Build-Benedictions

\$ buildben init-proj

Managing Multiple (Python) Projects & Dependencies

Dr. rer. nat. Martin Kuric

Academy of Sciences Göttingen · Germania Sacra / HisQu

buildben: Main Commands

(bube is the alias for buildben)

- \$ bube init-proj: Create a new project. 🗸 99% Done
- \$ bube add-experiment: Add a new experiment to a project. 🤞 80% Done
- \$ bube env-snapshot: Dockerize current project for reproducibility. 🤞 80% Done
- 🔸 💲 bube init-database : Create a new central database. 🔼 60% Done

Disclaimer

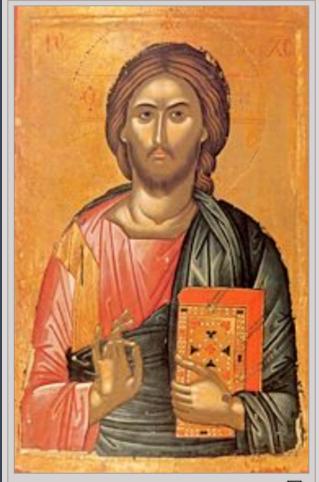
- buildben is very easy to use. (Goal is to make work simpler)
- This presentation is for python beginners.

But ...

- ... buildben solves a lot of behind-the-scenes-problems at once.
 - → The logic behind buildben is **not beginner-friendly**.
- Some problems are hard to understand if you haven't encountered them yet...
 (I myself don't understand them fully either, I simply trust the best practices..!)
- I'll give my best to explain python standards and my personal decisions.
- If anything is unclear, please ask immediately! (But expect some (un)organized chaos...)

How This all Started:

- I had one big mono-repository containing multiple projects. It was a MESS.
- After splitting into smaller repos: Managing multiple separate projects is painful, too..!
 - "Let's just start developing, I can add a setup.py later!"
 - "When did I last update the requirements.txt / setup.py ?"
 - "When anyone tries to use this code, the setup will probably break..."
- I had scripts to automate tasks, all of them poorly documented & scattered across repos!
- I needed one centralized standard to solve **all** my problems:
 - Think ahead, avoid problems, read my mind, etc.
 - Minimal interaction: No more than 1 CLI-command to do 100 things at once.
 - 🌼 (like a quick prayer doing miracles ... 🙏 😇)



Icon of Jesus Christ

Pantokrator by Theophanes
the Cretan. His right hand
is raised in benediction.

From Wikipedia:

"A **benediction** (Latin: bene, 'well' + dicere, 'to speak') is a short **invocation** for divine help, blessing and guidance [...]."

"Invocation is the act of calling upon a deity, spirit, or supernatural force, typically through prayer, ritual, or **spoken formula**, to seek guidance, assistance, or presence."

My Projects before buildben:

1. Make a virtual environment (.venv) for each project:

```
python -m venv ".venv" # Prevents polluting your OS with project-related chaos source .venv/bin/activate # Activate virtual environment
```

- 2. Collect my dependencies in a "proj-requirements.txt" file.
- 3. pip: Collects dependencies of my dependencies and installs everything:

```
pip install -r "proj-requirements.txt" # Resolve Environment & install dependencies
```

4. Compile all installed dependencies + versions for further reinstalls:

```
pip freeze > "requirements.txt" # Compile list of dependencies installed in current .venv
```

proj-requirements.txt

- Manually created by me: Whenever I pip install a new package, I add it to this file.
- Used by pip to "resolve the environment" (= collect dependencies of dependencies)

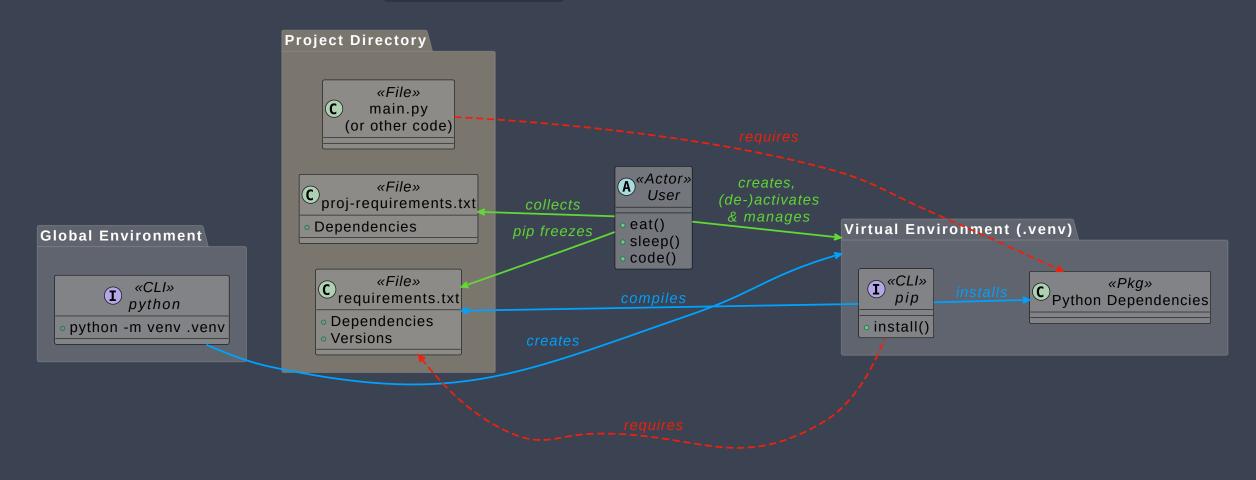
```
ipykernel
jupytext  # Convert .ipynb to .py
numpy
openpyxl  # For reading Excel files
pandas
matplotlib
seaborn  # Better plotting
pytest
```

