

Reproducibility in Action

My experiences writing a reproducible paper

Stephan Rasp
- LMU Munich -

Paper submitted to JAS (Talk about the science on Thursday morning):

Rasp, Selz and Craig, 2017. Variability and clustering of mid-latitude summertime convection: Testing the Craig and Cohen (2006) theory in a convection-permitting ensemble with stochastic boundary layer perturbations

Computation section in the manuscript

e. Computational details and reproducibility

This subsection closely follows the guidelines on publishing computational results proposed by Irving (2016). The analysis and plotting of model and observation data was done using Python. The Python libraries NumPy (Numerical Python; van der Walt et al. (2011)) and SciPy (Jones et al. 2001–) were used heavily. The raw data were read with the Python module cosmo_utils (code available upon request). The figures were plotted using the Python module Matplotlib (Hunter 2007). Plotting colors were chosen according to the Hue-Chroma-Luminance color space (Stauffer et al. 2015). Some plots were post-processed using the vector graphics program Inkscape.

To enable reproducibility of the results, this paper is accompanied by a version-controlled code repository (https://github.com/raspstephan/convective_variability_analysis)

and a Figshare repository (Rasp 2017), which contains a snapshot of the code repository at the time of submission and supplementary log files for each figure. These log files contain information about the computational steps taken from the raw data to the generation of the plots.

While the model code and initial data is not openly available, a detailed technical description of the model simulations can be found in the `cosmo_runscripts` directory of the code repository. The Jupyter notebooks (Kluyver et al. 2016) mentioned in the text are stored in the directory `jupyter_notebooks` of the repository. Links to non-interactive versions of the notebooks can be

found on the front page of the Github repository; rendered PDF versions are also added to the supplement of this paper.

Citation of software tools

Github repository

Figshare repository with log files

Jupyter notebooks

The github repository contains all code used from the raw data to the final figures with adequate documentation.

Repository for my work on convective variability and clustering

259 commits 1 branch 2 releases 1 contributor

Branch: master New pull request Create new file Upload files Find file Clone or download

File/Folder	Commit Message	Time Ago
aux_files	Restructured repository	6 months ago
config	Plotting changes;	2 months ago
cosmo_runscripts	Update README files for submission	a month ago
fortran_scripts	Restructured repository	6 months ago
jupyter_notebooks	Comment cosmo_utils import in RDF nb	14 days ago
python_scripts	Make cosmo_utils imports optional in helpers.py	14 days ago
synop_plots	Update README files for submission	a month ago
.gitignore	Updated documentation for variability.py	3 months ago
README.md	Update README files for submission	a month ago

Release Notes: submission

This is the version of the code repository at the time the paper was submitted. The Jupyter notebooks mentioned in the paper can be downloaded or viewed here:

- http://nbviewer.jupyter.org/github/raspstephan/convective_variability_analysis/blob/master/jupyter_notebooks/cloud_identification_and_rdf.ipynb
- http://nbviewer.jupyter.org/github/raspstephan/convective_variability_analysis/blob/master/jupyter_notebooks/beta_sample_size_dependency.ipynb

Convective Variability in COSMO ensembles

2016060800 Removed all unnecessary runscripts and extended README 5 months ago

README.md Update README files for submission a month ago

Description of INT2LM and COSMO runs

Disclaimer: Because Deutscher Wetterdienst (DWD) does not provide their models and data as open source, we are not able to provide any actual data or model code. With this limitation in mind, we nonetheless will try to provide a complete description of how our final data was produced. The hope is that this makes it easy for ther researchers with access to DWD data to set up similar experiments. Furthermore, it should provide internal (LMU) users with detailed instructions on the data structure and model setup. For this reason, all the specific paths are provided.

