Response to Reviewer #1

We would like to thank the reviewer for taking the time to review our manuscript. We provide our point-by-point responses to the reviewer comments below.

Reviewer comments:

The paper submitted by Ukkola et al. "FluxnetLSM R package (v1.0): A community tool for processing FLUXNET data for use in land surface modelling" presents a tool for the transformation and processing of FLUXNET data in order to make them directly available for LSM. The motivation is for sure important for the promotion of use of multiple data streams in LSM validation. However, the work presented doesn't have any relevant innovative concept or proposal. In fact, despite the import and export functions, change of format to NETCDF, renaming and unit conversions and summary plots (all steps that I don't think limits the use of data in LSM), there are no real innovations. The gapfilling of the meteorological drivers that is proposed (section 2.4.3) is an important step where gaps not filled in the timeseries are merged with the ERA-Interim versions, including the creation of a quality indicator. This activity however, looking to the variables description in FLUXNET available at http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/subset-data-product/, is already done in the FLUXNET product (e.g. from the table in the website TA_F = Air temperature, consolidated from TA_F_MDS and TA_ERA, TA_F_QC = Quality flag for TA_F 0 = measured; 1 = good quality gapfill; 2 = downscaled from ERA). For this reason the paper doesn't have the needed advances, novel concepts, ideas or tools to be considered for publication.

We agree that the gap-filling of meteorological data is an important step in processing eddy covariance data for use in LSMs. The reviewer is correct that the SUBSET product has been gap-filled using 'good-quality' statistical gap-filling and downscaled ERA-Interim data. However, as the FLUXNET documentation (http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/subset-data-product/) states, the SUBSET product contains minimal data quality and uncertainty information. It is suitable for those looking for an off-the-shelf data product, but does not provide the advanced user with the full resources to produce a dataset fit for purpose. The FULLSET product contains additional quality control information for the statistical gap-filling method used in FLUXNET2015 (Reichstein et al., 2005) that is absent in the SUBSET collection. As such, it provides the user with the full flexibility to use statistical and ERA-Interim based gap-filling, as facilitated by our R package. An important advantage of our R package is also the possibility to customise the gap-filling methods and add new methods to suit the user's requirements and datasets in a fully citeable and reproducible framework. We will clarify this in the revised manuscript.

In our experience, the discontinuities, varying data quality and incompatible data standards are real challenges for using flux tower data in LSMs. As many of these limitations are often resolved on an *ad hoc* basis, this hinders the reproducibility and transparency of many LSM studies using eddy covariance data, leads to under-utilisation of these data and wasted effort. Our R package aims to overcome these challenges and create a community standard for processing flux tower datasets. The reviewer indicated that they do not consider these as the main limitations hindering the use of flux tower datasets in LSMs. Unfortunately they do not elaborate what these limitations are in their opinion and we are thus unable to address these reviewer concerns in more detail.

References:

Reichstein, M., Falge, E., Baldocchi, D., Papale, D., Aubinet, M., Berbigier, P., Bernhofer, C., Buchmann, N., Gilmanov, T., Granier, A., Grünwald, T., Havránková, K., Ilvesniemi, H., Janous, D., Knohl, A., Laurila, T., Lohila, A., Loustau, D., Matteucci, G., Meyers, T., Miglietta, F., Ourcival, J. M., Pumpanen, J., Rambal, S., Rotenberg, E., Sanz, M., Tenhunen, J., Seufert, G., Vaccari, F., Vesala, T., Yakir, D. and Valentini, R.: On the separation of net ecosystem exchange into assimilation and ecosystem respiration: Review and improved algorithm, Glob. Chang. Biol., 11, 1424–1439, doi:10.1111/j.1365-2486.2005.001002.x, 2005.

Response to Reviewer #2

We would like to thank the reviewer for their helpful comments on our manuscript. In light of the reviewer comments, we propose to include several improvements to the package to provide a more flexible and generalised framework. These include providing:

1) Additional statistical gap-filling methods. The package currently gap-fills forcing variables using ERA-Interim estimates. The new statistical methods (such as linear interpolation or synthesis methods; Abramowitz et al., 2012) will allow the package to be applied to datasets for which ERA-Interim (or similar) estimates are not available and can be used to gap-fill both forcing and evaluation variables. See section 2.4.3 of the revised manuscript.

2) A model-specific look-up table for outputting site vegetation type as a plant functional type in addition to the IGBP vegetation type currently provided by the package. See section 2.3 of the revised manuscript.

3) An option to aggregate the data to a different output time step (e.g. daily). See section 2.4.5 of the revised manuscript.

4) The ability to use the package to also process the La Thuile Synthesis Dataset (http://fluxnet.fluxdata.org/data/la-thuile-dataset/). This dataset precedes the FLUXNET2015 data release that the R package is designed for but includes additional sites and may thus be the preferred dataset for some users.

We hope these will further enhance the utility of the package and provide for a wider range of applications. Below we address each of the reviewer comments in more detail.

General comments:

Ukkola et al. document an R package to convert FLUXNET data into forcing data for land surface models. This tool might be useful for all land surface models and may lead to more frequent use of FLUXNET data for model evaluation. As the general steps described here are necessary for using FLUXNET data for any land surface model, this can develop into a frequently cited reference. Reading data files, converting the units and writing them into netcdf is however not a big issue for most scientists. I therefore have some suggestions that could generalize the package more and hopefully lead to a more frequent use of the package.

1) the authors convert the driving data with respect to the units. It might also be useful to provide aggregation to different time steps, not all land surface models use the same time step in their forcing.

We thank the reviewer for this suggestion and agree that it would be useful to provide the option to aggregate the forcing data to a different time step. The package currently outputs the data at the same time step as the flux tower data is provided in but we have added an option to customise the time step in the revised package up to a daily resolution:

"By default, the package outputs the data in its original time resolution. However, a longer time step may be desired for some model applications. The package allows the aggregation of the data to up to a daily resolution. The aggregated time step size (in hours) is set by the argument aggregate and can be any number between the original resolution (usually 30 minutes) and 24 hours (daily), as long as it is divisible by 24 to allow a regular number of time steps to be aggregated. If any of the time steps being aggregated are missing, the new coarser time step will also be set to missing. The QC flags (if outputted) are assigned a fraction between 0-1, indicating the percentage of time steps used for aggregation that were observed."

2) The authors only mention that they include the IGBP vegetation classification. Many models however use plant functional types. For the package to be applicable in this respect for most land surface models a conversion to plant functional types would be necessary.

We acknowledge the reviewer's point that a conversion to plant functional types (PFT) may be necessary for other modelling groups. We have therefore added a new functionality to the package to output the vegetation type as a PFT.

As the PFTs used vary between individual models, we do not wish to provide an automated translation between the IGBP vegetation types and PFTs. The IGBP classification also does not distinguish between common model PFT types, such as C_3 and C_4 grass. Moreover, the choice of vegetation type for each site is model specific and at times a subjective choice. For example, a savanna site, such as Howard Springs, could be modelled as a C_4 grass, an evergreen broadleaf tree, or a combination of both PFTs depending on the model configuration and application (De Kauwe et al., 2015; Whitley et al., 2016).

To overcome these challenges, we will provide a model-specific look-up table for PFTs for each site, with the PFT type nominated by the user. This will be integrated with the site metadata file currently provided with the package (P5 L13). This will provide the user with flexibility to set each site's PFT to suit their model and application:

"This processing step connects key site metadata directly to each model forcing files. It can be extended to include additional metadata, such as site soil or vegetation properties, with minimal code modifications. For example, LSMs generally use plant functional types (PFT) instead of the International Geosphere-Biosphere Programme (IGBP; http://www.igbp.net/) vegetation types automatically retrieved by the package (Poulter et al., 2011). An example is provided for writing the PFT type for the CABLE LSM (Wang et al., 2011) and can be invoked by setting the model argument to the desired model name. Full instructions for adding model-specific parameters are provided in the package README file."

3) It would be interesting to check whether the unit conversion that is applied here is the one required for other models. The authors could gather a list with units for the most widely used land surface models and check whether additional unit conversions are necessary, and if so extend the package accordingly.

Our package uses the ALMA (Assistance for Land surface Modelling Activities; http://www.lmd.jussieu.fr/~polcher/ALMA/) convention. This has been the standard for land surface models since the mid-1990s (Polcher and Shao, 1996) and has been used for a number of model intercomparison projects, such as PILPS (Project for Intercomparison of Land surface Parameterisation Schemes; Lettenmaier, 2003; Polcher and Shao, 1996), and more recently PLUMBER (The Protocol for the Analysis of Land Surface Models (PALS) Land Surface Model Benchmarking Evaluation Project; Best et al., 2015) and GSWP3 (Global Surface Wetness Project Phase 3; http://hydro.iis.u-tokyo.ac.jp/GSWP3/). The outputs are also CF (Climate and Forecast) compliant. This is the prevailing metadata convention used across the climate science and forecasting community (http://cfconventions.org/). We recognise that some models (e.g. JULES) use a different format, but developing a package that accounts for every eventuality is not feasible. Instead what we have done is develop a generic community tool that could be easily adapted to a specific scenario (e.g. a model not compatible with ALMA or NetCDF). We are of course willing to work with individual groups, helping where possible.