requirements.txt

pip freeze > "requirements.txt" # Compile list of dependencies installed in current .venv

```
asttokens==3.0.0
build==1.2.2.post1
click==8.2.1
comm = = 0.2.2
debugpy==1.8.14
decorator==5.2.1
ipykernel==6.29.5
ipython==9.4.0
ipython_pygments_lexers==1.1.1
jedi==0.19.2
jupyter_client==8.6.3
jupyter_core==5.8.1
matplotlib-inline==0.1.7
# ...
```

My Projects before buildben: Architecture



"I will add a pyproject.toml once I need it!"

My Projects before buildben: Setup

```
git clone "<repo-url>"
                          # Download
 cd "<repo-name>"
 python -m venv ".venv" # Prevents polluting your OS with project-related chaos
 source .venv/bin/activate # Activate virtual environment
If there's only a "requirements.txt":
 pip install -r "requirements.txt" # Install only dependencies
If there's a pyproject.toml:
                                    # Editable install
 pip install -e .
```

My Projects before buildben: 2 Main Problems

1. Dependencies are pinned by hand:

requirements.txt must be manually updated.

2. Imports rely on current working directory:

- requirements.txt only holds dependencies, not the project structure.
- Cannot import anything outside the current working directory (no import ../module)
- VS Code (sometimes) struggles with refactoring & typing across packages.

Further Annoyances:

- 1. requirements.txt mixes runtime and development dependencies.
- 2. (De-)Activating .venv can be forgotten or annoying.
- 3. Too many CLI-commands to remember & type (especially when working with 4 Repos at the same time).
- 4. How to properly write unit-tests mid-development..?

>		
Solution	Why beginners should care	Standard
pyproject.toml	Single file that stores metadata and tool config	PEP 621
Editable install (pip install -e .)	Code changes are picked up without re-install	PEP 660
src/ layout	Forces you to test the installed package	PyPA guide
pip-tools	Auto-generates (and syncs) requirements*.txt	Jazzband docs
direnv	Activates the correct virtual env when you cd	direnv docs
just	Saves "one-liners" like just insco	just README

==== ID-based evaluation =====

Metric	Value
Hits Posctrl [total count]	2602
Hits AI [total count]	4372
Al TP [count]	1038
AI FP [count]	1105
AI FN [count]	1566
AI UNCLEAR [count]	662
ERROR [count]	1
Al precision [%]	48.4%
AI recall [%]	39.9%

Build-Benedictions: Minimal Workflow

bube proj # Shorthand for `buildben init-proj`

Build-Benedictions: Improving Setup & Maintenance

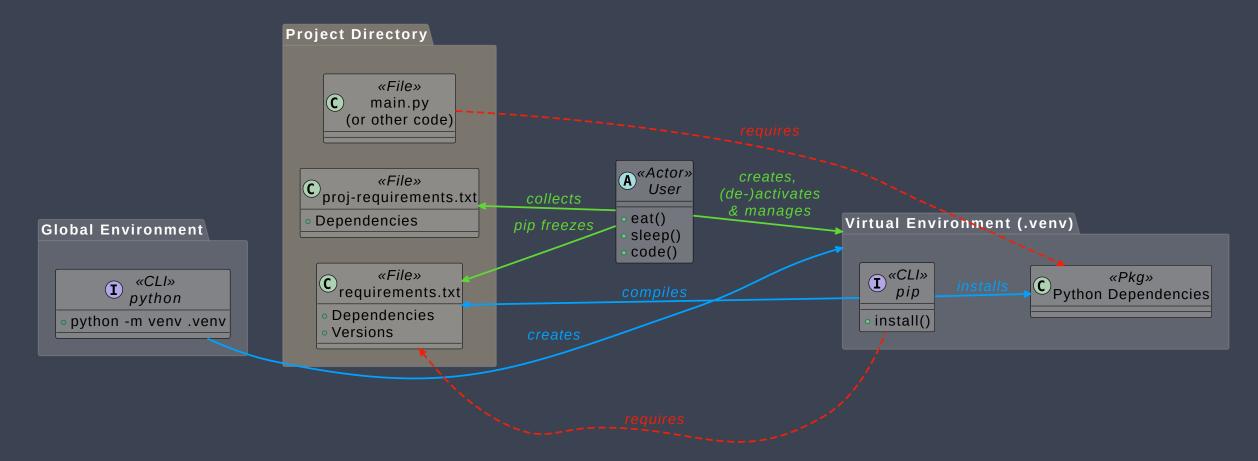
Standardize with template scaffolds:

