

Reliable and reproducible Earth System Model data analysis with ESMValTool

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Software ecosystem: ESMValCore and ESMValTool

ESMValCore: highly optimized, pure-Python package, responsible for **computationally-heavy pre-processing of data** (climate statistics, regridding, multi-model statistics etc) → **COMPUTING** and **DATA REDUCTION** are the outputs, **SMALL TECHNICAL TEAM (strong technical skills)** the developers

ESMValTool: main scientific analysis and diagnostics library (written in Python, NCL, R, and Julia) – responsible for **development of diagnostics and metrics (stored in recipes)**, with scientific output (plots, files etc) → SCIENCE is the main output, LARGE and DIVERSE (coding skills, technical knowledge) COLLABORATIVE group the developers

Software ecosystem: ESMValCore and ESMValTool

Common to both:

- lots of code (~200k lines, minimal code rot)
- complex dependency environments (100 direct dependencies, 500-1000 dependencies in any given environment)
- need for wide supported platforms
 (operating systems, Python versions etc)
- need for ease of installation, and maintenance
- complex configurations, but made as simple as possible for users



Testing is absolutely necessary to ensure correct functionality and portability, over long development cycles, with widely varied developers' skills and interests

Overall testing strategy - ESMValCore

ESMValCore package *ℯ*

```
docs passing DOI 10.5281/zenodo.3387139 matrix join chat PASSED codecov 93% code quality A docker build passing Anaconda.org 2.9.0 Test passing
```

► Highly optimized, pure-Python package, responsible for computationally-heavy pre-processing of data (climate statistics, regridding, multi-model statistics etc) → COMPUTING and DATA REDUCTION are the outputs, SMALL TECHNICAL TEAM the developers ->

Testing needs to be technically **diverse** and **comprehensive**

- ▶ Testing done for all supported operating systems and Python (as main language) versions
- ▶ Both **strict** and **in-depth** testing

Overall **testing strategy** - ESMValCore

ESMValCore package *∂*

```
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```

Both strict and in-depth testing:

Core system tests:

- software environment fitness (building the environment, and installing the package in it, regularily)
- backup environment recipe build and installation tests (conda-lock)
- Python package build tests
- Docker container(s) build and deploy tests

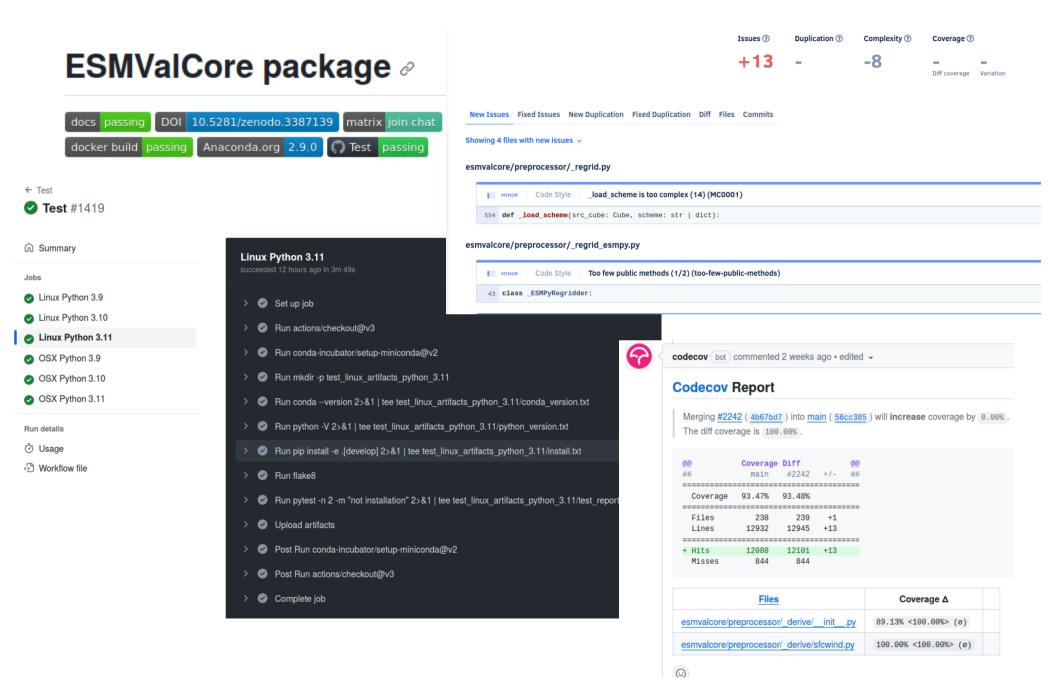
General purpose tests:

- unit/integration/regression (with sample data) tests
- coding standards tests (pylint and flake8)
- test coverage tests (when adding new code)

Documentation:

documentation build and deploy tests

Overall testing strategy (for separate packages)



Overall **testing strategy** - ESMValTool

ESMValTool



Main scientific analysis and diagnostics library – responsible for development of diagnostics and metrics (in recipes), with scientific output (plots, files etc) → SCIENCE is the main output, LARGE and DIVERSE COLLABORATIVE group the developers

Testing needs to ensure scientific correctness and allow for variability of developers' skills (ie not too restrictive, definitely not too lax, or "not great, not terrible")

- ▶ Testing done for all supported OS and Python versions
- Scientific output-oriented tests
- Still include some technical testing (like for ESMValCore, but less strict)

Overall **testing strategy** - ESMValTool

ESMValTool



- Scientific output-oriented tests include:
 - numerical and graphical output comparisons (with previous versions, and current version when changes occur; both manual and automated triggers) via a dedicated tool for recipe output comparison which is smart enough to handle small differences in numerical results in NetCDF files and small differences in plots through image hashing
 - EXIF and Mark I Eyeball testing (visualization of output)
 - input data specifications consistency tests
 - output provenance tests
- Still with some technical testing like for ESMValCore, but less strict:
 - FEWER unit/integration/regression (with sample data) tests
 - FEWER coding standards tests (pylint and flake8)
 - NO test coverage tests (when adding new code)

Provenance output and testing

all our software is stored on Zenodo for every release with a DOI we have docker containers that offer pretty good software environment reproducibility, we record the filenames and global NetCDF attributes of all input files.