We would also like to note that the output variable names are fully customisable and need not comply with those used in ALMA (as detailed on P6 L5). While only ALMA unit conversions are currently provided, addition of new conversions to the package is trivial. We will provide instructions for this in the package README file (https://github.com/aukkola/FluxnetLSM).

Specific comments:

p.2, l. 16-26: I think it would be good to distinguish between the forcing data and the flux measurements used to evaluate the model. The flux measurements do not necessarily need to be gapfilled if the model is compared with these data in high temporal resolution. Then you can simply only use the datapoints that were measured. Of course if you want to evaluate the annual sum the fluxes also need gapfilling.

The flux measurements are not currently gap-filled by the package. Only meteorological variables are gap-filled using ERA-Interim estimates (if this option is chosen by the user). We have added additional statistical gap-filling functions to the package that do not rely on ERA-Interim data to give the user the option to also gap-fill flux variables (see point 1) above). A number of gap-filling options (such as linear interpolation, copy-fill and synthesis based on other variables) are already provided in the PALS R package and have been integrated with the new package (see section 2.4.3 of the revised manuscript).

p.2 l. 35: what are Tier 1 sites?

The Fluxnet2015 data release has two data tiers with different data usage policies. The Tier 1 sites are those with an open data policy and are thus likely to be those used by the majority of users. We have clarified this in the revised manuscript (P2 L39).

p.3 l.21: is there any reference for this R package?

We have removed dependency on the PALS R package after identifying difficulties installing this package. Required PALS functions are now replicated in the FluxnetLSM package.

p.3 l. 22: "encourages screening of flux tower sites for model applications", what do you mean ? can you be more specific what this screening does?

The flux tower data have been gap-filled to various degrees and may have missing data periods. In many circumstances, these are not desirable for modelling applications. Our package provides an automated method for screening gap-filled and missing data. However, this may not detect all data periods and/or sites that are not desired in a particular application. The diagnostic plots generated by the package provide a final quality control step to complement the automated screening to verify that the data are realistic and as expected. For example, this will allow the user to check the magnitude and nature of variability of particular variables. We have clarified this in the revised manuscript:

"This facilitates the detection of data periods with unusual variability or variables exhibiting unusual magnitudes"

p.3 l. 26-30: please be more precise: "encourages better documentation", basically this paper is the documentation of the methods, right?

What we intended to say is that the use of the package will allow the data processing methods to be fully reproducible (by including as much metadata as possible in the data files, as well as metadata about the processing used to generate the files) and easily documented in a manuscript. We have clarified this in the revised manuscript.

"The package offers a useful tool for post-processing eddy covariance datasets for modelling applications and simplifies rigorous documentation of data processing methods in LSM studies to enhance their reproducibility. Specifically, future studies using these data would be able to explicitly demonstrate how the data were used, gap-filled, quality controlled and so on, and this could be reproduced by other users."

p.7, l. 30: please include all variables that are not gap filled.

We have named all variables that are not gap-filled in the revised manuscript.

p.10, l. 30: did you verify that the format is really directly usable by (many) LSMs? Formats might differ considerably between different models.

Our package uses the ALMA convention. This has been the standard format for the land surface modelling since the mid-1990s (Polcher and Shao, 1996) and has been used in several previous model intercomparison studies. See our response to reviewer comment #3 above for full details.

p.11, l.1: what are these specific applications?

The applications can range from model evaluation studies to addressing scientific questions using models at the site scales. For example, the user may wish to process the data differently if interested in evaluating models during short-term phenomena (such as heat waves) as opposed to longer seasonal to annual scales. We have clarified this in the revised manuscript.

"Simultaneously, it provides optional settings for an advanced user to produce flux tower datasets suited for specific applications. For example, the user may wish to process the data differently if interested in evaluating models during short-term phenomena (such as heat waves) compared to longer seasonal to annual scales."

Reference: Poulter, B., Ciais, P., Hodson, E., Lischke, H., Maignan, F., Plummer, S., and Zimmermann, N. E.: Plant functional type mapping for earth system models, Geosci. Model Dev., 4, 993-1010, doi:10.5194/gmd-4-993-2011, 2011.

References:

Abramowitz, G.: Towards a public, standardized, diagnostic benchmarking system for land surface models, Geosci. Model Dev., 5, 819–827, doi:10.5194/gmd-5-819-2012, 2012.

Abramowitz, G., Pouyanné, L. and Ajami, H.: On the information content of surface meteorology for downward atmospheric long-wave radiation synthesis, Geophys. Res. Lett., 39, 1–5, doi:10.1029/2011GL050726, 2012.

Best, M. J., Abramowitz, G., Johnson, H. R., Pitman, A. J., Balsamo, G., Boone, A., Cuntz, M., Decharme, B., Dirmeyer, P. A., Dong, J., Ek, M., Guo, Z., Haverd, V., van den Hurk, B. J. ., Nearing, G. S., Pak, B., Peters-Lidard, C., Santanello, J. A., Stevens, L. and Vuichard, N.: The plumbing of land surface models: benchmarking model performance, J. Hydrometeorol., 16, 1425–1442, doi:10.1175/JHM-D-14-0158.1, 2015.

De Kauwe, M. G., Kala, J., Lin, Y.-S., Pitman, A. J., Medlyn, B. E., Duursma, R. A., Abramowitz, G., Wang, Y.-P. and Miralles, D. G.: A test of an optimal stomatal conductance scheme within the CABLE land surface model, Geosci. Model Dev., 8, 431–452, doi:10.5194/gmd-8-431-2015, 2015.

Lettenmaier, D. P.: Preface, Glob. Planet. Change, 38, vii–ix, doi:10.1016/S0921-8181(03)00002-X, 2003.

Polcher, J. and Shao, Y.: A standard format for reporting PILPS experiments, Glob. Planet. Change, 13, 217–223, doi:10.1016/0921-8181(95)00047-X, 1996.

Whitley, R., Beringer, J., Hutley, L., Abramowitz, G., De Kauwe, M. G., Duursma, R., Evans, B., Haverd, V., Li, L., Ryu, Y., Smith, B., Wang, Y.-P., Williams, M. and Yu, Q.: A model inter-comparison study to examine limiting factors in modelling Australian tropical savannas, Biogeosciences, 13, 3245–3265, doi:10.5194/bgd-12-18999-2015, 2016.

Manuscript with track changes:

FluxnetLSM R package (v1.0): A community tool for processing FLUXNET data for use in land surface modelling

Anna M. Ukkola[1,3], Ned Haughton[1], Martin G. De Kauwe[2], Gab Abramowitz[1,3], Andy J. Pitman[1,3]

[1]ARC Centre of Excellence for Climate System Science, University of New South Wales, Sydney, NSW 2052, Australia
[2]Macquarie University, Sydney, NSW 2109, Australia
[3]Climate Change Research Centre, University of New South Wales, Sydney, NSW 2052, Australia

Correspondence to: A. M. Ukkola (a.ukkola@unsw.edu.au)

Abstract. Flux towers measure ecosystem-scale surface-atmosphere exchanges of energy, carbon dioxide and water vapour. The network of flux towers now encompasses ~900 sites, spread across every continent. Consequently, these data have become an essential benchmarking tool for land surface models (LSMs). However, these data as released are not immediately usable for driving, evaluating and benchmarking LSMs. Flux tower data must first be transformed into a LSM-readable file format, a process which involves changing units, screening missing data and varying degrees of additional gap-filling. All of this often leads to an under-utilisation of these data in model benchmarking. To resolve some of these issues, and to help make flux tower measurements more widely used, we present a reproducible, open-source R package that transforms the FLUXNET2015 and La Thuile data releases into community standard NetCDF files that are directly usable by LSMs. We note these data would also be useful for any other user or community seeking to independently quality control, gap fill or use the FLUXNET data.