Initial and Boundary data

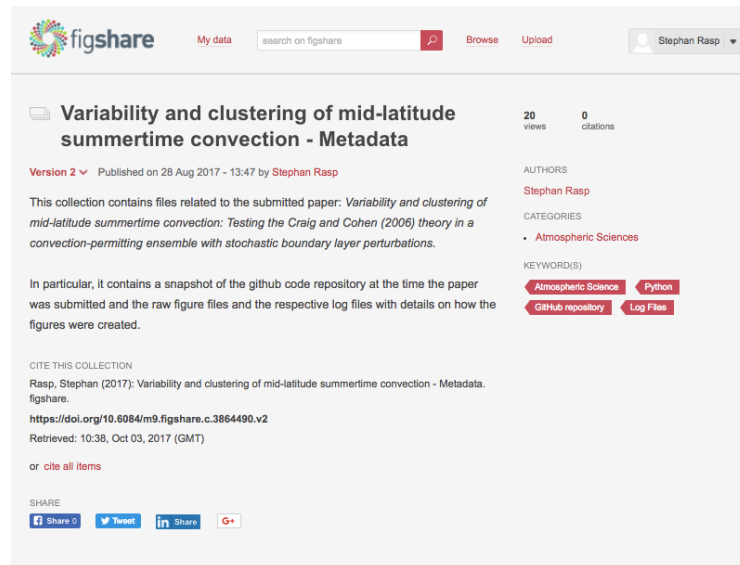
The initial and boundary data for these experiments are COSMO-EU operational analyses. A description of the COSMO-EU setup can be found here, but unfortunately only in German : https://www.dwd.de/SharedDocs/downloads/DE/modell/documentation/nwv/cosmo_eu/cosmo_eu_dbbeschr_201406.pdf?__blob=publicationFile&v=3

The COSMO-EU model runs with a horizontal grid spacing of 7 km and parameterized convection. It uses a nudging data assimilation system.

Since driving data and model source code are not open source as much information as possible about the model version and how to obtain the data are given. Additionally, the location of data and model are listed for internal users.

A figshare repository, which is referenced in the paper, contains a snapshot of the Github repository and the all raw figures and log files.

Rasp, S., 2017: Variability and clustering of mid-latitude summertime convection - metadata. Figshare, accessed 28 August 2017, doi:10.6084/m9.figshare.c.3864490.



Plotting log

```
#####
Time: 2017-08-01T12:41:32
```

Executed command

```
python weather_time_series.py --date_start 2016052800 --date_end 2016060800 --time_start 1 --time_end 24 --nens 50
--pp_name all_days_50mem --plot_name all_days_50mem --radar_mask day --plot_type prec_cape_comp
```

in directory: /home/s/S.Rasp/repositories/convective_variability_analysis/python_scripts

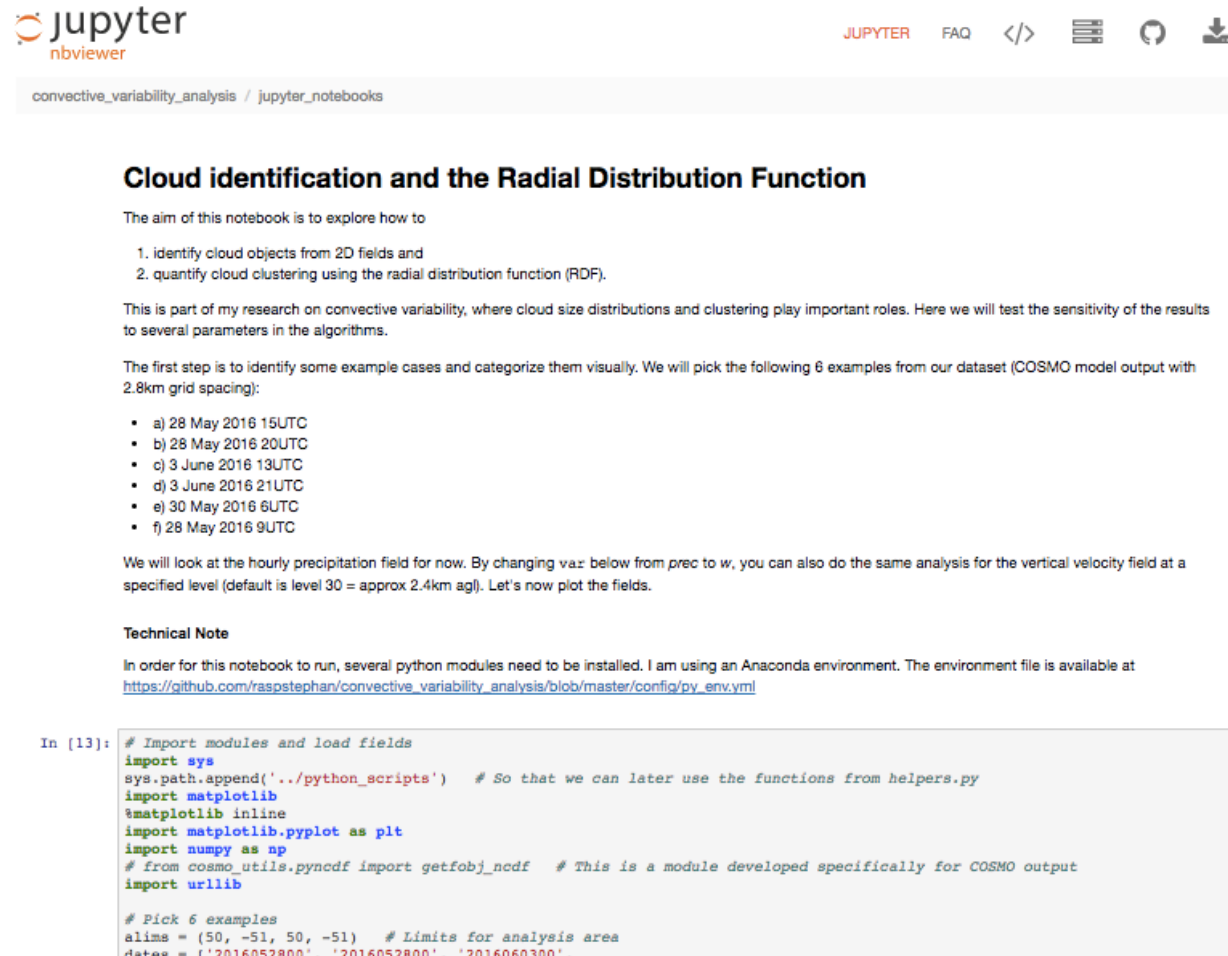
Git hash: f20fb9f16b9a0a32569d1ecea8db271400e3c96

