Reproducibility in atmospheric science - A minimum standard

Georgios Fragkoulidis

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Landshut, 9/10/2017

A MINIMUM STANDARD FOR PUBLISHING COMPUTATIONAL RESULTS IN THE WEATHER AND CLIMATE SCIENCES

BY DAMIEN IRVING

A procedure for publishing reproducible computational research is described that could be adopted as a minimum standard by journals in the weather and climate sciences.

The rise of computational science has led to unprecedented opportunities in the weather and climate sciences. Ever more powerful computers enable experiments that would have been considered impossible only a decade ago, while new hardware technologies allow data collection in even the most inaccessible places. To analyze the vast quantities of data now available to them, modern practitioners—most of whom are not computational experts—use an increasingly diverse set of software tools and packages. Today's weather or climate scientist is far more likely to be found debugging code written in Python, MATLAB, Interactive Data Language (IDL), NCAR Command Language (NCL), or R than to be poring over satellite images or releasing radiosondes.

This computational revolution is not unique to the weather and climate sciences and has led to something of a reproducibility crisis in published research (e.g., Peng 2011). Most papers do not make the data and code underpinning key findings available, nor do they adequately specify the software packages and libraries used to execute that code. This means it is impossible to replicate and verify most of the computational results presented in journal articles today. By extension (and perhaps even more importantly), it is also impossible for readers to interrogate the data processing methodology. If a reader cannot find out which Python library was used in regridding a particular dataset, how can they build upon that regridding method and/or apply it in their own context?

A movement within the computational science community has arisen in response to this crisis, calling for existing communication standards to be adapted to include the data and code associated with published findings (e.g., Stodden and Miguez 2014). The movement has also been active in producing best

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Problem:

- Today's weather and climate scientist is more likely to be found debugging MATLAB/Python/NCL/R code than observing satellite images or releasing radiosondes.
- A diverse set of software tools/packages/libraries is used without citation/specification, while there's no data/code disclosure.
- Replication / verification are impossible (e.g. if I cannot find out which Python library was used in regridding a particular dataset, or which exact method was used in an obscurely cited significance test)

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Proposed procedure that could enhance reproducibility...

Addition of computation section:

Cite the major software packages used and point readers to a “research-archiving" platform (e.g. **Figshare, Zenodo**) with:

(Nicolas and Bromwich 2014). These issues are less critical in our study because the primary focus is seasonal and interannual variability (as opposed to long-term trends or low-frequency variability), but they are still important to keep in mind.

b. ERA-Interim data

Reanalysis projects typically provide both analysis and forecast fields for download. The analysis fields are the output of the data assimilation cycle at each time interval, which for ERA-Interim is every 6 h. They represent arguably the most accurate possible depiction of the atmospheric state for several dozen variables that are all coherent on the calculation grid. These analysis fields are then used to initialize weather forecasts for the coming hours/days. ERA-Interim forecasts are initialized twice daily at 0000 and 1200 UTC, and forecast fields are available for 3, 6, 9 and 12 h after initialization.

In this study we analyze the daily average 500-hPa meridional wind (v), 500-hPa geopotential height (Z), surface air temperature, sea ice fraction, sea surface temperature, and mean sea level pressure, calculated as the mean of the 6-hourly analysis fields from ERA-Interim. For precipitation, the “total precipitation” forecast fields were used (i.e., the sum of the convective and large-scale precipitation, which is also provided separately). Each forecast field represents the accumulated precipitation since initialization, so the daily rainfall total was calculated as the sum of the two 12-h post initialization accumulated fields for each day. The horizontal resolution of the ERA-Interim data used here is 0.75° latitude × 0.75° longitude.

3. Computation procedures

The results in this paper were obtained using a number of different software packages. A collection of command line utilities known as the NetCDF Operators (NCO) and Climate Data Operators (CDO) were used to edit the attributes of netCDF files and to perform routine calculations on those files (e.g., the calculation of anomalies and climatologies), respectively. For more complex analysis and visualization, a Python distribution called Anaconda was used. In addition to the Numerical Python (NumPy; Van Der Walt et al. 2011) and Scientific Python (SciPy) libraries that come installed by default with Anaconda, a Python library called xray was used for reading and writing netCDF files and data analysis. Similarly, in addition to Matplotlib (the default Python plotting library; Hunter 2007), Iris and Cartopy were used to generate many of the figures.

