- 1 Predicting carbon and energy fluxes across global FLUXNET sites with regression
- 2 algorithms

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Use present time wherever possible!

Abstract

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Spatial-temporal fields of land-atmosphere fluxes derived from data-driven models can complement simulations by process-based Land Surface Models. While a number of strategies for empirical models with eddy covariance flux data have been applied, a systematic intercomparison of these methods has been missing so far. In this study, we perform a cross-validation experiment-for predicting carbon dioxide, latent heat, sensible heat and net radiation fluxes, in different ecosystem types with eleven machine learning (ML) methods from four different classes (kernel methods, neural network, tree methods, and regression splines). We emptoy two complementary setups: (1) eight days average fluxes based on remotely sensed data, and (2) daily mean fluxes based on meteorological data and mean seasonal cycle of remotely sensed variables. The pattern of predictions from different ML and setups were very consistent. There were systematic differences in performance among the fluxes, with the following ascending order: net ecosystem exchange (R²<0.5), ecosystem respiration (R²>0.6), gross primary production $(R^2>0.7)$, latent heat $(R^2>0.7)$, sensible heat $(R^2>0.7)$, net radiation $(R^2>0.8)$. ML methods predicted very well the across sites variability and the seasonal cycle (R²> 0.7) of the observed fluxes, while the weekly deviations from the mean seasonal cycle were not well predicted (R²< 0.5). Fluxes were better predicted at forested and temperate climate sites than at ones growing in extreme climates or less representated in training data (e.g. the tropics). The large ensemble of ML based models evaluated will be the basis of new global flux products.

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- Keywords: Machine learning, carbon fluxes, energy fluxes, FLUXNET, remote sensing,
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1. Introduction

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Improving our knowledge of the carbon, water, and energy exchanges between terrestrial ecosystems and the atmosphere is essential to better understand and model Earth's climate system (IPCC, 2007; Reich, 2010). In situ observations of these exchanges are obtained by the eddy covariance technique, which directly measures turbulent fluxes between ecosystems and the atmosphere (Aubinet at al., 2012; Baldocchi et al., 2014). The large-scale measurement network, FLUXNET integrates site observations of these fluxes globally and provides detailed time series of carbon and energy fluxes across biomes and climates (Baldocchi et al., 2008). However, eddy-covariance measurements are site-level observations, and spatial upscaling is required to estimate these fluxes at regional to global scales. The increasing number of eddy covariance sites across the globe has encouraged the application of data-driven models by machine learning (ML) methods such as Artificial Neural Networks (ANNs, Papale et al., 2003), Random Forest (RF, Tramontana et al., 2015), Model Trees (MTE, Jung et al., 2009; Xiao et al., 2008, 2010) or Support Vector Regression (SVR, Yang et al., 2006, 2007) to estimate surface-atmosphere fluxes from site level to regional or global scales (e.g. Beer et al., 2010, Jung et al., 2010, 2011; Kondo et al., 2015; Schwalm et al., 2010; Yang et al., 2007; Xiao et al., 2008, 2010). The ML upscaled outputs are also increasingly used to evaluate land surface models (e.g., Anav et al., 2013; Bonan et al., 2011; Ichii et al., 2009; Piao et al., 2013). The key characteristic of data-driven models compared the process-based ones are the the fact former's intrinsic observational nature, and that functional relationships are not

prescribed but rather emerge from the patterns found in the measurements. In this context, data-driven models extract multivariate functional relationships between the in situ measured fluxes of the network and explanatory variables in an empirical way. The originate explanatory variables are generally coming from satellite remote sensing, providing (VI's are only partially descriptive for vegetation state!) information on vegetation state (e.g., vegetation indices) and other land surface properties (e.g., surface temperature), along with continuous measurements of meteorological variables at flux towers. While ML-based upscaling provides a systematic approach to move from point-based flux estimates to spatially explicit gridded fields, various sources of uncertainty exist. For example, individual ML methods might have different responses especially when these models are applied beyond the conditions sampled by the training dataset (Jung et al., 2009; Papale et al., 2015). The information content of the driving input variables may not be sufficient to capture the variability of the fluxes in all conditions (Tramontana et al., 2015). Moreover, remotely sensed and meteorological gridded datasets are affected by uncertainties themselves. Remote sensing data contain noise, biases and gaps, and can be perturbed by atmospheric effects or by the presence of snow. Meteorological gridded datasets are known to contain product specific biases (Garnaud et al., 2014; Tramontana et al., 2015; Zhao et al., 2012). Thorough experiments using multiple data-driven models and explanatory variables are an essential step to identify and assess limitations and sources of uncertainty in the empirical upscaling approach. In this study, we present and evaluate an ensemble of ML based empirical models to predict carbon and energy fluxes across FLUXNET sites. The included in this study participating models were selected in the context of the FLUXCOM initiative, forming the basis of subsequent global flux products. We performed consistent cross-validation for two complementary experimental setups using: (1) eight days average fluxes based on