1 Introduction

Land surface models (LSMs) provide the lower boundary condition for climate and weather forecast models, simulating the exchange of carbon, water and energy fluxes between the soil, vegetation and the atmosphere (Pitman, 2003). Flux towers measure ecosystem-scale exchanges of carbon dioxide, water vapour fluxes and energy (Baldocchi, 2014) and have proven invaluable for LSM evaluation and benchmarking (Abramowitz et al., 2008; Best et al., 2015; Blyth et al., 2010; Haughton et al., 2016; Luo et al., 2012; Williams et al., 2009). Flux towers are particularly useful for modelling applications as they provide simultaneous observations of the meteorological data needed for forcing offline models as well as the key ecosystem variables against which models may be evaluated (e.g. sensible and latent heat) at time intervals similar to those used by LSMs, often over multiple years. As such, they are ideal for characterising the interactions between climate and ecosystem processes and allow the evaluation of LSMs over time periods ranging from sub-daily through to seasonal and inter-annual time scales (e.g. Blyth et al., 2010; Bonan et al., 2011; Mahecha et al., 2010; Matheny et al., 2014; Powell et al., 2013; Ukkola et al., 2016; Wang et al., 2011; Whitley et al., 2016). The investment in flux tower measurements is considerable and there are multiple benefits to these data being more widely used. First, the use of these data for LSM evaluation and benchmarking helps realise the value of existing investments. Second, where flux tower measurements identify biases in how LSMs represent processes, the potential exists to improve how well these models simulate the surface energy, water and carbon balances. Since LSMs are central to the simulation of key phenomena including droughts, water resource availability, carbon storage and feedbacks on heatwaves this has direct policy implications. Thirdly, greater use of flux tower measurements by the LSM and climate science community could help with the argument in support of on-going resourcing of flux tower measurements. In short, the effective and widespread use of flux tower measurements is beneficial across the science and policy communities.

Before data from flux tower sites can be used in models they commonly require significant pre-processing. In principle, flux towers provide near-continuous observations of ecosystem fluxes but, in practice, the measurements often include discontinuities due to instrument failure or unfavourable weather conditions (Reichstein et al., 2005). As LSMs must be provided with continuous meteorological forcing data, flux tower datasets require varying degrees of gap-filling of missing time steps. This also poses challenges for using these data for model evaluation and benchmarking. Ideally, models should be evaluated against high-quality observations. Due to data gaps, as well as measurement biases (e.g. Leuning et al., 2012), flux tower measurements do not provide reliable observations representative of the true ecosystem dynamics in all circumstances. Arguably therefore, the full breadth of flux tower data available across the entire network is unlikely to be suitable to the role of evaluating LSMs.

FLUXNET, an international network of flux tower sites, comprises of >900 sites globally (http://fluxnet.fluxdata.org/). The latest FLUXNET data release (FLUXNET2015; http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/) provides flux tower measurements for 212 sites. It was preceded by the La Thuile Synthesis Dataset (http://fluxnet.fluxdata.org/data/la-thuile-dataset/), which comprises of 252 flux tower sites, 141 of which are not currently available in FLUXNET2015. The available data overcome some of the limitations of raw eddy covariance measurements through significant post-processing and gap-filling. Despite this, these datasets cannot be employed directly by

LSMs. Critically, not all FLUXNET data releases are provided with temporally continuous observations of all essential meteorological variables (e.g. precipitation and wind speed) for forcing LSMs. For example, across 155 FLUXNET2015 "FULLSET" open data policy (Tier 1) sites reporting half-hourly observations, nearly all sites include gaps in rainfall and 77% of the sites have missing air temperature observations with up to 61% (median 5%) of the time series missing despite this variable being nominally gap-filled. Further, evaluation variables, such as latent and sensible heat, are generally gap-filled but to vastly different extents depending on the site and variable. For example, between 0% and 89% (median 31%) of the latent heat time series and 0% and 83% (median 25%) of the sensible heat time series have been gap-filled across the 155 sites. This poses a challenge for utilising these data for LSM applications and additional post-processing is necessary. A specific concern is that individual land surface modellers are very likely to post-process flux data in different ways, with different assumptions and varying levels of acceptance on how many gaps represent a worthwhile data set. When the gap-filled data are subsequently used and published, the detail of how all the possibilities around post-processing the data are resolved is rarely fully documented. This leads to difficulties in interpreting model evaluation studies, a lack of reproducibility and, given many groups process data individually, wasted effort.

In an effort to resolve some of these problems and to connect the flux tower researchers with the LSM researchers more strongly, we present the R package "`FluxnetLSM`" to facilitate the processing of FLUXNET datasets for use in LSMs. The package serves several important functions. Firstly, it enables the creation of fully gap-filled meteorological forcing datasets for running LSMs. Past studies have relied on various (often ad-hoc) gap-filling methods that are rarely fully documented in the literature. Worryingly, it would be virtually impossible to reproduce many existing LSM evaluation and benchmarking studies although we note some exceptions (Best et al., 2015). The R package provides a community tool for creating LSM forcing datasets in a fully citeable and reproducible framework. Secondly, the package assists with the quality controlling of the data. It enables the selection of good-quality measurement periods and sites through automated screening of heavily gap-filled or missing data periods according to user-defined thresholds. To complement the automated quality controlling, the package also provides tools for creating diagnostic plots to visualise output data periods. This facilitates the detection of data periods with unusual variability or variables exhibiting unusual magnitudes. Finally, the package converts the flux tower data into the community standard NetCDF format used by the climate modelling and LSM community and collates metadata on data variables, flux tower sites as well as processing steps in the output files.

The package offers a useful tool for post-processing eddy covariance datasets for modelling applications and simplifies rigorous documentation of data processing methods in LSM studies to enhance their reproducibility. Specifically, future studies using these data would be able to explicitly demonstrate how the data were used, gap-filled, quality controlled and so on, and this could be reproduced by other users. In the following sections, we describe the different functionalities of the package.

Anna Ukkola 18/7/2017 1:31 PM
Deleted: using the Protocol for the Analysis of Land Surface models (PALS) R package.

Anna Ukkola 18/7/2017 1:31 PM
Deleted: and encourages screening of flux tower sites for model applications.

2 Package description

The `FluxnetLSM` package (v1.0) was developed to serve as a community tool to facilitate the use of flux tower measurements in LSMs. It is written in the open-source R language (https://www.r-project.org/) and is freely accessible in a version-controlled repository (see Code Availability for full details). Instructions for installation are provided in the following section.

The package has two processing streams: the collection of site metadata and processing of high frequency temporally varying variables. These are described in sections 2.3 and 2.4, respectively. The package outputs a separate NetCDF file for meteorological and evaluation variables, with metadata stored in each file. Additionally, a log file is produced detailing output file names, potential warnings and errors. The package also provides the option to produce diagnostic plots for further data exploration. Figure 1 illustrates the general workflow with each component described in detail below.

2.1 Installation and requirements

`FluxnetLSM` requires R version ≥3.1.0. It relies on base R functions as well as three additional packages: `R.utils`, `ncdf4` and `rvest`. These packages should be installed prior to the installation of `FluxnetLSM`. The `devtools` package is also recommended to aid installation.

The `R.utils`, `ncdf4`, `rvest` and `devtools` packages can be installed directly in R with the command `install.packages("package_name")`. The `FluxnetLSM` package can be downloaded from the Github repository at https://github.com/aukkola/FluxnetLSM and installed within R by typing:

```
devtools::install_github("aukkola/FluxnetLSM")
```

Alternative installation methods are provided in the package github repository. After installation, the `FluxnetLSM` package can be loaded into the R session by typing `library(FluxnetLSM)`. Other required packages are loaded automatically by the `FluxnetLSM` package.

2.2 Running FluxnetLSM

The package is run by invoking a single R function called `convert_fluxnet_to_netcdf`:

```
convert_fluxnet_to_netcdf(site_code, infile, era_file=NA, out_path,
                          conv_opts=get_default_conversion_options(),
                          plot=c("annual", "diurnal", "timeseries"),
                          ...)
```

Anna Ukkola 18/7/2017 1:31 PM
Deleted: The Protocol for the Analysis of Land Surface Models (`pals`) R package can be obtained from the Github repository at https://github.com/dudek313/palsR and installed in R with the command: ... [1]

The user must set three arguments (`infile`, `site_code` and `out_path`), with all other arguments being optional. Each argument and its default value is described in Table 1 and discussed in detail in the following sections. A full example for usage is provided in Section 3. Three example scripts are also provided with the package and are stored in `examples/FLUXNET2015` and `examples/LaThuile` for the FLUXNET2015 and La Thuile data releases, respectively. In each directory, the `example_conversion_single_site.R` file shows an example for processing a single site. The `example_conversion_multiple_sites.R` and `example_conversion_multiple_sites_parallel.R` files show an example for processing multiple sites using serial and parallel programming, respectively.

