Build-Benedictions

Aliases: buildben, bube

Managing Multiple (Python) Projects & Dependencies

using

\$ bube init-proj

Dr. rer. nat. Martin Kuric

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..!
 - → expect some (un)organized chaos...

PLEASE INTERRUPT ME AT ANY POINT!

What's buildben?

ChatGPT:

"buildben is like **Cookiecutter** plus automatic virtual-env creation, dependency locking, and helper tasks."

... and what's a Cookiecutter?

"A **Cookiecutter** is a project template that can be used to create new projects with a predefined structure and configuration. It is a tool that helps developers quickly set up new projects by providing a standardized starting point."

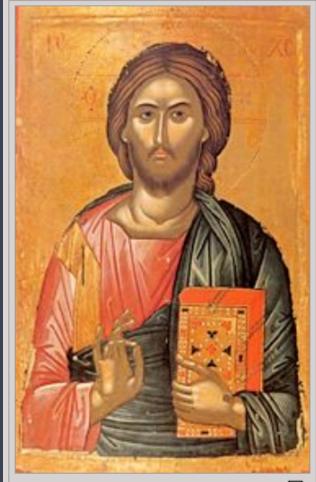
Aliases: buildben, bube

Main Modules:

- \$ 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

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..!
 - o "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.
 - o (like a quick prayer for a miracle ... 🙏 😇)



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)

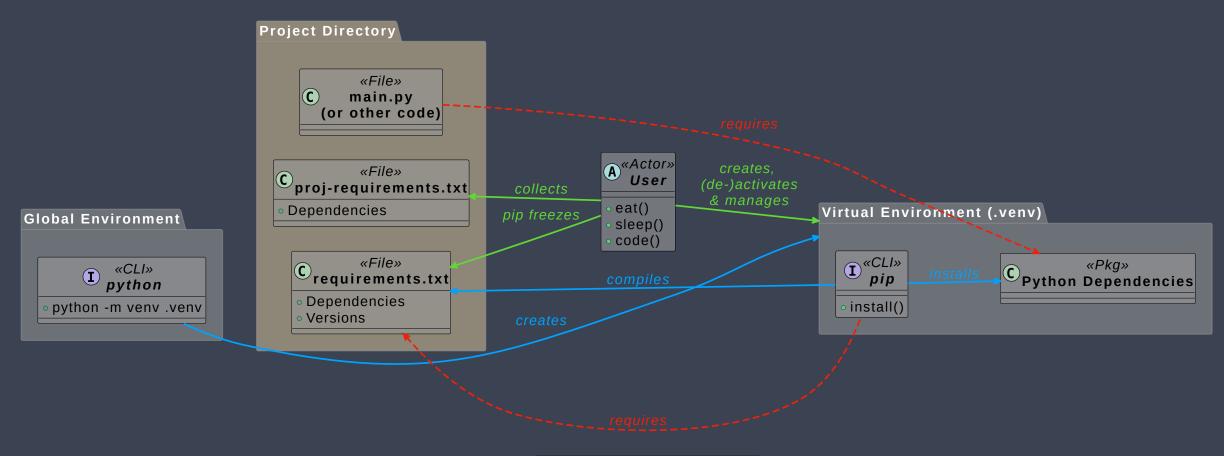
```
ipykernel
jupytext  # Convert .ipynb to .py
numpy
openpyxl  # For reading Excel files
pandas
matplotlib
seaborn  # Better plotting
pytest
```

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 later..!"

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..?
- 5. Where to keep .secrets.env ..?

Solutions:

Building Block	Why beginners should care	Standard
pyproject.toml	Single file that stores metadata and tool config	PEP 621
pip install -e	Code changes are picked up without re-install	PEP 660
src/ layout	Forces tests to run on the installed package	PyPA guide
pip-tools	Compiles *requirements.txt & syncs it with venv	(realpython.com)
direnv	Activates the correct virtual env when you cd	(direnv docs)
just	Saves "one-liners" like just insco	(just README)

bube proj : Workflow

1. \$ bube proj sets up a ready-to-use project directory (Cookie-Cutter):

- pyproject.toml: Pre-configured for src -layout, basic dependency list, etc.
- .envrc: Tells direnv to create & activate virtual environment automatically.
- justfile: Comes with working recipes (functions) to install, etc.
- Many more...