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remotely sensed data, and (2) daily mean fluxes based on remotely sensed and meteorological data. The ML tools span the full range of commonly applied algorithms: from model tree ensembles, multiple adaptive regression splines, artificial neural networks, to kernel methods, with several representatives of each family. The different ML algorithms were trained with consistent sets of predictor variables. Our overarching aim is to understand how well fluxes of carbon (gross primary production (GPP), terrestrial ecosystem respiration (TER) and net ecosystem exchange (NEE)), and energy (latent heat (LH), sensible heat (H) and net radiation (Rn)) can be predicted by an ensemble of ML methods. More specifically, we address the following questions:

- 1. Are the patterns of predicted fluxes consistent between the two experimental setups?
- 2. How different are the predictions of the various ML algorithms?
 - 3. How does the performance differ among capturing the across-sites, seasonal and the deviations from the mean seasonal cycle variability?
 - 4. How does the performance differ among climate zones or ecosystem types?

2. Material and methods

2.1 Data

2.1.1 Eddy covariance study sites

We used eddy covariance data from 224 flux-tower sites (supplementary material, Sect. S1), which originate from the FLUXNET La Thuile synthesis dataset and CarboAfrica network (Valentini et al., 2014). The study sites are distributed globally and cover most plant functional types (PFT) and biomes over the globe (Table 1, Giri et al., 2005).

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2.1.2 Observation-based carbon and energy fluxes

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All flux measurements were post-processed using standardized procedures of quality 138 control and gap-filled following Reichstein et al. (2005) and Papale et al. (2006). Estimates 139 140 of GPP and TER were derived from half-hourly NEE measurements using two independent flux partitioning methods: (1) following Reichstein et al. (2005), where the temperature 141 142 sensitivity of ecosystem respiration is initially estimated from night-time NEE data and . This is done then extrapolated to daytime to estimate TER and GPP, by subtracting NEE (negatively 143 According to signed for the carbon uptake) from TER; (2) following Lasslop et al. (2010), where daytime 144 NEE data ⁴⁹ used to constrain a hyperbolic light response curve to directly estimate GPP 145 146 and TER. In the following we reference GPP and TER derived by Reichstein et al. (2005) as 147 GPP_R and TER_R; whereas estimates based on the Lasslop et al. (2010) method are referred 148 to as GPP_L and TER_L. The half-hourly data were aggregated to daily values and screened according to multiple 149 quality criteria, as follow: 150 151 1) we excluded data when more than 20% of the data were based on gap-filling with low 152 confidence (Reichstein et al., 2005); 2) we identified and removed obviously erroneous periods due to non-flagged instrument 153 or flux partitioning failures based on visual interpretation; 154

3) we excluded data-points where the two flux-partitioning methods provided extremely different patterns. Specifically, we computed for each site a robust linear regression between (a) $TER_R - GPP_L$ and NEE, and (b) GPP_R and GPP_L . Data points with a residual outside the range of \pm 3 times of the inter-quartile range were removed. This criterion removed only the extreme residuals, systematic differences between methods were not removed;

4) we removed the 5% of data-points with the largest friction velocity (u*) uncertainty, defined as data points above the 95th percentile of daily u* uncertainty (measured as inter-quartile range of 100 bootstrap samples).

Similarly to the carbon fluxes, we applied the same criteria 1) and 2) for the energy fluxes. Additionally, we removed data with inconsistent energy fluxes, i.e. when the residual of a robust linear regression between LE + H and Rn for each site was outside three-times the inter-quartile range of the residuals.

2.1.2 Remote sensing data

We collected data coming from Moderate Resolution Imaging Spectroradiometer (MODIS) which provides data at a spatial resolution of 1km or better (Justice et al., 2002). We used the cutout surroundings of 3×3 km pixels centered on the towers. We collected and processed the following MODIS products: MOD11A2 Land Surface Temperature (LST; Wan et al., 2002), MOD13A2 Vegetation Index (Normalized Difference Vegetation Index (NDVI) and Enhanced Vegetation Index (EVI); Huete et al., 2002), MOD15A2 Leaf Area fAPAR Index (LAI) and Fraction of Absorbed Photosynthetic Active Radiation (FPAR; Myneni et al., 2002), and MCD43A2 and MCD43A4 Bidirectional Reflectance Distribution Function

(BRDF) corrected surface reflectances (Schaaf et al., 2002). The BRDF-corrected surface reflectance data were further processed to calculate the Normalized Difference Water Index (NDWI) (Gao, 1996) and the Land Surface Water Index (LSWI) (Xiao et al., 2002). These data were obtained from http://daac.ornl.gov/MODIS/.