2.3 Collation of site metadata

The package collates metadata on the flux tower sites and stores these as attributes in the output NetCDF files. These include information required for modelling such as site coordinates, elevation and vegetation type. The primary source for metadata is a site attribute file provided with the package (stored in `data/Site_metadata.csv`). This file includes metadata detailed in Table 2 for the Tier 1 sites of the FLUXNET2015 November 2016 release (see http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/ for more information). The metadata were collated by the code developers from the site information provided on the FLUXNET website as well as individual flux tower network websites (see `data/README.md` for full details). The metadata file can be edited by the user to include additional sites or to modify existing data. The code first extracts site metadata from the CSV file. If any metadata cannot be found in the provided file, the code attempts to retrieve missing metadata from the FLUXNET website (http://fluxnet.fluxdata.org), followed by the Oak Ridge National Laboratory (ORNL) FLUXNET website (https://fluxnet.ornl.gov/) by using functions for reading html webpages provided in the `rvest` library.

Additionally, the code stores the dataset name and version (as set by the `datasetname` and `datasetversion` arguments to the main function), as well as the processing options, time and date as attributes in the output files. The code also calculates the mean annual precipitation for the output period when precipitation is outputted. It is stored as an attribute in the meteorological output file and can be useful particularly for rescaling precipitation for LSM spin-up so that each year's precipitation during the spin-up matches the site average.

This processing step connects key site metadata directly to each model forcing files. It can be extended to include additional metadata, such as site soil or vegetation properties, with minimal code modifications. For example, LSMs generally use plant functional types (PFT) instead of the International Geosphere-Biosphere Programme (IGBP; http://www.igbp.net/) vegetation types automatically retrieved by the package (Poulter et al., 2011). An example is provided for writing the PFT type for the CABLE LSM (Wang et al., 2011) and can be invoked by setting the `model` argument to the desired model name. Full instructions for adding model-specific parameters are provided in the package README file.

2.4 Processing of high frequency data variables

2.4.1 Output variables

The package is supplied with a suggested list of output variables that will be processed by the package for each site, where available. Separate lists are provided for FLUXNET2015 FULLSET and SUBSET, and La Thuile data releases due to different naming conventions and variables (stored in `data/Output_variables_FLUXNET2015_FULLSET.csv`, `data/Output_variables_FLUXNET2015_SUBSET.csv` and `data/Output_variables_LaThuile.csv`, respectively) The output variables are categorised as meteorological or evaluation variables, and a separate NetCDF output file is produced for each category. Where possible, the output variables are named using the Assistance for Land-surface Modelling Activities (ALMA) convention (http://www.lmd.jussieu.fr/~polcher/ALMA/convention_output_3.html) commonly employed by LSMs. The package also performs common unit conversions between the original FLUXNET and ALMA convention units (see section 4.4). The output variables are fully customisable according to user requirements by removing or adding variables to the output variable list. The information required for each output variable is shown in Table 3.

2.4.1.1 Meteorological variables

The meteorological variables include the data variables typically required to force LSMs. The meteorological variables processed by the package by default are detailed in Supplementary Table 1. The user can also nominate essential meteorological variables that must be available and processed by modifying the `Essential_met` field in the output variable list (see Table 3). By default, these include air temperature, downward shortwave radiation (or photosynthetically active radiation), vapour pressure deficit, precipitation and wind speed. If any of these variables are not provided in the input data file, the code will terminate and the site will not be processed. The code provides several options for gap-filling meteorological variables if required (see Section 2.4.3 for details).

2.4.1.2 Evaluation variables

The evaluation variables include the data variables typically predicted by land surface models and used to evaluate model outputs. The default evaluation variables processed by the package are provided in Supplementary Table 2. The user can nominate preferred evaluation variables by modifying the `Preferred_eval` field in the output variable list (see Table 3). By default these include net radiation, latent (LE) and sensible (H) heat and net ecosystem exchange (NEE). If none of the preferred variables are available in the input data file, the site will not be processed. The evaluation variables can be gap-filled by the package using statistical methods (Section 2.4.3).

In addition to common evaluation variables, the package also processes and outputs uncertainty estimates provided with the FLUXNET2015 release by default. These include uncertainty bounds for LE, H and NEE, as well as error estimates for gross primary productivity (GPP). Several estimates for NEE and GPP are also included to reflect the inherent uncertainties in deriving these variables from eddy covariance data (Papale et al., 2006; Reichstein et al., 2005; Supplementary Table 2).

2.4.2 Gap-filled and missing values

The code produces NetCDF files with whole years of data only, to ensure LSM automated spin-up procedures remain relatively unbiased. It determines which years are included in its output according to user-defined thresholds for gap-filled and missing values as detailed below.

A threshold must be set for the maximum percentage of missing values per year (argument `missing`, 15% by default). The code checks for the percentage of missing values for each data variable during each year. If *any* essential meteorological variables or *all* preferred evaluation variables have missing values in excess of this threshold, the year is not processed.

Additionally, thresholds can be set for the maximum percentage of all gap-filling (default option; set by argument `gapfill_all` using 20% as the default) or separately for "good", "medium" and "poor" quality gap-filling (arguments `gapfill_good`, `gapfill_med` and `gapfill_poor`, respectively; see section 4.3). The percentage of gap-filled values is then checked for each data variable with a corresponding quality control flag during each year. If *any* essential meteorological variable or *all* preferred evaluation variables include gap-filled values in excess of the threshold(s), the year is not processed. Note the November 2016 FLUXNET2015 release has gaps in quality control flags for latent and sensible heat variables even when data are present. A fix has been provided (http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/known-issues/) but if not implemented, the data quality cannot be ascertained from the flags (D. Papale, pers. comm.) and is treated by the package as poor-quality gap-filling.

If a threshold for gap-filling is set, the percentage of both gap-filled and missing values must not exceed their respective thresholds for a year to be processed. If no years fulfilling the criteria are found, or the time period is shorter than the user-defined minimum number of consecutive years (set by argument `min_yrs`, by default 2 years), the site it not processed. If several, non-consecutive, time periods fulfilling the criteria are found, these are written to separate output files.

Provided that at least one evaluation variable has fewer gaps than the user-defined thresholds, all evaluation variables are written to the output file by default, with the exception of any variables that

Anna Ukkola 18/7/2017 1:31 PM
Deleted: (Papale et al., 2006; Reichstein et al., 2005; Supplementary Table 2)

Anna Ukkola 18/7/2017 1:31 PM
Formatted: English (UK)

Anna Ukkola 18/7/2017 1:31 PM
Deleted: some evaluation

Anna Ukkola 18/7/2017 1:31 PM
Formatted: English (UK)

Anna Ukkola 18/7/2017 1:31 PM
Deleted: In this case,

Anna Ukkola 18/7/2017 1:31 PM
Formatted: English (UK)

Anna Ukkola 18/7/2017 1:31 PM
Formatted: English (UK)

only contain missing values. An option is provided to discard any evaluation variables with gaps exceeding the user-defined thresholds by setting the argument `include_all_eval` to `FALSE`.

2.4.3 Gap-filling variables

LSMs require continuous forcing data, but a number of essential meteorological variables (rainfall, wind speed, incoming longwave radiation and air pressure) are not fully gap-filled in the FLUXNET2015 "FULLSET" and/or La Thuile releases. The package provides two methods for gap-filling meteorological variables: statistical and ERA-Interim (Dee et al., 2011; Vuichard and Papale, 2015). Additionally, statistical methods are provided for gap-filling evaluation variables.

2.4.3.1. ERA-Interim –based gap-filling

Downscaled ERA-Interim reanalysis estimates are provided as part of the FLUXNET2015 dataset for gap-filling meteorological variables. These are available only in the "FULLSET" version of the FLUXNET2015 release (http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/fullset-data-product/), whereas the "SUBSET" version of the dataset has already been gap-filled using ERA-Interim but offers the user less flexibility for controlling for gap-filling quality (with missing, medium- and poor-quality gapfilled time steps readily gapfilled with ERA-Interim).

This gapfilling option is chosen by setting the argument `met_gapfill` to "ERAinterim" and by providing the name of the ERAinterim input file to argument `era_file`. The ERA-Interim variable corresponding to each meteorological variable is set in the output variable list (`ERAinterim_variable` field; Table 2). If an ERA-Interim estimate is available for a given variable, the code gap-fills any missing time steps with the corresponding ERA-Interim data value. The package saves information on the gap-filled time steps in quality control flag variables (see Section 2.4.4 for details).

2.4.3.2 Statistical gap-filling

Alternatively, meteorological, as well as evaluation, variables can be gap-filled using statistical methods using a combination of methods depending on the length of missing periods. This gap-filling option can be chosen for meteorological and evaluation variables by setting arguments `met_gapfill` and `flux_gapfill` to "statistical", respectively.