2. Use just recipes for everyday tasks:

- Installing your project: just install-compile
- Resetting environment: just reset-venv
- Upgrading dependencies: just upgrade-deps
- You can add more yourself!

bube proj : Demonstration

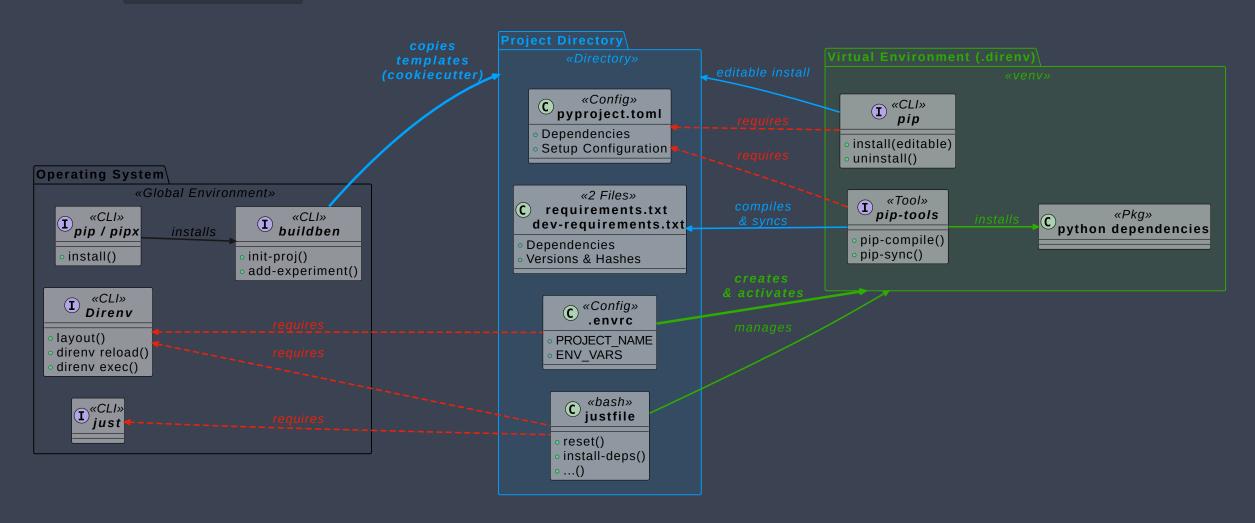
```
bube -h
                                 # Show help message
                                 # Shorthand for `buildben init-proj -h`
bube proj -h
bube proj "sheesh" -t . -g -u "<your_github_username>" # Cookiecutter project
cd "sheesh"
                                 # Change to project directory
direnv allow
                                 # Trust & execute .envrc
# A .direnv directory is created containing the virtual environment
                                 # Show available recipes
just
just install-compile
                                 # Install project, compile requirements.txt
cd ...
                      # Demonstrate auto-deactivation of direnv
cd bla_a
                      # Demonstrate auto-activation of direnv
cd ../sheesh
                      # Demonstrate auto-deactivation and activation of direnv
just reset-venv
               # Fully Nuke the virtual environment, start fresh!
```