The remote sensing data were further processed to improve data quality and data gaps which were filled to create continuous time-series data, and to minimize non-land surface signals. We adopted the following processing scheme: we identified good quality pixels control by the using the quality assurance/quality criteria (QA/QC) included in the MODIS product. If more than 25% of pixels had good quality at the time of snapshot, the average of good quality pixels were assigned as the actual value. Otherwise, the data at the time snapshot were marked as blank (no data). Then, we created the mean seasonal variations from 2000-2012 using only good pixels data and the data gaps in the processed data were filled using the mean seasonal variation. Only MOD13 is provided with 16 days (Which type of composite?) composite, and eight days data were created by assigning the 16 days composite value to

2.1.3 Meteorological data

the corresponding two eight days periods.

The in situ measured air temperature (Tair), global radiation (Rg), VPD, and precipitation applied

were used after data screening according to the criteria 1) and 2) as for the measured the

fluxes (see Sect. 2.1.2). We also used long-term time series of these variables from ERA-dataset (Reference?)

These data

Interim for the period 1989-2010 (Dee et al., 2011), which were bias-corrected for each

site based on the overlapping period of in situ measurements (see http://www.bgc-dena.mpg.de/~MDIwork/meteo/). These long-term meteorological data are primarily

used to calculate consistent metrics of climatological variables (e.g. mean annual for temperature) across all sites given the temporal coverage of data of the different sites. In addition, we use a composite of these ERA-Interim data based and in situ measured data, to obtain a gap-free time series for calculating a simple soil Water Availability Index (WAI, see Sect. 2.3.2 and supplementary material, Sect. S3).

2.2 Participating ML methods

We chose 11 ML algorithms for regression from four broad families: tree-based methods, regression splines, neural networks, kernel methods. Moreover a comprehensive review of ML algorithms in biophysical parameter estimation can be found in Verrelst et al. (2015).

Tree based methods

These methods construct hierarchical binary decision trees. The inner nodes of the tree hold decision rules according to explanatory variables (e.g. less/greater than X1), recursively splitting the data into subspaces. The leaf nodes at the end of the decision tree contain models for the response variable. Because a single tree is generally not effective enough to cope with strong non-linear multivariate relationships, ensembles of trees are often used. We applied two different tree ensemble methods: (1) Random Forests (RF) which combines regression trees grown from different bootstrap samples and randomly selected features at each split node (Breiman, 2001; Ho, 1998); and (2) Model Tree Ensembles (MTE) which combine model trees (Jung et al., 2009). The main difference between regression and model trees is the prediction model in the leaf node: a

simple mean of the target values from training in regression trees and a parametric function (here a multiple linear regression) in model trees. In this study, we used three different variants of MTE, which differ mainly with respect to different cost functions for determining the splits, and the technique to create an ensemble of model trees. Further details are described in the supplementary material (Sect. S2).

Regression splines

Multivariate regression splines (MARS) are an extension of simple linear regression that can adapt to non-linear response surfaces—using piecewise (local) functions—by which a target variable is predicted by the sum of regression splines and a constant value (Alonso Fernández, 2013; Friedman et al., 1991).

Neural networks

Neural networks are based on nonlinear and nonparametric regressions. Their base unit is the neuron, where nonlinear regression functions are applied. The neurons are interconnected and organized in layers. The output of m neurons in the current layer are the inputs for n neurons of the next layer. We used two types of neural networks: the artificial neural network (ANN) and the group of method for data handle (GMDH). In an ANN, each neuron performs a linear regression followed by a non-linear function. Neurons of different layers are interconnected by weights that are adjusted during the training (Haykin et al., 1999; Papale et al., 2003). The GMDH is a self-organizing inductive method (Ungaro et al., 2005) building polynomials of polynomials; the neurons are pairwise connected through a quadratic polynomial to produce new neurons in the next layer (Shirmohammadi et al., 2015).

Kernel methods

Kernel methods (Shawe-Taylor and Cristianini, 2004) owe their name to the use of kernel measure functions, which measures similarities between input data examples. Among the available kernel methods we used: (1) support vector regression (SVR) (Vapnik et al., 1997), (2) kernel ridge regression (KRR) (Shawe-Taylor and Cristianini, 2004), and (3) Gaussian process regression (GPR) (Rasmussen, 2006; Verrelst et al., 2012). The SVR defines a linear prediction model over mapped samples to a much higher dimensional space, which is non-linearly related to the original input (Verrelst et al., 2012, Yang et al., 2007). The KRR is considered as the kernel version of the regularized least squares linear regression (Shawe-Taylor and Cristianini, 2004, Verrelst et al., 2012). The GPR is a probabilistic approximation to nonparametric kernel-based regression, and both a predictive mean (point-wise estimates) and predictive variance (error bars for the predictions) can be derived. We also used a hybrid approach combining RF with simple decision stumps in the inner nodes and GPR for prediction in the leaf nodes (Fröhlich et al., 2012).