\$ bube init-proj : Create a new project

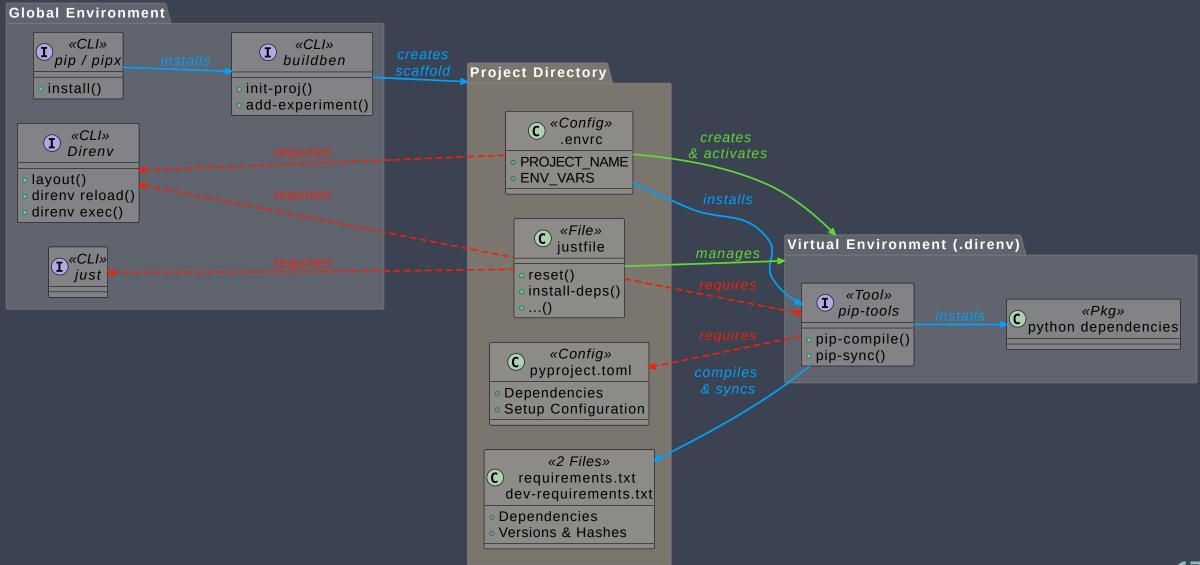
Automate workflow by integrating popular CLI-tools:

- direnv : Automate virtual environments & variables.
- pip-tools: Automate dependency management.
- just: Summarize tasks into one-liners: just install, just upgrade, etc.
- docker: Snapshot current state of project.

Without buildben:



With buildben:



Project Directory: src -Layout

```
# src layout (good)
                                 # flat layout (risky)
myproject/
                                 myproject/
   src/
    └─ myproject/
           main.py
                                     main.py
            package/module.py
                                     package/module.py
    tests/
                                     tests/
    test_module.py
                                     test_module.py
    README.md
                                     README.md
```

Benefits:

- Avoids imports from working directory via PYTHONPATH
 - → Forces tests to run on installed code: pip install -e . → Catches import bugs
- Builds clean wheels: Stray files never ship to PyPI
- Recommended by Python Packaging Authority (PyPA)

Project Directory: Inside src

```
myproject/
    src/
                      # Single directory, same name as project root (Recommended)
         myproject/
              __init__.py  # Marks directory as package; runs on first import!
main.py  # Optional CLI entry-point (wired in via pyproject.toml)
              sheesh.py # >>> import myproject.sheesh
clients/ # >>> import myproject.clients
                  __init__.py  # Sub-package "clients"
llm.py  # >>> import myproject.clients.llm
                  - llm.py
                   embedding.py # >>> import myproject.clients.embedding
              utils/
                                    # >>> import myproject.utils
                  __init__.py # Sub-package "utils"
                 - cooltool.py # >>> import myproject.utils.cooltool
                 - module6.py # >>> import myproject.utils.module6
```

Project Directory: Auxiliary Files in Project Root

```
myproject/
   .venv/
                         # Virtual environment (or .direnv!)
                         # Environment variables (& secrets)
   .env
   .gitignore
   .git/
                         # Repository metadata
  - src/
    └─ myproject/
                  # Separate source code from tests!
   tests/
    test_module1.py # Tests for module1
   justfile
                         # Development tasks
   pyproject.toml
                         # Project metadata, Setup!
   requirements.txt # Dependencies
   requirements-dev.txt # Development dependencies
   README.md
    LICENSE
```