bube proj : Minimal Example

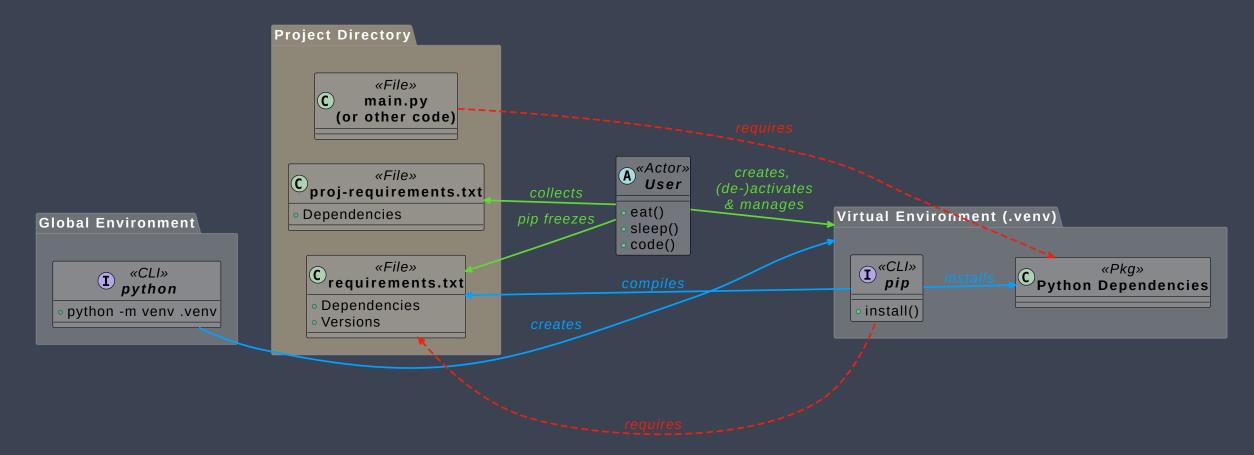
4 Lines to set up a new pip -installable project.

```
bube proj "sheesh" -t . -g -u "<your_github_username>"
cd "sheesh"
direnv allow
just install-compile
```

With buildben:



Without buildben:



src/ -Layout

Project Structure: 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

Project Structure: Inside src/

```
myproject/
   src/
                   # Single directory, same name as project root (Recommended)
        myproject/
             <u>__init___.py</u> # Marks directory as package; runs on first import!
                    # Optional CLI entry-point (wired in via pyproject.toml)
            main.py
           shishkebab.py # >>> import myproject.shishkebab
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
               - 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
```

just, justfiles & Recipes

just, justfiles & Recipes

• A "Recipe" is a bash function that can be called from the command line.

```
# Docstring for the recipe (optional)
recipe-name *ARGS:
    echo "Hello, World!"
    echo "This is a recipe."
    rm {{ARGS}}  # Pass arguments
alias rcp-nm:=recipe-name # Create an alias for the recipe
```

- All Recipes are stored in a file called justfile in the project root.
- just auto-detects the justfile and provides a CLI to run the recipes.

pyproject.toml

pyproject.toml

- Contains project metadata:
 - Dependencies (it replaced my proj-requirements.txt file).
 - Build system (e.g. setuptools, poetry, uv).
- Used by pip & pip-sync to install the project and its dependencies.
- Used by pip-compile to generate lock-file: requirements.txt.

pyproject.toml : Main Dependencies

- Whenever you pip install a package, add it to the list (like I did with my projrequirements.txt)
 - → Otherwise it will be forgotten when you re-install the project

```
[project]
  dependencies = [
    "numpy",
    "openpyxl",
    "matplotlib==3.5.1",  # You can pin a specific version
    "pandas>=2.0.0,<3.0.0",  # You can pin a version range
    "IPython",  # Unpinned versions will be resolved by pip or pip-compile
    "...",  # Add more dependencies here
]</pre>
```

pyproject.toml: Private / Unpublished Projects as Dependencies

- pip install <package> only works for packages published on PyPI.
 - o (We don't bother with PyPI, yet. Also, GitHub-Submodules are <u>scary</u>)
- Any pip -installable projects can be added via Git-URL or local path:

```
[project.dependencies]
"<my_project> @ file://../<my_project>", # Local path (easiest).
"<my_project2> @ git+https://github.com/HisQu/<my_project2>.git", # Git-URL
```