To facilitate the reproducibility of the results presented, an accompanying Figshare repository has been created to document the computational methodology (Irving 2015). In addition to a more detailed account (i.e., version numbers, release dates, and web addresses) of the software packages discussed above, the Figshare repository contains a supplementary file for each figure in the paper, outlining the computational steps performed from initial download of the ERA-Interim data through to the final generation of the plot. (A version-controlled repository of the code referred to in those supplementary files can be found at https://github.com/DamienIrving/climate-analysis.)

4. Methods for quantifying planetary wave activity

a. Overview of existing methods

In analyzing SH planetary wave activity (i.e., the ZW1 and/or ZW3 patterns), previous studies have tended to define metrics based on either a stationary pattern or Fourier decomposition. With respect to the former, Raphael (2004) defines a ZW3 index that is essentially the average 500-hPa geopotential height zonal anomaly across three key points (the annual average location of the ridges of the ZW3 pattern in the 500-hPa geopotential height field), while Yuan and Li (2008) use the principal component of the leading empirical orthogonal function (EOF) mode of the surface monthly meridional wind. The stationary nature of these approaches means they cannot fully capture the subtle (approximately 15° of longitude on average) seasonal migration in the phase of the ZW3 (van Loon and Rogers 1984; Mo and White 1985) or the occurrence of patterns whose phase does not approximately coincide with the location of the three analysis points or leading EOF mode.

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Software packages:

- **netCDF Operators. 4.0.8.** April 2011. netCDF Operators Project. *http://sourceforge.net/projects/nco/*
- **Climate Data Operators. 1.5.3.** October 2011. Max Plank Institut fur Meteorologie. Hamburg, Germany. *https://code.zmaw.de/projects/cd*
- **Python. 2.7.10.** May 2015. Python Software Foundation. *https://www.python.org/*
- **Anaconda. 2.0.1.** July 2014. Continuum Analytics. Austin, Texas. *http://docs.continuum.io/anaconda/*
- **NumPy. 1.9.2.** March 2015. NumPy Developers. *http://www.numpy.org/*
- **SciPy. 0.14.0.** May 2014. SciPy Developers. *http://www.scipy.org/scipylib/index.html*
- **xray. 0.5.1.** June 2015. xray Developers. *http://xray.readthedocs.org/en/stable/*
- **windspharm. 1.3.1.** June 2014. Andrew Dawson. *http://ajdawson.github.io/windspharm/*
- **Matplotlib. 1.4.0.** August 2014. Matplotlib Development Team. *http://matplotlib.org/*
- **Iris. 1.8.0.** April 2015. Met Office. Exeter, England. *http://scitools.org.uk/*
- **Cartopy. 0.10.0.** January 2014. Met Office. Exeter, England. *http://scitools.org.uk/*

Operating system:
- **Ubuntu. 12.04.** April 2012. Canonical Ltd. *http://www.ubuntu.com/*

(https://doi.org/10.6084/m9.figshare.1385387.v8)

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3) Log files that outline all computational steps performed (data download / handling –> plot generation) in producing each key result