2.3 Experimental design

2.3.1. Experiment setups

We defined two complementary experimental setups, which differ in the choice of explanatory variables, and the temporal resolution of the target fluxes: 1) at eight days temporal resolution using exclusively remote sensing data (hereafter RS); and 2) at daily

temporal resolution using meteorological data together with the mean seasonal cycle (MSC) of remote sensing data (hereafter RS+METEO). In the latter case, the MSC of remote sensing data were smoothed and interpolated to daily time step. Each setup has advantages and disadvantages. While RS can provides products with high spatial of 1 km or less resolution (up to 1km), data are limited to the MODIS era (2000-present) and has a coarse (weekly) temporal resolution. The uncertainties of remote sensing data at tower locations due to finer scale spatial heterogeneity may also degrade the performance of the ML methods. RS+METEO can take advantage of information from meteorological variables, and is resistant to the noise of remote sensing time series because only mean seasonal cycle of data from satellite were used. RS+METEO allows for upscaled products over a longer time period (because not constrained by the availability of MODIS data) and capacity finer time scale (daily). However the predictive skill of this setting was conditioned by the (phenology) missing of information regarding the interannual variability of vegetation greenness. In addition the use of meteorological gridded datasets introduces another source of uncertainty coming from potential dataset specific biases and by their typically coarse spatial resolution (0.5 degrees or larger).

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2.3.2. Variable selection

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Combining remote sensing and meteorological data (see Sect. 2.1.2 and 2.1.3) we created model input additional variables for model inputs. In the case of RS+METEO setup we derived the Water Availability Index (WAI) that it is based on a simple soil water balance model (for more details see supplementary material, Sect. S3) as an attempt to better represent water stress ed conditions. For both setups we derived proxies for absorbed radiation as

fAPAR

the product between vegetation greenness (e.g. EVI, NDVI, FPAR) and available energy (e.g. daytime LST, Rg, and potential radiation). Other derived variables include the mean (phenology) seasonal cycle (MSC) of dynamic variables and associated metrics (minimum, maximum, amplitude, and mean). For remote sensing predictors, the MSC and associated metrics are based on the period 2001-2012 while for climate variables are based on the bias corrected daily long-term ERA-Interim data reference period (1989-2010). In total, 216 potential explanatory variables were created for RS and 231 for RS+METEO (see supplementary material S4 for details).

Optimally suitable
For each setup we selected a small subset of variables best-suited to predict the target

fluxes using a variable selection search algorithm. Variable selection is an important since it improves while component in the spatial upscaling because the accuracy of predictions improves and the computational costs of the global predictions are minimized. We used the Guided Hybrid Genetic Algorithm (GHGA) published by Jung and Zscheischler (2013), which was designed for variable selection problems with many candidate predictor variables and computationally expensive cost functions. The GHGA requires the training of a regression algorithm (here RF) to estimate the cost associated with selected variable subsets (see S5 for details).

Instead of doing a computationally demanding variable selection for each individual flux,

variable selection runs were performed for the RS and RS+METEO setups and separately

for carbon and energy fluxes. This procedure has the advantage that the resulting global

products originate from a consistent set of predictor variables. The selected variables for

the prediction of carbon and energy fluxes are listed in Table 2.

2.3.3. Model training

The capability of ML methods to spatially extrapolate carbon and energy fluxes has been evaluated by a 10-fold cross-validation strategy. The training datasets were stratified into a 10-folds, each one roughly containing 10% of the data. Entire sites were assigned to each fold (Jung et al., 2011). The target values for each fold were predicted based on the training using the remaining nine folds. Due to computational expense of the RS+METEO setup, only one method representing each "family" – multiple regressions, RF, MARS, ANN and KRR – was trained.

ML methods base settings have been before the training (for further details, see supplementary material S6). These hyper-parameters account for regularization in order to avoid overfitting, as well as for the shape and smoothness constraints. Instead, the model parameters were estimated for each ML every time in each fold.

2.3.4. Model evaluation

In order to highlight the differences between the RS and RS+METEO setups, the daily has been output from RS+METEO were aggregated to eight days time steps; the same periods and have been sites were used for the comparison. Besides the statistical analysis of the individual ML focussed cross-validation results, we focus on the ensemble median estimate, here defined as the median predicted value across all ML for a given setup and time step. The advantages of the median ensemble estimate is the robustness of the predictions for the contribution of outliers many ML that reduced the risk of outlier in the extrapolation exercise.

We used different metrics to evaluate the ML performance such as the Nash and Sutcliffe model efficiency (MEF), the root mean square error (MSE), the empirical BIAS, the

Pearson's linear correlation coefficient (ρ), the coefficient of determination (R²) and the ratio of variance (ROV).