• Git version control: Add @<branch> , @<tag> or @<commit_hash> after the Git-URL:

```
"<my_project3> @ git+https://github.com/HisQu/<my_project3>.git@<commit>"
```

pyproject.toml: Optional Dependencies

- Unnecessary dependencies risk breaking the project for users who don't need them.
- Development-tools are only needed for development, make them optional:

```
[project.optional-dependencies]
  dev = [  # Name of the optional dependency group
   "pytest",
   "...",  # Add more dependencies here
]
```

• Include optional dependencies on installation:

```
pip install -e .[dev] # Install dependencies + development-dependencies
```

pyproject.toml : Packaging

- Packaging = Collecting all files needed to run the project into a single distributable.
- Python packages are usually distributed as wheels (.whl files).
- By default, Python uses setuptools to auto-package projects (PEP 517).
 - Other packaging-tools use pyproject.toml, too (poetry, flit, uv).
- setuptools scans for any, and packages them automatically.

pyproject.toml: Packaging Nomenclature

Component	Defintion	Contains
Module	single .py file	vars, funcs, classes
Package (pkg)	directory withinitpy	modules & sub-pkgs
Namespace pkg	directory withoutinitpy (PEP 517)	modules & sub-pkgs
Sub-package	nested package	modules (& sub-pkgs)
Project	collection of code units	pkgs, modules, assets, etc.

pyproject.toml : Packaging of .py files

Modules & Packages inside package-dir will be copied into
 ".venv/**/<my_project>".

```
[tool.setuptools]
package-dir = { "" = "src"} # "<my_project>/src/" --> ".venv/**lib**/<my_project>"
```

• Auto-discovery (and exclusion) of packages:

```
[tool.setuptools.packages.find]
where = ["src"]  # Scan "<my_project>/src/" for packages (subdirectories)
```

• This determines the import -paths:

```
from <my_project>.<package>.<module> import <your_class>, <your_variable>
```

Table / key	Purpose	Why it matters
<pre>[tool.setuptools] → package- dir</pre>	Maps <i>import</i> package path to real files ("" = "src")	Tells pip to copy code from src/into the installed wheel
[tool.setuptools.packages.find]	Auto-discovers packages under where = ["src"]; supports include, exclude, namespaces	Avoids hand-listing sub-packages; you can still override when needed
Other [tool.*] subtables	Config for linters, type- checkers, docs, etc. ([tool.black], [tool.mypy])	Keeps all project config in one file, reducing boilerplate

pyproject.toml: Packaging strategy of buildben

- \$ bube proj returns a pyproject.toml pre-configured with a conservative strategy:
 - Use the src/ -layout
 - Use a *single* parent directory as the root of the project.

Why the single src/ directory is good practice:

- **Keeps import statements short & stable**: e.g. from my_project.subpkg.mod import Foo just works after pip install -e .
- Yes, you could nest multiple roots, flat-layout, mixed C-extensions...
 - But every extra path mapping adds maintenance cost.
 - For most apps the single-dir rule of thumb is "99 % right, 0 % regrets"

pyproject.toml: Packaging non- .py files

- Anything that's not a .py -file must be explicitly added:
- The path-logic is

```
[tool.setuptools.package-data]
"<my_project>" = [
    "data/**/*.xlsx",  # Located in "src/<my_project>/data/"
    "images/**/*.{png,jpg}",  # Located in "src/<my_project>/images/"
]
```

pyproject.toml: Manual Configurations after \$ bube init-proj

Do immediately:

• Add description, license, authors, etc. under [project]

