```

# Why Docker?

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- Pros:
  - Supported most places
  - Easy to hack fixes in
  - Works with Dev Containers! 💖
- Cons:
  - Installing and learning Docker is not trivial
  - Easy to hack fixes in
  - Devices may not support





Something is missing...

A thick, wavy purple line is positioned horizontally below the text, spanning approximately the first half of the text's width.



nix.dev

# Advanced Declarative: Nix

A language for declarative environments

# Nix ecosystem

## Nixpkgs

- The largest, most up-to-date software distribution in the world, and written in the Nix language.

## NixOS

- Entire operating system that bootstraps from the nix package manager and nix-shell

## nix-shell

- Declarative shell environments

# Advanced Declarative: `nix-shell`

```
[nix-shell:~]$ nix-shell -p python3
```

```
this path will be fetched (11.42 MiB download, 62.64 MiB unpacked):
```

```
  /nix/store/pwy30a7siqrkki9r7xd1lksyv9fg4l1r-python3-3.10.11
```

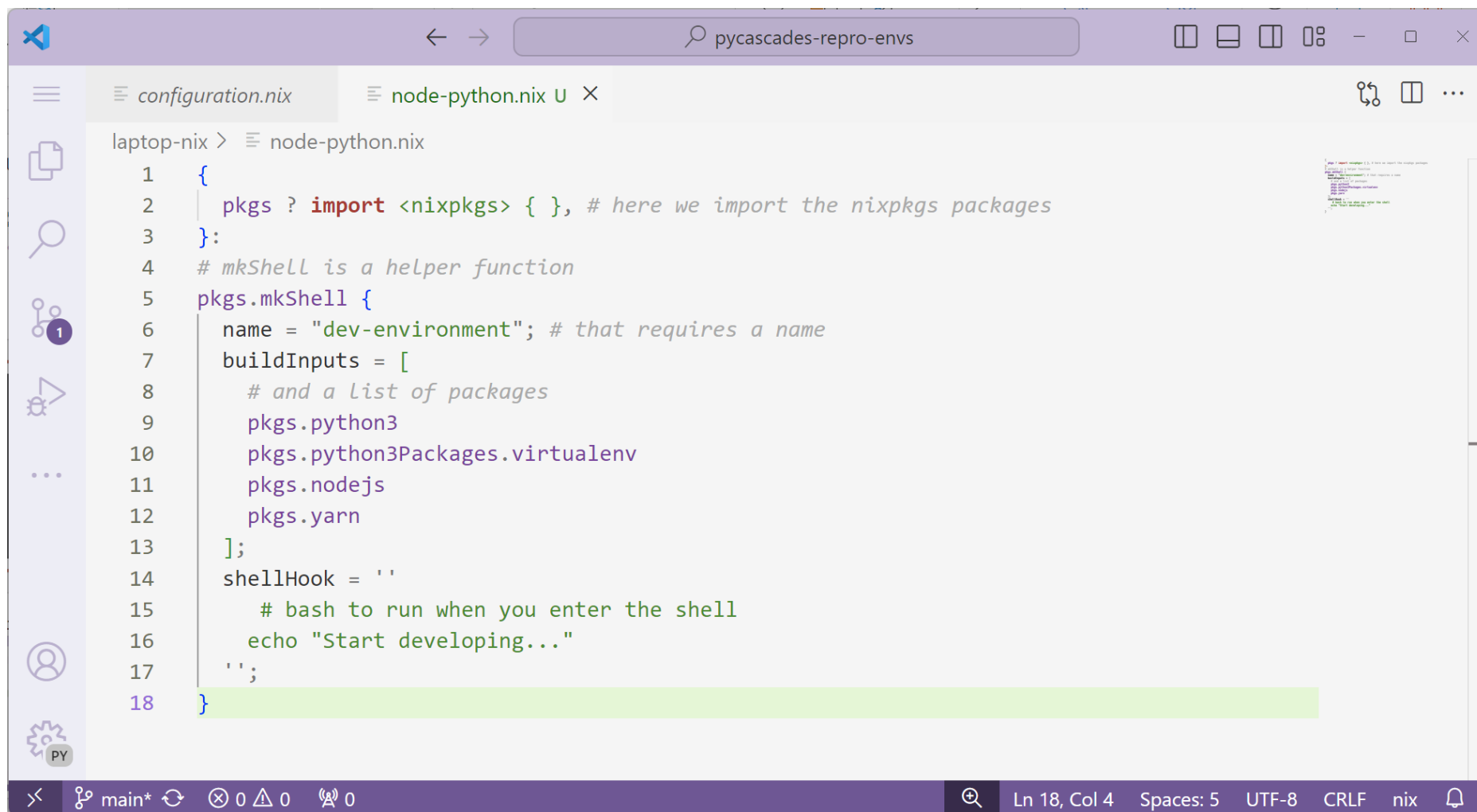
```
copying path '/nix/store/pwy30a7siqrkki9r7xd1lksyv9fg4l1r-python3-3.10.11'  
from 'https://cache.nixos.org' ...
```