Surface air pressure and incoming longwave radiation are synthesised using empirical functions (Abramowitz et al., 2012). Air pressure is calculated from air temperature and elevation using the barometric formula as detailed in Supplementary Section S.1.1. Three methods for synthesising longwave radiation are provided ("Abramowitz_2012", "Swinbank_1963" and "Brutsaert_1975") and are set by the argument `lwdown_method`. "Swinbank_1962" calculates longwave radiation based on air temperature, whereas "Abramowitz_2012" (default) and "Brutsaert_1975" calculate it from air temperature and relative humidity. Each of these methods is detailed in Supplementary Section S.1.2.

For all other meteorological and evaluation variables, short data gaps (by default up to 4 hours, set by argument `linfill`) are first gap-filled using linear interpolation between the previous and next available time steps. This prevents the introduction of abrupt variations, but leads to a loss of some subdiurnal variability.

For meteorological variables, longer gaps (by default up to 10 days, set by argument `copyfill`) are then gap-filled by taking the average of the corresponding time steps during other years (Blyth et al., 2010). Data gaps that are longer than set by `copyfill` are not gap-filled due to the limitations of statistical gap-filling for stochastic variables, such as rainfall.

For evaluation variables, longer gaps (by default up to 30 days, set by argument `regfill`) are gap-filled using a linear regression of each evaluation variable against one or several meteorological variables (adapted from Best et al., 2015). When incoming shortwave radiation, air temperature and humidity (relative humidity or vapour pressure deficit) are available, the code will perform a multiple linear regression against these variables. Else, if only shortwave radiation is available, a linear regression against this variable is performed. All available time steps are used to construct a linear regression model separately for day- and night-time (using incoming solar radiation of 5 W m^{-2} as the day-night threshold; Abramowitz et al., 2012). The linear regression models are then used to predict missing values at each time step. If none of the meteorological variables are available, or data gaps are longer than set by `regfill`, the evaluation variables are not gap-filled. If `copyfill` is preferred over `regfill`, the code will default to this option if `regfill` is set to `NA`.

After performing the gap-filling, the code checks for missing values (as per Section 2.4.2). If missing values remain in *any* essential meteorological variables or *all* preferred evaluation variables at a given year, the year is removed from the outputs. If the remaining time period is shorter than the user-defined minimum number of consecutive years, the site is not processed.

2.4.4 Quality control flags

The code retains and outputs the original FLUXNET quality control (QC) flags, when these are included in the output variable list. These flags are set to 0 for measured data, and 1, 2 and 3 for good, medium and poor quality gap-filling, respectively, for La Thuile and FLUXNET2015 "FULLSET" data (Reichstein et al., 2005; http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/). FLUXNET2015 "SUBSET" QC flags are as per "FULLSET" for measured and good-quality gapfilled data, with flags set to 2 for ERA-Interim gapfilled time steps.

Additionally, the code produces QC flags for meteorological variables when they are gap-filled using ERA-Interim data or statistical methods. The QC flag is set to 4 when a time step is gap-filled with ERA-Interim data and 5 for statistical gap-filling. If a QC flag does not exist for a given variable, the code creates a QC flag variable with measured time steps set to 0 and ERA-Interim or statistically gap-filled time steps set to 4 or 5, respectively. This flag is automatically stored as a variable in the meteorological data output file and is named as the output variable plus the extension "_qc" (e.g. Precip_qc). See below for QC flag conventions when aggregating data to coarser time steps.

2.4.5 Aggregation to coarser time steps

By default, the package outputs the data in its original time resolution. However, a longer time step may be desired for some model applications. The package allows the aggregation of the data to up to a daily resolution. The aggregated time step size (in hours) is set by the argument `aggregate` and can be any number between the original resolution (usually 30 minutes) and 24 hours (daily), as long as it is divisible by 24 to allow a regular number of time steps to be aggregated. If any of the time steps being aggregated are missing, the new coarser time step will also be set to missing. The QC flags (if outputted) are assigned a fraction between 0-1, indicating the percentage of time steps used for aggregation that were observed.

2.4.6 Unit conversions

The package uses ALMA convention units for outputs by default where possible (as indicated in Supplementary Tables 1 and 2). These differ from the original FLUXNET units for a number of variables and a conversion is performed in each case. Available conversions are detailed in Table 4. If a conversion is not available for the specified units, the code will produce an error and terminate. Additionally, the package provides functions for converting i) vapour pressure deficit to relative humidity, ii) relative humidity to specific humidity and iii) photosynthetically active radiation (PAR) to incoming shortwave radiation (SW_{down}).

For these conversions, saturated vapour pressure (e_{sat}) is first calculated from air temperature (T_{air}; °C) (Jones, 1992) at each time step as

$$e_{sat} = 613.75 * \exp[17.502 * T_{air} / (240.97 + T_{air})] \quad (1)$$

Relative humidity (R_h; %) is then determined from e_{sat} and vapour pressure deficit (D; Pa) as

$$R_h = 100 * (1 - (D * 100) / e_{sat}) \quad (2)$$

To calculate specific humidity (Q_{air}; kg kg^{-1}), specific humidity at saturation (w_s; kg kg^{-1}) is derived from e_{sat} and air pressure (ρ_{air}; Pa) as

$$w_s = 0.622 * e_{sat} / (\rho_{air} - e_{sat}) \quad (3)$$

Q_{air} is then calculated as

$$Q_{air} = (R_h / 100) * w_s \quad (4)$$

PAR (µmol m^{-2} s^{-1}) is converted to SWdown (W m^{-2}) following Monteith and Unsworth (1990):

$$SW_{down} = PAR * (1/2.3) \quad (5)$$

Negative PAR values are set to 2.17 W m^{-2} (equivalent to 5 µmol m^{-2} s^{-1}) to avoid problems forcing LSMs with negative SW_{down}.

2.4.7 Visualisation of outputs

The package provides an option to visualise outputs variables. Three types of plots can be produced: a mean annual cycle, a mean diurnal cycle by season and a time series figure. This is controlled by the argument `plot` that can be set to any combination of `annual`, `diurnal` and `timeseries` for the three plot options, respectively. Examples of each plot are provided in Figure 2.

The outputs are retrieved from the output NetCDF files and all data variables are plotted with separate figures produced for meteorological and evaluation variables. Any missing values are ignored during plotting, but their presence is noted in the figure, when applicable. The data are plotted in their output units, with the exception of air temperature (converted from Kelvin to Celsius) and rainfall (converted from mm/s to mm/time step). It is envisaged the plots will complement the automated quality control performed during data processing and enable further detection of unsuitable data periods or sites.

3 Example application

Here we present an example application using "FluxnetLSM" for processing FLUXNET2015 "FULLSET" data at the Howard Springs (Australia) flux tower site. This example is provided in full with the package and stored in `examples/FLUXNET2015/example_conversion_single_site.R`. It is also reproduced in Supplementary section S.2 for convenience. Meteorological data is gap-filled using ERA-Interim estimates in this example but this functionality can be disabled if desired by setting `met_gapfill` argument to NA (see below). The user must provide four inputs, with the following inputs used in this example:

```
infile    <- "FLX_AU-How_FLUXNET2015_FULLSET_HH_2001-2014_1-3.csv"
ERA_file  <- "FLX_AU-How_FLUXNET2015_ERAI_HH_1989-2014_1-3.csv"
site_code <- "AU-How"
out_path  <- "~/FluxnetLSM/Outputs"
```

The data can then be processed by invoking:

```
convert_fluxnet_to_netcdf(infile, site_code, ERA_file out_path,
                          met_gapfill="ERAinterim")
```

All other arguments are left to their default values in this example (see Table 1 for argument descriptions). The package automatically selects output years based on the default thresholds (as detailed in Section 2.3.2). Figure 3 shows the full time series of essential meteorological variables and two example evaluation variables at Howard Springs. The code helps exclude time periods with extensive missing periods, such as the first year (2001) of the time series, as well as heavily gap-filled time periods (e.g. around January 2007). Extended periods with missing QC flags (see Section 2.2.3) are also excluded for evaluation variables due to unknown data quality (Figure 3b). Based on the default thresholds, the time period 2010-2014 is chosen and outputted, indicated by grey shading in Figure 3. The rest of the data are discarded. Thresholds can of course be modified by the user to change this result.

Once the data have been processed and outputted, they can be visualised. Three types of plots are produced by default: mean annual and diurnal cycles and a time series plot. Figure 2 shows an example of each type of output plot produced by the package. These plots can be used for further quality controlling to detect any anomalous data periods not automatically excluded by the package.

4 Discussion and Conclusions

Efforts to better utilise existing observational data provide multiple benefits, including bringing research communities together, evaluating models against broader data, and providing further support to groups seeking to maintain primary observations. To maximise the use of observed data by communities other than those that collect the data, it is advantageous to make the data as accessible and easy to use as possible. In the case of the FLUXNET data, one major community is the land surface modelling sciences. Land surface models are key components in climate modelling and are therefore critical to broader science and policy communities. It is important to take any opportunities to improve the evaluation of land surface models that exist, and making FLUXNET datasets more reliably and easily available to the land surface modelling community removes a significant hurdle in that process.