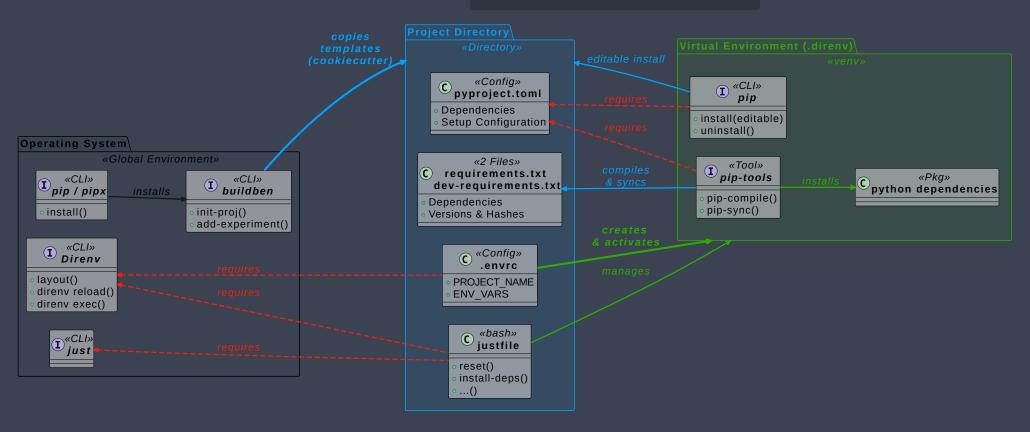
Do mid-development:

- Add emerging dependencies to [project]
- Add emerging non- .py files to [tool.setuptools.package-data]

Don't Do unless you know what you're doing:

- Modify the [build-system] section
- Change single directory src/ layout [tool.setuptools], [tool.setuptools.packages.find]

pip-tools



pip-compile:

- Compiles a requirements.txt file from the pyproject.toml file (unlike pip freeze).
- Automatically resolves dependencies and their versions.
- Generates a requirements.txt file with pinned versions.

pip-sync :

- Synchronizes the virtual environment with multiple lock files (e.g. *requirements.txt):
 - Installs packages from the lock files.
 - Un-installs packages not listed in lock-files (unlike pip install).

Capability	pip freeze	pip-compile
Locks transitive deps deterministically	♠ best- effort	✓ topologically sorted
Separates direct vs indirect deps	×	comments show who pulled what
Generates securehash= pins	X	generate-hashes flag
Selective upgrades (e.gupgrade-package flask)	×	✓ built-in
Understands modern metadata (PEP 621 pyproject.toml)	×	

Installation of buildben

Prerequisites:

- Python installed on your OS (and you know its executable in your \$PATH)
- A Package manager (apt, brew, winget, etc.)

Quick & Dirty:

```
git clone https://github.com/markur4/buildben.git
pip install -e buildben # venv recommended. (Also, you might want just & direnv.)
```

Full Install (recommended):

1. Install pipx:

To use buildben globally and to keep the OS-python clean, we recommend pipx.

```
sudo apt install pipx  # For Ubuntu
# brew install pipx  # For MacOS
# py -m pip install --user pipx  # For Windows (Not tested!)
pipx ensurepath  # Add pipx to PATH, if not already done
pipx upgrade-all  # !! Never run pipx with sudo !!
```

2. Clone & install buildben:

```
git clone https://github.com/markur4/buildben.git
cd buildben  # Needed, `pipx install buildben` does NOT work!
pipx install -e .  # Editable for direct modifications.
```

Full Install (recommended):

3. Install just:

```
sudo apt install just  # For Ubuntu
# brew install just  # For MacOS
# pipx install rust-just # Windows requires the cross-platform version (not tested!)
```

4. Install direnv & hook it into your shell:

- Either follow the instructions for install & hook,
- Or run src/buildben/setup_zsh.sh to install both zsh & other useful plugins, including direnv.

Summary

Summary – Key Takeaways

- One command, full scaffold: bube init-proj drops a ready-to-run project (src/, pyproject.toml, .envrc, justfile, tests) in seconds.
- **Standards-first:** Uses PEP 621 for metadata & PEP 660 for editable installs, so your code works with modern packaging tools.
- Automated dependency locking: pip-compile + pip-sync generate and enforce reproducible requirements*.txt.
- **Zero-friction environments:** direnv creates & activates the correct venv every time you cd into the folder.
- Repeatable recipes: just gives you memorable one-liners (just insco, just reset-venv) for daily tasks.

Build once → code everywhere. Less worry, more science 🙎 🦖