MEF (Nash and Sutcliffe, 1970), if the capability of a model to estimate a target variables is better than a reference model. If the reference model is the mean value of the target,

359 MEF can be calculated as:

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$$MEF = 1 - \frac{\sum_{i=1}^{n} (x_i - y_i)^2}{\sum_{i=1}^{n} (y_i - \overline{y})^2}$$
 (1)

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where χ_i and γ_i were the predicted and the observed values respectively and \overline{y} is the mean value of the observations (here the reference model). MEF can vary between -inf to capacity

1; if MEF > 0 the predictive skill of the model is better than the mean (MEF = 1 for the capacity

ideal model), if MEF=0 the predictive skill of the model is equivalent to the mean, finally if capacity

MEF < 0, the predictive skill of the mean value of the target is better than the model.

is

The RMSE was estimates as the root square of the mean value of the squared residuals:

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$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (x_i - y_i)^2}{n}}$$
 (2)

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372 The BIAS was evaluated as the differences between the mean value of model's residuals

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$$BIAS = \frac{\sum_{i=1}^{n} (x_i - y_{i)}}{n}$$
 (3)

Following Gupta et al. (2009) the importance of bias on the overall uncertainty was evaluated as the ratio between the square of BIAS and Mean Square Error, the latter estimated as the square value of RMSE.

The Pearson's linear correlation coefficient (ρ) is the ratio between the covariance between the modeled and observed values (σ_{xy}) and the product of the standard deviation of modeled (σ_x) and observed (σ_y) values:

$$\rho = \frac{\sigma_{xy}}{\sigma_x \sigma_y} \tag{4}$$

 R^2 was estimated as the squared value of ρ ; finally ROV was evaluated as the ratio between predicted and observed standard deviation.

capacity

We evaluated the overall predictive skill of the models, evaluating the consistency among trained ML approaches and across the experimental setup. Then we evaluated the capability of the regression models to predict site-specific mean fluxes, mean seasonal cycle (MSC), and anomalies (Jung et al., 2011). The MSC per site was calculated using the averaged values for each eight days period across all available years, but only when at least two values (i.e., years) for each eight days period were available. To assess the mean values of the study sites, we calculated the mean of the MSC if at least 50% of the are

46 eight daily values were present, whereas the weekly anomalies were calculated as the deviation of a flux value from the MSC. Finally, the mean site value was removed from the MSC to disentangle the seasonal variation from the mean, thus making the MSC and mean complementary.

We also analyzed the performance for the different Köppen climate zonesand IGBP plant (PFT's) functional types. In particular, we computed for each flux, setup and tower site the

400	performances of ML median estimate. Then, for each setup, we estimated the median
401	value of the site-by-site statistics per PFT and climate zone.
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404	3. Results and Discussions
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407	3.1 Overview
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409	S The ensemble median estimate always outperformed the median performance of ML-
410	specific methods (the median value of metrics calculated for individual ML) (Table 3;
411	(what does skill mean here? Unclear phrasing) Appendix A). Individual ML methods also exhibited higher skill than multiple linear
412	regressions (higher MEF and lower RMSE; Fig. 1). This highlights the added value of ML
413	methods as these are able to account for nonlinearities in either explanatory variables or
414	fluxes. Overall, using the ensemble median estimate gives a representative overview of
415	ML-based flux predictions.
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418	capacity 3.2 Predictive skill of carbon and energy fluxes
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420	capacity Predictive skill of the ensemble median estimate clustered into tiers whereby energy
421	fluxes are uniformly better predicted than carbon fluxes: Rn > H/LE/GPP > TER > NEE
422	predicitve capacity (Table 3). The highest skill levels as exhibited by net radiation shows near perfect
423	agreement; Rn displays a model efficiency (MEF) of 0.91-0.92 and a correlation of 0.96.
424	predicitve capacity The decline in skill for the second tier fluxes is ca. 15% to 20%: MEE for H. LE. and GPP is

425	0.79, 0.75-0.76, and 0.71 respectively. The lowest two tiers exhibits 20% and 40%
426	declines in MEF (0.57-0.64 and 0.43-0.46 for TER and NEE respectively). These relative
427	rankings are unchanged regardless of skill metric used—apart from RMSE where the
428	difference in fluxes units and magnitude, confounds a direct comparison (Table 3)—
429	suggesting that accuracy and precision scale linearly.
430	There were only minor performance differences between the two carbon fluxes
431	partitioning methods (Table 3), although for the RS setup, the performance of TER_L were
432	comparatively lower than TER_R (lower MEF, ρ and ROV). A similar trend was not found in
433	the case of RS+METEO setup.
434	predicitve capacity The overall skill profile in this study confirms previous upscaling efforts (Jung et al., 2011;
435	predicitve capacity Yuan et al., 2010). This relatively stable cross-study skill gradient reflects the information
436	content of the available predictor variables. The spatiotemporal variability of remotely
437	sensed land surface properties is well-suited to predict the top tier fluxes (Rn, H, LE, and
438	GPP) (Jung et al., 2008; Tramontana et al., 2015; Xiao et al., 2010; Yang et al., 2007)
439	predicitve capacity The higher skill associated with energy fluxes suggests that these fluxes are more easily
440	predictable using the drivers selected in particular respect to NEE. In fact NEE is strongly
441	controlled by external factors such management and disturbances (Amiro et al., 2010;
442	Thornton et al., 2002) and by lag and memory effects (Bell et al., 2012; Frank et al., 2015,
443	Papale et al., 2015; Paruelo et al., 2005), which are both poorly captured by predictor
444	variables typically used in upscaling and poorly constrained in general, i.e., data limited.
445	Another reason for the low performances in NEE simulation can be in the uncertainties in
446	the measurements that are larger compared to H and LE and have an important effect
447	being NEE the difference between two large components (GPP and TER).
448	Among the carbon fluxes, GPP is the best predicted probably because the seasonal cycle
449	are and canopy properties, which were strongly related to GPP, were well represented by the

