

ESMValTool

Earth System Model Evaluation Tool

Reliable and reproducible Earth System Model data analysis with ESMValTool

Valeriu Predoi (NCAS-CMS University of Reading, UK) and Bouwe Andela (Netherlands eScience Centre, The Netherlands) for the ESMValTool Technical Lead Team

It facilitates the analysis of Earth system model's data.



What is ESMValTool?

What is ESMValTool?

Documentation https://docs.esmvaltool.org/en/latest/ GitHub https://github.com/ESMValGroup Website https://esmvaltool.org/ Video https://www.youtube.com/watch?v=sidM4EB6Sbo



What can ESMValTool do for you?

- Helps to analyze climate data
- Provides provenance and citation information.
- Supports several programming languages and operating systems.
- Helps efficient data processing.



GitHub https://github.com/ESMValGroup Website https://esmvaltool.org/ Video https://www.youtube.com/watch?v=sidM4EB6Sbo

Software ecosystem: ESMValTool and ESMValCore

ESMValTool: scientific analysis and diagnostics library (written in Python, NCL, R, and Julia) – contains reproducible recipes with scientific output (plots, data files etc) \rightarrow SCIENCE is the main output, LARGE and DIVERSE (coding skills, technical knowledge) COLLABORATIVE group the developers



ESMValCore: Python package for working with CMIP(-like) data, responsible for running ESMValTool recipes. It finds and optionally downloads the input data, applies preprocessor functions (climate statistics, regridding, multi-model statistics etc) and passes the resulting NetCDF files on to the scientific analysis codes \rightarrow COMPUTING and DATA REDUCTION are the outputs, SMALLER TECHNICAL TEAM (strong technical skills) the developers



Software ecosystem: ESMValCore and ESMValTool

ESMValTool

lots of code (~200k lines)
many dependencies (~100 direct dependencies, ~600 indirect dependencies), but should be easy to install
provides ~100 recipes and diagnostics, which are fairly independent of each other

ESMValCore

- relatively compact codebase
- only a few dependencies
- reliability is key because it is used by every recipe



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 @



- Testing needs to be technically diverse and comprehensive
- Testing done for Linux and OSX and all recent Python versions
- Both strict and in-depth testing

Overall testing strategy - ESMValCore

ESMValCore package @

docs passing	DOI	10.5281/zenodo.3387139	matrix join chat	② PASSED	Codecov	93%	🔿 code quality	А
docker build pa	assing	Anaconda.org 2.9.0	Test passing					

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 (mypy, pylint, and flake8)
- code coverage check by Codecov, 100% coverage required for changes

Documentation:

- documentaton build and deploy tests

Overall **testing strategy** (for separate packages)

ESMValCo	ore package @		Issues ⑦ Duplication ⑦ + 13 -	Complexity ⑦ Coverage ⑦ -8 Diff coverage Variation			
docs passing DOI 10. docker build passing A	5281/zenodo.3387139 matrix join chat naconda.org 2.9.0 💭 Test passing	New Issues Fixed Issues New Duplication Fixed Du Showing 4 files with new issues ~ esmvalcore/preprocessor/_regrid.py	uplication Diff Files Commits				
← Test ✓ Test #1419		Image: Code Style _load_scheme is too complex (14) (MC0001) 554 def _load_scheme(src_cube: Cube, scheme: str dict): esmvalcore/preprocessor/_regrid_esmpy.py Image: Code Style Too few public methods (1/2) (too-few-public-methods)					
G Summary	Linux Python 3.11 succeeded 12 hours ago in 3m 49s						
 Linux Python 3.9 Linux Python 3.10 Linux Python 3.11 OSX Python 3.9 	 Set up job Run actions/checkout@v3 Run conda-incubator/setup-miniconda@v2 	43 class _ESMPyRegridder:	codecov (bot) commented 2 weeks ago • edited	•			
OSX Python 3.10OSX Python 3.11	 Run mkdir -p test_linux_artifacts_python_3.11 Run condaversion 2>&1 tee test_linux_artifacts_python_3.11 	acts_python_3.11/conda_version.txt	Codecov Report				
Run detalls ඊ Usage ① Workflow file	 Run python -V 2>&1 tee test_linux_artifacts_p Run pip install -e .[develop] 2>&1 tee test_linux Run flake8 Run pytest -n 2 -m "not installation" 2>&1 tee Upload artifacts Post Run conda-incubator/setup-miniconda@v. Post Run actions/checkout@v3 	python_3.11/python_version.txt ux_artifacts_python_3.11/install.txt test_linux_artifacts_python_3.11/test_report 2	Merging #2242 (4b67bd7) into main (56cc385 The diff coverage is 100.00% . @@ Coverage Diff @@ ## main #2242 +/- Coverage 93.47% 93.48%) will increase coverage by 0.00%.			
	> 🥥 Complete job		Files esmvalcore/preprocessor/_derive/initpy esmvalcore/preprocessor/_derive/sfcwind.py	Coverage Δ 89.13% <100.00%> (0) 100.00% <100.00%> (0)			

Overall testing strategy - ESMValTool

ESMValTool



- ► ESMValTool: scientific analysis and diagnostics library (written in Python, NCL, R, and Julia) – contains reproducible recipes with scientific output (plots, data files etc) → SCIENCE is the main output, LARGE and DIVERSE (coding skills, technical knowledge) 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")
- Basic 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, scientifically approved versions
 - 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
 - Testing workflow is at the moment manual for every release, working on automation by setting up a "recipe test workflow"
- Mark I Eyeball testing (visualization of output) comparison with figures in papers
- Input data specifications consistency tests
- Still with some technical testing like for ESMValCore, but less strict:
 - Limited unit/integration tests, only for a few shared components
 - More relaxed on coding standards (pylint and flake8)
 - No code coverage checks

FAIR research software

- Software releases are stored on Zenodo with a DOI
- Docker containers for reproducible software environments for every release
- A recipe with fixed input data versions is recorded for each recipe run
- ESMValCore records provenance, which includes the filenames and global NetCDF attributes of all input files used to create a figure.

For more information on FAIR research software, see:

Barker, M., Chue Hong, N.P., Katz, D.S. et al. Introducing the FAIR Principles for research software. Sci Data 9, 622 (2022). https://doi.org/10.1038/s41597-022-01710-x

ESMValTool: take home message

- The tools have a modular design in which community members of varying skill level are able to contribute without compromising reliability and user experience for others
- Test and code quality requirements are adjusted to how many users and developers will be affected if a component breaks
- FAIR research software for doing open science