To enhance transparency, to help reproducibility and as a platform for further community efforts we have presented an R package that transforms FLUXNET data into a form directly useable by LSMs. As released, FLUXNET data cannot be directly employed in LSMs due to data gaps, incompatible units and non-standard (land surface community) file format (CSV rather than NetCDF). The R package also collates metadata on data processing steps and the flux tower sites and stores these in the output files for easy access, and to permit more reliable reproducibility for modelling experiments. Finally, the package generates visualisations of outputs to facilitate further quality control of flux tower data and to help inform appropriate site selection, an important step in applying these data to modelling studies.

The package is open source, fully documented and simple to use, requiring minimal input from the user. It allows multiple sites to be processed into a form usable by LSMs in a short R script. Simultaneously, it provides optional settings for an advanced user to produce flux tower datasets suited for specific applications. For example, the user may wish to process the data differently if interested in evaluating models during short-term phenomena (such as heat waves) compared to longer seasonal to annual scales. Importantly, the package provides a tool for producing flux tower datasets for modelling applications in a fully citeable and reproducible framework. The package is stored in a publicly available repository and is being actively developed with community contributions encouraged.

Code availability

The `FluxnetLSM` code can be downloaded from the Github repository at https://github.com/aukkola/FluxnetLSM. Other required packages (`R.utils`, `ncdf4` and `rvest`) can be installed directly in R with the command `install.packages("package_name")`. See section 2.1 for further details on installation.

Anna Ukkola 18/7/2017 1:31 PM
Deleted: The code relies on the Protocol for the Analysis of Land Surface Models (PALS) R package. This package can be downloaded from the Github repository at https://github.com/dudek313/palsR.

Acknowledgements

We acknowledge the support of the Australian Research Council Centre of Excellence for Climate System Science (CE110001028). M.G. De Kauwe was supported by Australian Research Council Linkage grant LP140100232. This work used eddy covariance data acquired and shared by the FLUXNET community, including these networks: AmeriFlux, AfriFlux, AsiaFlux, CarboAfrica, CarboEuropeIP, CarboItaly, CarboMont, ChinaFlux, Fluxnet-Canada, GreenGrass, ICOS, KoFlux, LBA, NECC, OzFlux-TERN, TCOS-Siberia, and USCCC. The ERA-Interim reanalysis data are provided by ECMWF and processed by LSCE. The FLUXNET eddy covariance data processing and harmonization was carried out by the European Fluxes Database Cluster, AmeriFlux Management Project, and Fluxdata project of FLUXNET, with the support of CDIAC and ICOS Ecosystem Thematic Center, and the OzFlux, ChinaFlux and AsiaFlux offices.

References

Abramowitz, G., Leuning, R., Clark, M. and Pitman, A.: Evaluating the performance of land surface Models, J. Clim., 21, 5468–5481, doi:10.1175/2008JCLI2378.1, 2008.
Abramowitz, G., Pouyanné, L. and Ajami, H.: On the information content of surface meteorology for downward atmospheric long-wave radiation synthesis, Geophys. Res. Lett., 39, 1–5, doi:10.1029/2011GL050726, 2012.
Baldocchi, D.: Measuring fluxes of trace gases and energy between ecosystems and the atmosphere - the state and future of the eddy covariance method, Glob. Chang. Biol., 20, 3600–3609, doi:10.1111/gcb.12649, 2014.
Best, M. J., Abramowitz, G., Johnson, H. R., Pitman, A. J., Balsamo, G., Boone, A., Cuntz, M., Decharme, B., Dirmeyer, P. A., Dong, J., Ek, M., Guo, Z., Haverd, V., van den Hurk, B. J. ., Nearing, G. S., Pak, B., Peters-Lidard, C., Santanello, J. a., Stevens, L. and Vuichard, N.: The plumbing of land surface models: benchmarking model performance, J. Hydrometeorol., 16, 1425–1442, doi:10.1175/JHM-D-14-0158.1, 2015.
Blyth, E., Gash, J., Lloyd, A., Pryor, M., Weedon, G. P. and Shuttleworth, J.: Evaluating the JULES Land Surface Model Energy Fluxes Using FLUXNET Data, J. Hydrometeorol., 11, 509–519, doi:10.1175/2009JHM1183.1, 2010.
Bonan, G. B., Lawrence, P. J., Oleson, K. W., Levis, S., Jung, M., Reichstein, M., Lawrence, D. M. and Swenson, S. C.: Improving canopy processes in the Community Land Model version 4 (CLM4) using global flux fields empirically inferred from FLUXNET data, J. Geophys. Res., 116, 1–22, doi:10.1029/2010JG001593, 2011.
Dee, D. P., Uppala, S. M., Simmons, A. J., Berrisford, P., Poli, P., Kobayashi, S., Andrae, U., Balmaseda, M. A., Balsamo, G., Bauer, P., Bechtold, P., Beljaars, A. C. M., van de Berg, L., Bidlot, J., Bormann, N., Delsol, C., Dragani, R., Fuentes, M., Geer, A. J., Haimberger, L., Healy, S. B., Hersbach, H., Holm, E. V., Isaksen, L., Kållberg, P., Köhler, M., Matricardi, M., Mcnally, A. P., Monge-Sanz, B. M., Morcrette, J. J., Park, B. K., Peubey, C., de Rosnay, P., Tavolato, C., Thepaut, J. N. and Vitart, F.: The ERA-Interim reanalysis: Configuration and performance of the data assimilation system, Q. J. R. Meteorol. Soc., 137, 553–597, doi:10.1002/qj.828, 2011.
Haughton, N., Abramowitz, G., Pitman, A. J., Or, D., Best, M. J., Johnson, H. R., Balsamo, G., Boone, A., Cuntz, M., Decharme, B., Dirmeyer, P. A., Dong, J., Ek, M., Guo, Z., Haverd, V., van den Hurk, B. J. J., Nearing, G. S., Pak, B., Santanello, J. A., Stevens, L. E. and Vuichard, N.: The plumbing of land surface models: is poor performance a result of methodology or data quality?, J. Hydrometeorol., JHM-D-15-0171.1, doi:10.1175/JHM-D-15-0171.1, 2016.
Jones, H. G.: Plants and microclimate: A quantitative approach to environmental plant physiology, Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA., 1992.
Leuning, R., van Gorsel, E., Massman, W. J. and Isaac, P. R.: Reflections on the surface energy imbalance problem, Agric. For. Meteorol., 156, 65–74, doi:10.1016/j.agrformet.2011.12.002, 2012.
Luo, Y. Q., Randerson, J. T., Abramowitz, G., Bacour, C., Blyth, E., Carvalhais, N., Ciais, P., Dalmonech, D., Fisher, J. B., Fisher, R., Friedlingstein, P., Hibbard, K., Hoffman, F., Huntzinger, D., Jones, C. D., Koven, C., Lawrence, D., Li, D. J., Mahecha, M., Niu, S. L., Norby, R., Piao, S. L., Qi, X., Peylin, P., Prentice, I. C., Riley, W., Reichstein, M., Schwalm, C., Wang, Y. P., Xia, J. Y., Zaehle,

S. and Zhou, X. H.: A framework for benchmarking land models, Biogeosciences, 9, 3857–3874, doi:10.5194/bg-9-3857-2012, 2012.

Mahecha, M. D., Reichstein, M., Jung, M., Seneviratne, S. I., Zaehle, S., Beer, C., Braakhekke, M. C., Carvalhais, N., Lange, H., Le Maire, G. and Moors, E.: Comparing observations and process-based simulations of biosphere-atmosphere exchanges on multiple timescales, J. Geophys. Res. Biogeosciences, 115, 1–21, doi:10.1029/2009JG001016, 2010.

Matheny, A. M., Bohrer, G., Stoy, P. C., Baker, I. T., Black, A. T., Desai, A. R., Dietze, M. C., Gough, C. M., Ivanov, V. Y., Jassal, R. S., Novick, K. a., Schäfer, K. V. R. and Verbeeck, H.: Characterizing the diurnal patterns of errors in the prediction of evapotranspiration by several land-surface models: An NACP analysis, J. Geophys. Res. Biogeosciences, 1458–1473, doi:10.1002/2014JG002623, 2014.

Monteith, J. and Unsworth, M.: Principles of Environmental Physics, Academic Press, Oxford, United Kingdom., 1990.