ML drivers. The intermediate skill of TER, relative to carbon fluxes only, is supported by its tight coupling to the well-predicted GPP and the availability of predictor variables that capture the temperature dependency of respiration. However specific drivers for TER could be still missing. In fact in contrast to GPP, the canopy properties are less important drivers of TER, while the soil properties, carbon pools and their turnover rates are key for respiratory processes (Amiro et al., 2010) but not available to be used as drivers. This likely explains the poor performance for TER in comparison with GPP.

3.3 Are the flux predictions consistent between RS and RS+METEO?

predicitve capacity

Skills, in terms of both performance tiers and absolute value of skill metrics, are similar for both RS and RS+METEO approaches with some differences, in particular: (1) RS and predictive capacity RS+METEO diverged more for those fluxes and showed lower overall skill levels, in particular for NEE (Fig. 1, Table 3); (2) MEF and correlation values were slightly larger for RS than RS+METEO, excluding TER_L where the opposite was found, indicating an important role of the meteorological data for this version of the ecosystem respiration. It can be should be considered that the differences in performances could be also due to a different ensemble size, with the RS composed of 11 individual ML-based ensemble members, whereas RS+METEO is based on only four. The overall good performance of the RS setup implies that carbon and energy fluxes can be mapped exclusively based on remotely sensed inputs allowing high-spatial resolution products and reduction of uncertainty due to the meteorological drivers spatialization (Tramontana et al., 2015).

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3.4 How different are the predictions of the various ML algorithms	3.4 How di	ifferent are t	the predictions	of the various	ML algorithms
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Pair-wise R^2 values for model outputs (Table 4) were close to unity ($R^2 \ge 0.90$), regardless 478 of experimental setup, with NEE showing a slightly lower value (R² = 0.84). Among 479 corresponding model residuals (Table 4), R² values ranged from 0.79 (Rn) to 0.89 (TER_L). 480 Comparing the same ML technique but using different experimental setups (Table 4, RS 481 vs. RS+METEO) showed similarly high, albeit somewhat diminished level of consistency 482 (R² range ranged from 0.71 to 0.80 for model residuals). These finding highlights that the 483 ML methods were mapping between explanatory variables and target fluxes both reliably 484 and robustly. Across the all three consistency checks there was also a tendency for better 485 predicted fluxes (e.g., H) to exhibit higher pair-wise R² values than poorly predicted fluxes 486 (e.g., NEE). This is expected as more robust patterns—and therefore those that lead to 487 greater predictive skill—are easier to extract regardless of ML algorithm and 488 experimental setup in this study; thus increasing consistency. While this broad 489 consistency confirms that the extracted patterns are robust, the decline in R² when 490 comparing the same ML trained with different drivers (RS vs RS+METEO) respect to the 491 492 correlation among ML methods with the same drivers, suggests that the choice of the explanatory variable had higher impact than the choice of the ML technique for the 493 494 pattern of predictions.

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3.5 How does the performance differ among capturing the across-sites, seasonal and the deviations from the mean seasonal cycle variability?

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500 Decomposing FLUXNET data into across-sites variability, mean seasonal cycle, and interannual variability components (Sect. 2.3.4) revealed clear gradients in predictive skill 501 (Table 5 and Fig. 2). Across-sites variability was in general well-captured by the ML (R² 502 range: 0.61 to 0.81 except for NEE) and the best predicted pattern for GPP and TER. This 503 suggests that ML are suitable to reproduce the spatial pattern of mean annual fluxes. 504 The variability in the mean seasonal cycle (at weekly time scale) was also uniformly well 505 predicted (R² between 0.67-0.77 for GPP and TER, and between 0.86-0.98 for the energy 506 507 fluxes) and the best predicted pattern for energy fluxes in particular for LE and Rn. phenology The importance of seasonality in carbon and energy annual fluxes is known (Joiner et al., 508 phenological 2014; Jung et al., 2011; Merbold et al., 2009; Wolf et al., 2011) and biases in its dynamic s 509 510 (e.g. in the growing season length) could lead to biases into the predicted fluxes (Ichii et 511 al., 2010). A clear benefit of the ML upscaling approach used here is that none of the parameters controlling seasonality are prescribed, reducing the possibility of biases. 512 In contrast, interannual variability is generally poorly captured by all the ML approaches 513 used with only H and Rn showing an R² greater than 0.4. This low predictive skill holds 514 regardless of whether weekly, monthly (Jung et al., 2011), or annual time steps are used 515 516 (data not shown). This is likely due to a combination of missing predictor variables (e.g. 517 disturbances, management, legacy effects) and the noise/uncertainty in both predictor and target variables that plays a major role when small differences (like in the interannual 518 variability) are predicted. The slightly better performances when sensible heat flux is 519 estimated could be due to the lower uncertainty in this flux respect to the others (only 520 521 one sensor used, the sonic anemometer, in contract with the other fluxes where also the 522 gas analyzer is used) but also to the fact that it is strongly and directly related to the LST used as driver. In any case, predicting interannual variability remains one of the largest 523 challenges in the context of empirical upscaling. 524

