Packaging research* encourages good habits, improves transparency, and enables collaboration.

Adantages

Encourages good habits
- Structure helps work effectively, ideally community/peer’s conventions are used
- Tools & workflows for Openness often increase efficiency at the same time
- Tidy well-documented virtual laboratory (keep input, methods, output separate)
- Packaging process can even simulate and independent reproduction (starting from scratch in container)
- Quality of work improves with good programming practices, (perceived) overhead pays off quickly
- Prepare for requirements by funders and journals (Open Science will become Science)

Improves transparency
- Easier to understand (readers, students, self)
- More convincing and inspectable (reviewers)
- Higher trust and confidence in results because of independent re-execution

Enables collaboration
- Future you is your best collaborator!
- Data, methods, and software are demonstrated to work, which improves reuse and discoverability
- Extensibility through good practices

Examples
[Images from left to right.]

* As research compendium, ERC, Docker/Singularity image/container, VM, Binder, ReproZip package, Tale, Compute Capsule, ...

GeoSimulation model with PCRaster/Python
https://github.com/2JudithVerhagen/PLUC_Mozambique/

GeOBIA workflow
doi:10.3390/rs9030290

Environmental citizen science
doi:10.5281/zenodo.1135139

Containerisation/VMs & UI
- x11docker makes sharing of display between host and container simple and secure (Linux)
- Web-based UI (incl. API) best
- Special UI encourages deliberate communication
- Containers scripted (Dockercfile) and better for reuse and "making"
- VMs larger, good for dissemination, but for use only...when did the Kernel ever break?

Research Compendium
https://research-compendium.science/
- Accompanies/enhances/a scientific publication
- Container for data, code, docs, notebooks; under clear licenses; distribution & managing
- "package-pendium": based on programming language modules, e.g. PyPI, CRAN, npm.

Executable Research Compendium (ERC)
https://o2r.info/erc-spec/
- Notebook serves as control file and input for display file (dual entry points)
- Software includes container for runtime environment
- UI bindings provide interactivity & linking of parts

"An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship."
(Crowfoot & Detoni 1999) doi:10.7187/0146-7221-57.2.198

Assisted Containerisation

More & References