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EXAMPLE LOG FILE

The following is the log file corresponding to Fig. SB1. It shows every command line entry executed in creating the figure from the initial download of the underlying data to the final generation of the figure. Details regarding the software and code referred to in the log file are provided in the "Example computation section."

```
Tue Jun 30 08:57:37 2015: /
usr/local/anaconda/bin/
python /home/STUDENT/
dbirving/climate-analysis/
visualisation/plot_hilbert.
py/mnt/meteo0/data/simmonds/
dbirving/ERAInterim/data/
va_ERAInterim_500 hPa_030day-
runmean_native.nc va /
mnt/meteo0/data/simmonds/
dbirving/ERAInterim/
data/zw/figures/hilbert_
zw_w19_va_ERAInterim_500
hPa_030day-runmean_native-
55S_1986-05-22_2006-07-29.
png 1 2 --latitude -55
--dates 1986-05-22 2006-07-29
--wavenumbers 1 9 --figure_size
15 6 (Git hash: 1a906a7)

Tue Jun 30 07:35:49 2015: cdo
runmean,30 /mnt/meteo0/data/
simmonds/dbirving/ERAInterim/
data/va_ERAInterim_500
hPa_daily_native.nc /mnt/
meteo0/data/simmonds/
dbirving/ERAInterim/data/
va_ERAInterim_500 hPa_030day-
runmean_native.nc

Wed Mar 18 17:17:14 2015: cdo
mergetime va_ERAInterim_500
hPa_daily-2014-06-01-
to-2014-12-31_native.nc ../
data/va_ERAInterim_500 hPa_
daily_native_orig.nc ../data/
va_ERAInterim_500 hPa_daily_
native.nc

Mon Nov 10 17:15:49 2014:
ncatted -O -a level,va,o,c,500
hPa va_ERAInterim_500 hPa_
daily_native.nc

Mon Nov 10 16:31:05 2014:
ncatted -O -a long_
name,va,o,c,northward_wind
va_ERAInterim_500 hPa_daily_
native.nc

Thu Aug 21 10:57:46 2014:
ncatted -O -a axis,time,c,c,T
va_ERAInterim_500 hPa_daily_
native.nc

Thu Aug 21 10:34:46 2014:
ncrename -O -v v,va va_
ERAInterim_500 hPa_daily_
native.nc

Thu Aug 21 10:26:49
2014: cdo invertlat
-sellonlatbox,0,359.9,-90,90
-daymean va_ERAInterim_500
hPa_6hourly_native.nc va_
ERAInterim_500 hPa_daily_native.
nc

Thu Aug 21 10:14:59
2014: cdo mergetime ../
download/va_ERAInterim_500
hPa_6hourly-1979-1988_
native_unpacked.nc ../
download/va_ERAInterim_500
hPa_6hourly-1989-1998_
native_unpacked.nc ../
download/va_ERAInterim_500
hPa_6hourly-1999-2008_
native_unpacked.nc ../
download/va_ERAInterim_500
hPa_6hourly-2009-2014_native_
unpacked.nc va_ERAInterim_500
hPa_6hourly_native.nc

Thu Aug 21 10:13:35 2014:
ncpdq -P upk va_ERAInterim_500
hPa_6hourly-2009-2014_
native.nc va_ERAInterim_500
hPa_6hourly-2009-2014_native_
unpacked.nc

Wed Aug 20 23:16:22 2014:
Initial download of 6 hourly,
500 hPa meridional wind ERA-
Interim data in 5 or 10 year
chunks (e.g., va_ERAInterim_500
hPa_6hourly-2009-2014_native.
nc) from http://apps.ecmwf.
int/datasets/data/interim-
full-daily/
```

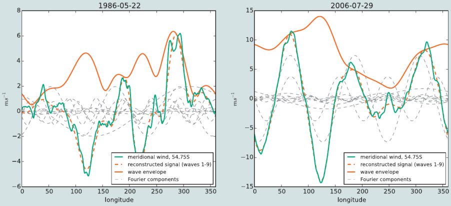

Fig. SB1. Wave envelope of the ERA-Interim, 30-day running mean, 500-hPa meridional wind for 22 May 1986 and 29 Jul 2006 at 54.75°S. See IS2015 for details.

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Author guidelines (set by the journals):

"If computer code is central to any of the paper's major conclusions, then the following is required as a minimum standard:

- 1) A statement describing whether (and where) that code is available and setting out any restrictions on accessibility.
- 2) A high-level description of the software used to execute that code (including citations for any academic papers written to describe that software).
- 3) A supplementary file outlining the precise version of the software packages and operating system used. This information should be presented in the following format: name, version number, release date, institution, and DOI or URL.
- 4) A supplementary log file for each major result (including key figures) listing all computational steps taken from the initial download/attainment of the data to the final result (i.e., the log files describe how the code and software were used to produce the major results).

It is recommended that items 1 and 2 are included in a "computation procedures" (or similarly named) section within the manuscript itself. Any practical issues preventing code sharing will be evaluated by the editors, who reserve the right to decline a paper if important code is unavailable. While not a compulsory requirement, best practice for code sharing involves managing code with a version control system such as Git, Subversion, or Mercurial, which is then linked to a publicly accessible online repository such as GitHub or Bitbucket. In the log files a unique revision number (or hash value) can then be quoted to indicate the precise version of the code repository that was used. Authors are not expected to produce a brand new repository to accompany their paper; an "everyday" repository that also contains code not relevant to the paper is acceptable. Authors should also note that they are not obliged to support reviewers or readers in repeating their computations."

Reviewer guidelines (set by the journals):

"If computer code is central to any of those conclusions, then reviewers should ensure that the authors are compliant with the minimum standards outlined in the author guidelines. *It should be noted that reviewers are not obliged to assess or execute the code associated with a submission. They must simply check that it is adequately documented.*"

Proposed procedure that could enhance reproducibility:

1) Addition of computation section in the article referring to software description, code repository and logs of data processing steps

2) Author and reviewer guidelines by the academic journal