Full argparse parameters

```
-----
--plot_type prec_cape_comp
--recompute False
--time_start 1
```

The log file lists the exact command executed and the computational environment. For an example of a simple log file creation in Python: <https://raspstefhan.github.io/2017/08/24/reproducibility-hack.html>

Jupyter notebooks allow for literate programming. Great for data exploration, code examples and simple analysis. In combination with a VCS literate programming can make decisions more reproducible. For R: R Markdown



jupyter
nbviewer

convective_variability_analysis / jupyter_notebooks

Cloud identification and the Radial Distribution Function

The aim of this notebook is to explore how to

1. identify cloud objects from 2D fields and
2. quantify cloud clustering using the radial distribution function (RDF).

This is part of my research on convective variability, where cloud size distributions and clustering play important roles. Here we will test the sensitivity of the results to several parameters in the algorithms.

The first step is to identify some example cases and categorize them visually. We will pick the following 6 examples from our dataset (COSMO model output with 2.8km grid spacing):

- a) 28 May 2016 15UTC
- b) 28 May 2016 20UTC
- c) 3 June 2016 13UTC
- d) 3 June 2016 21UTC
- e) 30 May 2016 6UTC
- f) 28 May 2016 9UTC

We will look at the hourly precipitation field for now. By changing `var` below from `prec` to `w`, you can also do the same analysis for the vertical velocity field at a specified level (default is level 30 = approx 2.4km agl). Let's now plot the fields.