525 NEE is confirmed to be the most difficult and consequently poorest predicted flux (Table Predicitive capacity for is 3). NEE shows considerably lower skill relative to the other fluxes for across-sites 526 variability ($R^2 = 0.46$), the mean seasonal cycle ($R^2 = 0.59$), and interannual variability ($R^2 = 0.46$) 527 528 0.13, TER₁ is lowest at 0.10). 529 530 3.6 How does the performance differ among climate zones or ecosystem types? 531 532 Using climate zone and plant functional type (PFT) to disaggregate ML methods 533 performances we find that in general energy fluxes are better predicted than carbon 534 between fluxes among the different climate zone and PFTs (Fig. 3 and Appendix C). The median R² 535 between simulation and observation for carbon fluxes (excluding NEE) is greater than 0.6 536 for more than 75% of the PFT and climate zone, while in the energy fluxes an R² greater 537 than 0.7 is found for more than the 85% of the PFT and climate zone (in all sites for Rn). 538 NEE is again consistently poorly predicted (low R² and high relative RMSE; Fig. 3), apart 539 from deciduous broadleaf forests (DBF) and MF where a marginal improvement is 540 elicited evident. The better performance in these two vegetation types could be related to the 541 higher seasonal variance of NEE in comparison with the other PFTs that is a pattern more 542 consistent with the seasonal variance of the used drivers. 543 tropical Overall the ML methods show poor prediction capability in tropics and evergreen 544 broadleaf forests (EBF). Possible explanations are the absence of a clear seasonal cycle 545 traceable by the remote sensing signal (evergreen vegetation) and a low variance in their 546 seasonal cycle that is challenging to explained mathematically and capture with a model. 547

(Sims et al., 2008; Yebra et al., 2015; Yuan et al., 2010). In addition, the difficulty in

acquiring cloud-free remotely sensed data introduces additional uncertainty in the drivers.

Reason for low performances can be also the lack of important driving variables, that are is probably the main explanation for cropland where management information are missing (e.g. irrigation, fertilization, tillage) and also for cold and dry environments where the extreme nature of the environments characterized by water limitation (for dry sites) and the extreme low temperature (for cold sites) would require probably more targeted drivers such direct estimations of soil water content. In addition, cold and dry sites are characterized by both low magnitude and low variance of fluxes, making it difficult to explain the fluxes in these ecosystems types by empirical models.

4. Conclusions

The ML methods presented and evaluated in this study have shown high capability to predict carbon and energy fluxes, in particular the between-site variability and the seasonal variations, with a general tendency of increasing performance in the following order: NEE, TER, GPP, LE, H, and Rn. The relatively poor performance for NEE likely results from factors that cannot be easily accounted for in ML based modelling approaches, such as legacies of site history (e.g. disturbances, management, age and stocks). Future progress in this direction requires the reconstruction of the relevant management and disturbance history, trying to integrate information from forest inventories, high resolution satellites such LANDSAT and high resolution biomass data from radar and LIDAR with the aim to improve model performance. The better results obtained for the energy fluxes (LE and H) in comparison to the carbon fluxes (GPP and TER) could be related to more complex mechanisms driving the carbon cycle that are also not

575 represented in the drivers used, in addition to a relatively higher uncertainties in the GPP and TER due to the use of flux partitioning methods based on NEE measurements. 576 We found no substantial bias in the predictions of the ML models for most vegetation 578 types or biomes. However, the predictions have deviated more from the observations for 579 evergreen broadleaf forests, croplands, the tropics and extreme climates. The growing number of eddy-covariance sites, in particular new sites in poorly represented regions will likely improves the predictive skill in the future. This is particularly relevant since tropical areas account for a disproportionate share of the global water and carbon cycle 582 583 (Beer et al., 2010). The deviations from the mean seasonal cycle (weekly anomalies) are still poorly captured by the ML methods. We expected the RS+METEO approach to perform better regarding 585 586 the prediction of anomalies as meteorological drivers were included and the noise in remote sensing time series was greatly reduced by using smoothed seasonal cycle. 588 However, this was not the case, which indicates that either, the weekly anomalies of both, the flux data, and the drivers, are strongly affected by the uncertainties, or that the 590 anomalies are dominated by management and disturbance (or other factors) not accounted for in the predictors. Hence, the prediction of interannual anomalies remains a 592 major unresolved research topic. The predictions for ecosystem fluxes across FLUXNET by different ML techniques and by 593 594 different explanatory variable sets (RS vs RS+METEO) are highly consistent, indicating that 595 the extracted patterns by the trained models are robust, realistic and not subject to 596 severe overfitting. The differences in predictions among the RS and RS+METEO setups are slightly larger than among different ML methods, suggesting that future activities should concentrate on identifying new driver variables to further improve the performance of 598 fluxes predictions. Nevertheless, we recommend using the ensemble median estimate of

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multiple ML techniques for analyzing global flux products because extrapolation beyond the FLUXNET-sampled conditions can generate larger differences among methods than discernible from our cross-validation comparison.