Papale, D., Reichstein, M., Aubinet, M., Canfora, E., Bernhofer, C., Kutsch, W., Longdoz, B., Rambal, S., Valentini, R., Vesala, T. and Yakir, D.: Towards a standardized processing of Net Ecosystem Exchange measured with eddy covariance technique: algorithms and uncertainty estimation, Biogeosciences, 3, 571–583, doi:10.5194/bg-3-571-2006, 2006.

Pitman, A. J.: The evolution of, and revolution in, land surface schemes designed for climate models, Int. J. Climatol., 23, 479–510, doi:10.1002/joc.893, 2003.

Poulter, B., Ciais, P., Hodson, E., Lischke, H., Maignan, F., Plummer, S. and Zimmermann, N. E.: Plant functional type mapping for earth system models, Geosci. Model Dev., 4, 993–1010, doi:10.5194/gmd-4-993-2011, 2011.

Powell, T. L., Galbraith, D. R., Christoffersen, B. O., Harper, A., Imbuzeiro, H. M. a, Rowland, L., Almeida, S., Brando, P. M., da Costa, A. C. L., Costa, M. H., Levine, N. M., Malhi, Y., Saleska, S. R., Sotta, E., Williams, M., Meir, P. and Moorcroft, P. R.: Confronting model predictions of carbon fluxes with measurements of Amazon forests subjected to experimental drought, New Phytol., 200, 350–365, doi:10.1111/nph.12390, 2013.

Reichstein, M., Falge, E., Baldocchi, D., Papale, D., Aubinet, M., Berbigier, P., Bernhofer, C., Buchmann, N., Gilmanov, T., Granier, A., Grünwald, T., Havránková, K., Ilvesniemi, H., Janous, D., Knohl, A., Laurila, T., Lohila, A., Loustau, D., Matteucci, G., Meyers, T., Miglietta, F., Ourcival, J. M., Pumpanen, J., Rambal, S., Rotenberg, E., Sanz, M., Tenhunen, J., Seufert, G., Vaccari, F., Vesala, T., Yakir, D. and Valentini, R.: On the separation of net ecosystem exchange into assimilation and ecosystem respiration: Review and improved algorithm, Glob. Chang. Biol., 11, 1424–1439, doi:10.1111/j.1365-2486.2005.001002.x, 2005.

Ukkola, A. M., De Kauwe, M. G., Pitman, A. J., Best, M. J., Abramowitz, G., Haverd, V., Decker, M. and Haughton, N.: Land surface models systematically overestimate the intensity, duration and magnitude of seasonal-scale evaporative droughts, Environ. Res. Lett., 11, 104012, doi:10.1088/1748-9326/11/10/104012, 2016.

Vuichard, N. and Papale, D.: Filling the gaps in meteorological continuous data measured at FLUXNET sites with ERA-Interim reanalysis, Earth Syst. Sci. Data, 7, 157–171, doi:10.5194/essd-7-157-2015, 2015.

Wang, Y. P., Kowalczyk, E., Leuning, R., Abramowitz, G., Raupach, M. R., Pak, B., van Gorsel, E. and Luhar, A.: Diagnosing errors in a land surface model (CABLE) in the time and frequency domains, J. Geophys. Res., 116, G01034, doi:10.1029/2010JG001385, 2011.

Whitley, R., Beringer, J., Hutley, L., Abramowitz, G., De Kauwe, M. G., Duursma, R., Evans, B., Haverd, V., Li, L., Ryu, Y., Smith, B., Wang, Y.-P., Williams, M. and Yu, Q.: A model inter-comparison study to examine limiting factors in modelling Australian tropical savannas, Biogeosciences, 13, 3245–3265, doi:10.5194/bgd-12-18999-2015, 2016.

Williams, M., Richardson, A. D., Reichstein, M., Stoy, P. C., Peylin, P., Verbeeck, H., Carvalhais, N., Jung, M., Hollinger, D. Y., Kattge, J., Leuning, R., Luo, Y., Tomelleri, E., Trudinger, C. M. and Wang, Y.-P.: Improving land surface models with FLUXNET data, Biogeosciences, 6, 1341–1359, doi:10.5194/bg-6-1341-2009, 2009.

Tables

Table 1: Input arguments to the main `convert_fluxnet_to_netcdf` function. Conversion options can be passed directly into the function or retrieved using `get_default_conversion_options()` (see example in Supplementary section S.1).

Argument	Description	Default value
`infile`	FLUXNET2015 or La Thuile file(s) containing data variables	-
`site_code`	FLUXNET site ID (see Table 2)	-
`out_path`	User-defined output path	-
`era_file`	FLUXNET2015 file containing ERA-interim variables	NA
`conv_opts`	List of conversion options (by default retrieved automatically)	get_default_conversion_options()
`plot`	Output plots to be produced. Set to NA if not required	c("annual", "diurnal", "timeseries")
Conversion options:		
`datasetname`	Name of the dataset being processed (FLUXNET2015 or LaThuile)	FLUXNET2015
`datasetversion`	User-defined dataset version. Stored as metadata in output files.	n/a
`flx2015_version`	FLUXNET2015 version (FULLSET or SUBSET)	FULLSET
`fair_use`	La Thuile data policy/ies the output dataset should comply with.	Fair_Use
`fair_use_vec`	A vector of La Thuile data use policies for each year in the data files. Retrieved automatically from `data/LaThuile_site_policy.csv`.	NA
`aggregate`	Time step (in hours) to aggregate data to	NA
`met_gapfill`	Method to gapfill meteorological data: "ERAinterim", "statistical" or NA (no gapfilling)	NA
`flux_gapfill`	Method to gapfill flux data: "statistical" or NA (no gapfilling)	NA
`missing`	Max. percentage of time steps allowed to be missing in any given year	15
`gapfill_all`	Max. percentage of time steps allowed to be gap-filled (any quality) in any given year	20
`gapfill_good`	Same as above for good-quality gap-filling	NA
`gapfill_med`	Same as above for medium-quality gap-filling	NA
`gapfill_poor`	Same as above for poor-quality gap-filling	NA
`min_yrs`	Min. number of consecutive years to process	2
`linfill`	Max. consecutive length of time (in hours) to be gap-filled using linear interpolation	4
`copyfill`	Max. consecutive length of time (in number of days) to be gap-filled using copyfill	10
`regfill`	Max. consecutive length of time (in number of days) to be gap-filled using multiple linear regression	30
`lwdown_method`	Method to synthesise incoming longwave radiation. One of "Abramowitz_2012", "Swinbank_1963" and "Brutsaert_1975".	Abramowitz_2012

`include_all_eval`	Should all evaluation values be outputted, regardless of data gaps? If set to FALSE, any evaluation variables with missing or gap-filled values in excess of the thresholds will be discarded	TRUE
`model`	Name of land surface model. Allows additional model parameters to be stored as metadata in output files	NA

Anna Ukkola 18/7/2017 1:31 PM
Deleted: `min_yrs` ... [2]

Table 2: Site metadata provided with the package. All attributes are provided for each Tier 1 site, with the exception of tower and canopy height.

Attribute	Description
SiteCode	FLUXNET site ID*, e.g. AU-How
Fullname	FLUXNET site name*, e.g. Howard Springs
SiteLatitude	Latitude (degrees north)
SiteLongitude	Longitude (degrees east)
SiteElevation	Elevation (metres)
IGBP_vegetation_short	Short IGBP vegetation type, e.g. WSA
IGBP_vegetation_long	Long IGBP vegetation type, e.g. Woody Savannas
TowerHeight	Height of measurement tower (metres)
CanopyHeight	Height of canopy at site (metres)
Tier	FLUXNET2015 site tier*
Exclude	Should site be excluded? Allows sites with known problems to be excluded *a priori*. Set to TRUE or FALSE.
Exclude_reason	Reason why site should be excluded (user-defined)

*See http://fluxnet.fluxdata.org/sites/site-list-and-pages/

Table 3: Attributes required for each output variable (stored separately for FLUXNET2015 and La Thuile data releases in `data/Output_variables_*.R`).

Field name	Description	Value
Fluxnet_variable	Original FLUXNET variable name[1]	e.g. TA_F_MDS
Fluxnet_unit	Original FLUXNET variable unit[1]	e.g. C
Fluxnet_class	Variable data type. Used to define the `colClasses` argument in the R `read.csv` function when reading the input data file. Set to "numeric" if not known.	"numeric" or "integer"
Output_variable	Output variable name	User-defined, e.g. Tair
Output_unit	Output unit (note section 2.4.6 for unit conversions)	User-defined, e.g. K
Longname	Long variable description. Written as a variable attribute in the output file.	User-defined, e.g. Near surface air temperature
Standard_name	Climate and Forecast (CF) convention standard name[2]. Written as a variable attribute in the output file.	User-defined, e.g. air_temperature
Data_min	Minimum acceptable data value. Used to check data ranges (using output units).	User-defined, e.g. 200
Data_max	Maximum acceptable data value. Used to check data ranges.	User-defined, e.g. 333
Essential_met	Sets variable as essential when set to `TRUE` (see section 2.4.1.1)	"TRUE" or "FALSE"
Preferred_eval	Sets variable as preferred when set to `TRUE` (see section 2.4.1.2)	"TRUE" or "FALSE"
Category	Determines if the variable is written in the meteorological or evaluation NetCDF output file.	"Met" or "Eval"
ERAinterim_variable	Name of ERA-interim variable[1]	e.g. "TA_ERA"
Aggregate_method	Method used to aggregate the variable (mean or sum).	e.g. mean

[1]Must match naming conventions on http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/ for FLUXNET2015 and http://fluxnet.fluxdata.org/data/la-thuile-dataset/ for La Thuile.

