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

**Advantages**

- **Encourages good habits**
  - Structure helps to 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**

- Geosimulation model with PCRaster/Python
- GEOBIA workflow
- Environmental citizen science

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

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**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 (Dockerfile) 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/is a scientific publication
- Container for data, code, docs, notebooks; under clear licenses; distribution & managing
- “package-panium”: 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 (Jupyter etc.)

"An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship."

(Engelkamp & Donnay 1999; doi:10.1109/MC.1999.750064)

**Assisted Containerisation**

Binder, CODE OCEAN, ReproZip

**More & References**

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