Technical Note

In order for this notebook to run, several python modules need to be installed. I am using an Anaconda environment. The environment file is available at https://github.com/raspstephan/convective_variability_analysis/blob/master/config/py_env.yml

```
In [13]: # Import modules and load fields
import sys
sys.path.append('../python_scripts') # So that we can later use the functions from helpers.py
import matplotlib
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
# from cosmo_utils.pyncdf import getfobj_ncdf # This is a module developed specifically for COSMO output
import urllib

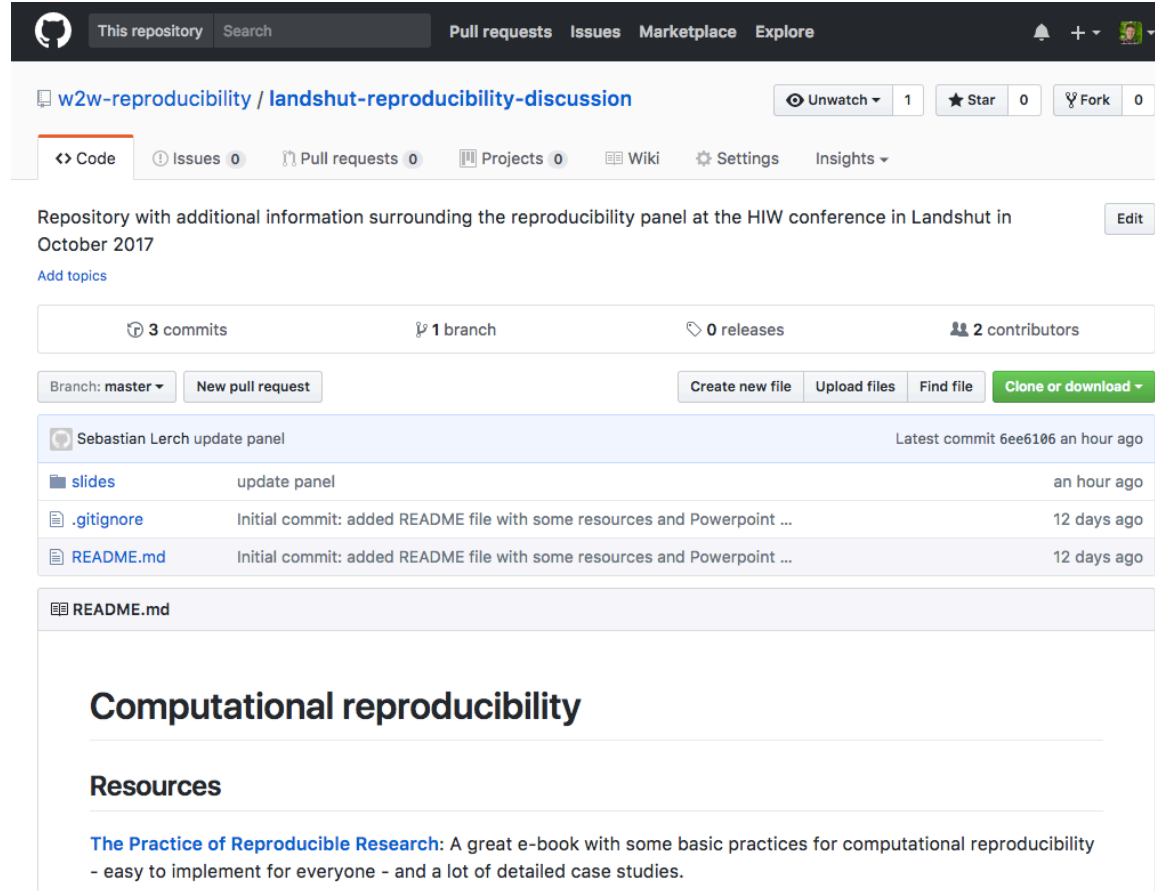
# Pick 6 examples
alims = (50, -51, 50, -51) # Limits for analysis area
dates = ['2016052800', '2016052800', '2016060300']
```

Final thoughts from my side:

- Striving to write reproducible code made me really think about my analysis.
- The initial (re)structuring of the code is time-consuming. Few examples to look at.
- In the long run, reproducible code probably saves time, personally and for the community.
- Uncertainty how to deal with non-open source data and model code.
- Lack of software development education for computational scientists (almost everyone!)

Resources available at <https://github.com/w2w-reproducibility/landshut-reproducibility-discussion>

Link on HIW Webpage: <https://hiw2017.wavestoweather.de>



The screenshot shows the GitHub interface for the repository 'w2w-reproducibility / landshut-reproducibility-discussion'. The repository has 1 star, 0 forks, and 0 issues. It was created by Sebastian Lerch and has 3 commits, 1 branch, and 0 releases. The repository description states: 'Repository with additional information surrounding the reproducibility panel at the HIW conference in Landshut in October 2017'. The file list includes 'slides', '.gitignore', and 'README.md'. The 'README.md' file is expanded, showing the title 'Computational reproducibility' and a section 'Resources' with a link to 'The Practice of Reproducible Research'.

Repository with additional information surrounding the reproducibility panel at the HIW conference in Landshut in October 2017

3 commits 1 branch 0 releases 2 contributors

Branch: master New pull request Create new file Upload files Find file Clone or download

Sebastian Lerch update panel Latest commit 6ee6106 an hour ago

File	Commit Message	Time
slides	update panel	an hour ago
.gitignore	Initial commit: added README file with some resources and Powerpoint ...	12 days ago
README.md	Initial commit: added README file with some resources and Powerpoint ...	12 days ago

README.md

Computational reproducibility

Resources

[The Practice of Reproducible Research](#): A great e-book with some basic practices for computational reproducibility - easy to implement for everyone - and a lot of detailed case studies.

Panel and open discussion:

Jenny Sun, NCAR - Julia Keller, WMO - Hannah Christensen, NCAR - Linus Magnusson, ECMWF

- Why is so little research currently computationally reproducible in the weather and climate sciences?
- What are the biggest problems related to reproducibility at the moment?
- How can these problems be tackled by the community?
- Should there be strict guidelines and requirements regarding reproducibility? Who enforces them (funding agencies, journals, universities, ...)?