[2]see http://cfconventions.org/standard-names.html

Table 4: Available unit conversions.

Variable	Variable name		Original unit	Converted unit
	FLUXNET2015*	La Thuile		
Air temperature	TA_F_MDS	Ta_f	C	K
Rainfall	P	Precip_f	mm	kg m^{-2} s^{-1}
Air pressure	PA	-	kPa	Pa
Atmospheric CO_2 concentration*	CO2_F_MDS	CO2	µmol CO_2 mol^{-1}	ppm

*Note these units are equal and the conversion is included to allow different notations

*FULLSET variable names reported here

Figures

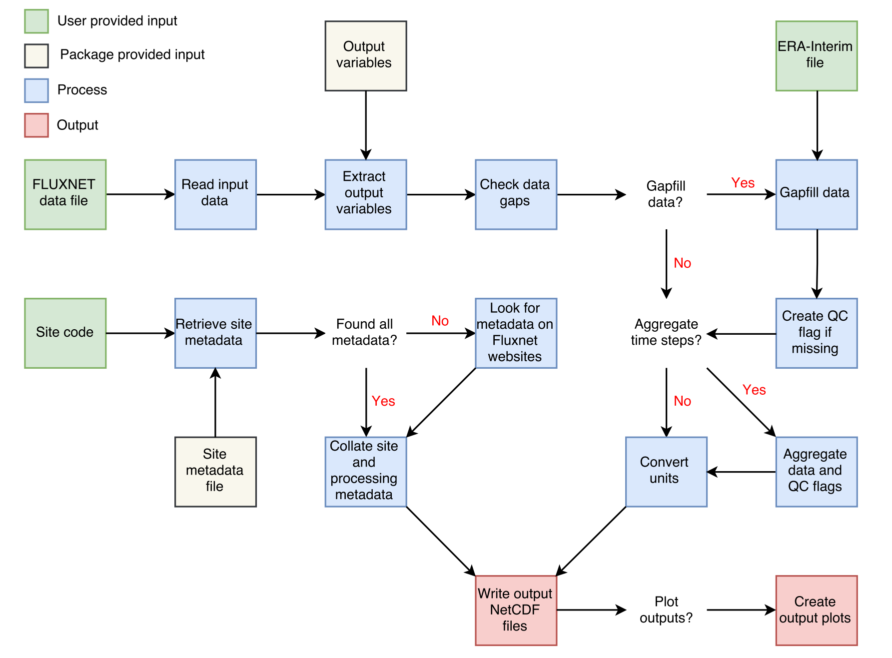

Figure 1: General workflow of the FluxnetLSM R package.

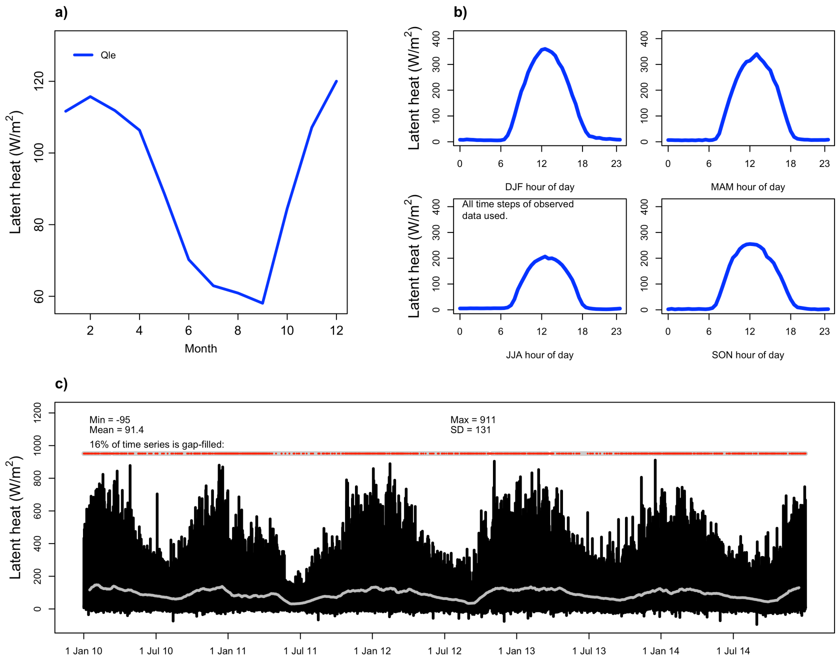

Figure 2: Examples of output plots produced by the package. Mean annual cycle by month is shown in panel a) and mean diurnal cycle by season in panel b). A time series is plotted in panel c), with the full time series shown in black and a smoothed 14-day running mean in grey. Gap-filled periods are indicated in red.

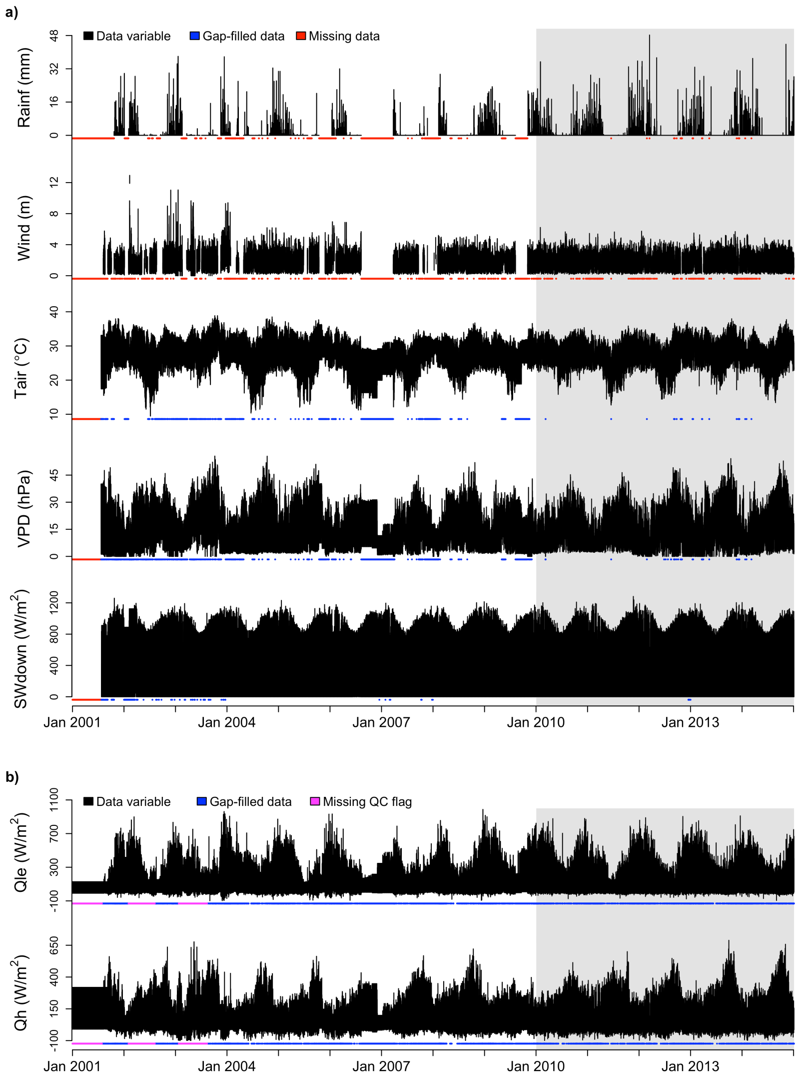

Figure 3: Time series of (a) essential meteorological variables and (b) select evaluation variables in Howard Springs. Meteorological variables include precipitation (Rainf), wind speed (Wind), air temperature (Tair), vapour pressure deficit (VPD) and incoming shortwave radiation (SWdown). Latent heat (Qle) and sensible (Qh) are shown as examples of evaluation variables. Gap-filled periods are indicated in blue and missing periods in data variables in red. For evaluation variables, periods with missing quality control (QC) flags are shown in pink.