```
[nix-shell:~]$ python --version
```

```
Python 3.10.11
```



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```
laptop-nix > node-python.nix
1  {
2    pkgs ? import <nixpkgs> { }, # here we import the nixpkgs packages
3  }:
4    # mkShell is a helper function
5    pkgs.mkShell {
6      name = "dev-environment"; # that requires a name
7      buildInputs = [
8        # and a list of packages
9        pkgs.python3
10       pkgs.python3Packages.virtualenv
11       pkgs.nodejs
12       pkgs.yarn
13     ];
14     shellHook = ''
15       # bash to run when you enter the shell
16       echo "Start developing..."
17     '';
18 }
```

Ln 18, Col 4 Spaces: 5 UTF-8 CRLF nix



NixOS 21.11

<https://nixos.org/>

## Software

KDE Plasma Version: 5.23.3

KDE Frameworks Version: 5.87.0

Qt Version: 5.15.3

Kernel Version: 5.10.117 (64-bit)

Graphics Platform: Wayland

## Hardware

Processors: 2 × Intel® Core™ i5-3427U CPU @ 1.80

Memory: 1.9 GiB of RAM

Graphics Processor: SVGA3D; build: RELEASE; LLVM;

# Why Nix?

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- Pros:
  - Package manager covers whole system
  - Uses similar container infra to Docker so it can interoperate
  - Efficient cache management
- Cons:
  - Not as widespread in Python community
  - Can be harder to write in the first place to get it just right

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◦ • Ok, what should  
I choose? 🌀

\*Opinions are my own, your mileage may vary



In a vacuum, I would go fully  
declarative via Nix.

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# In real life, why not both?!

Start with  
Nix:

- Make a shell.nix to specify a project environment
- Add Python and any other tools needed (e.g.: LLVM, Clang, Fortran, etc.)
- Use direnv/pipenv to activate a Nix environment when you enter a directory



add Docker  
when it gets  
hard:

- Use nix-shell in a Docker container for portability
- Describe the steps that are hard to make declarative
- Export nix package to an OCI images for interoperability

# Sample python project config

---

```
# shell.nix
let
  pkgs = import <nixpkgs> {};
in pkgs.mkShell {
  packages = [
    (pkgs.python3.withPackages (python-pkgs: [
      # select Python packages here
      python-pkgs.pandas
      python-pkgs.requests
    ]))
  ];
}
```

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  - Case study:  
My home lab





# Requirements:

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- Needs to be portable across devices/hardware
- Runs/hosts Docker containers and local services
  - Home Assistant
  - PiHole
  - Wiki
  - Networking
  - Etc.
- Easy to maintain and back up





# The NixOS experiment

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- Declare the entire operating system and put it in source control
- Needed to use docker to hack some pieces in we couldn't get to work right
- We are still learning 😊

# Sample NixOS file: Hardware

```
{ config, pkgs, ... }:  
  
{  
  imports =  
    [ # Include the results of the hardware scan.  
      ./hardware-configuration.nix  
      <home-manager/nixos>  
    ];  
  
  # Bootloader.  
  boot.loader.systemd-boot.enable = true;  
  boot.loader.efi.canTouchEfiVariables = true;  
  
  # Define your hostname.  
  networking.hostName = "nixos-demo";  
  
  # Enable networking  
  networking.networkmanager.enable = true;  
  
  services.tailscale.enable = true;  
  services.flatpak.enable = true;  
  
  # Set your time zone.  
  time.timeZone = "America/Los_Angeles";
```

# Sample NixOS file: Users

```
# Define a user account.
users.users.demouser = {
  isNormalUser = true;
  description = "demouser";
  extraGroups = [ "networkmanager" "wheel"
"docker" ];
  packages = with pkgs; [
    discord
    slack
    signal-desktop
    element-desktop
    hyper
  ];
};
```

# Sample NixOS file: Home manager

```
home-manager.users.demouser = { pkgs, ... }:  
{  
  home.packages = [ pkgs.atool pkgs.httpie ];  
  programs.bash.enable = true;  
  programs.nushell.enable = true;  
  programs.starship.enable = true;  
  programs.starship.settings = {  
    username = {  
      show_always = true;  
      style_user = "bg:purple";  
      style_root = "bg:purple";  
      format = "[ ✨ ]($style)";  
    };  
    directory = {  
      style = "bg:red";  
      format = "[ $path ]($style)";  
      truncation_length = 3;  
      truncation_symbol = ".../";  
    };  
  };  
  home.stateVersion = "23.11";  
};
```

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# Conclusions

# Reproducible Environments

We need **declarative** and **imperative** descriptions of our projects

Docker containers are great, but can be hard to maintain

Nix is a declarative language for environments that can improve reproducibility





I declare... an environment

# Thanks! 🌟💖

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[aka.ms/pycascades-repro-envs](https://aka.ms/pycascades-repro-envs)

[aka.ms/pyc24](https://aka.ms/pyc24)

[aka.ms/python-discord](https://aka.ms/python-discord)

[mathstodon.xyz/@crazy4pi314](https://mathstodon.xyz/@crazy4pi314)

[sckaiser.com](https://sckaiser.com)