The ML based models presented and extensively evaluated here form the basis of an extensive archive of global gridded flux products, which is currently under development. The thorough cross-validation experiment presented in this paper helps users understanding the products' strengths and weaknesses. The good performance of the ML methods, the availability of an ensemble of them, and the detailed analysis of their uncertainties will make this archive an unprecedented data stream to study the global land-atmosphere exchange of carbon, water and energy.

Appendix A: Median performance of the methods.

In table A1 we reported, for both setups, the median value of skill metrics (MEF, RMSE, and absolute value of BIAS) realized by singular ML and their related variability such estimated as the median absolute deviation (MAD) from the median multiplied per 1.4826 (see Jung et al., 2009 for details)

Appendix B: scatterplot between the observations and the predictions by the median ensemble of ML.

In Fig. B1 and B2 we reported the scatterplots between eddy covariance observations and the modeled median ensemble estimates respetively for RS and RS+METEO setup. We

reported the overall eight days time series, and the comparison for the across site variability, the mean seasonal cycle and the weekly deviations (or anomalies) from the mean seasonal cycle.

Appendix C Median value of site-by-site performance per vegetation and climate type.

At follow we reported the median estimate of site-by-site R², RMSE, and absolute bias per PFT and climate zones.

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 Table 1. Distribution of flux tower sites across plant functional types (PFT) and climate zones.

PFT	N° of sites	Climate zone	N° of sites
Evergreen needleleaf forest	66	Temperate	111
Grassland	38	Subtropical - Mediterranean	47
Cropland	27	Boreal	34
Deciduous broadleaf forest	24	Tropical	14
Evergreen broadleaf forest	19	Dry	13
Wetland	17	Artic	5
Shrubland	12		
Mixed forest	11		
Savannah	10		

Table 2. Selected predictors for both setup for carbon fluxes (GPP, TER and NEE) and energy fluxes (H, LE and Rn). List of acronyms: Enhanced Vegetation Index (EVI), fraction of photosynthetically active radiation absorbed by a canopy (fPAR), Leaf Area Index (LAI), daytime Land Surface Temperature (LST_{Day}) and nighttime Land Surface Temperature (LST_{Night}), Middle Infrared Reflectance (band 7) (MIR⁽¹⁾), Normalized Difference Vegetation Index (NDVI), Normalized Difference Water Index (NDWI), Plant Functional Type (PFT), incoming global Radiation (Rg), top of atmosphere potential Radiation (Rpot), Index of Water Availability (IWA), Relative humidity (Rh), Water Availability Index lower (WAI_L), and upper (WAI_U) (for details see supplementary material, Sect. S3), Mean Seasonal Cycle (MSC). Interaction between A and B is shown as (A, B)

Setup	Type of variability	Carbon fluxes	Energy fluxes			
RS	Spatial	PFT	PFT			
		Amplitude of MSC of EVI	Maximum of MSC of			
			(fPAR, Rg)			
		Amplitude of MSC of MIR ⁽¹⁾	Minimum of MSC of			
			(NDVI, Rg)			
		Maximum of MSC of LST _{Day}				
	Spatial & seasonal	MSC LAI	MSC of (EVI, LST)			
			Rpot			
	Spatial, seasonal &	NDWI	Rg			
	interannual	LST _{Day}	LST _{Day}			
		LST _{Night}	Anomalies of LST _{Night}			
		(NDVI, Rg)	Anomalies of (EVI, LST)			
RS+METEO	Spatial	PFT	PFT			
		Amplitude of MSC of NDVI	Maximum of MSC of			
			(NDVI, WAI _U)			
		Amplitude of MSC of band	Mean of MSC of band 6			

4 BRDF reflectance⁽²⁾ BRDF reflectance⁽²⁾

Minimum of MSC of NDWI

Amplitude of MSC of

(NDVI, WAI_L)

Spatial & Seasonal MSC of LST_{Night} Rpot

MSC of (FPAR, LST) MSC of NDWI

 $MSC \ of \ (NDVI, \ Rg) \\ \hspace{1cm} MSC \ of \ LST_{Night}$

MSC of (NDVI, Rg, IWA)

Spatial & Seasonal & Tair Rain

Interannual Rg

Rh

^{1020 (1)} derived from the MOD13 product; (2) derived from MCD43 product.

Table 3. Statistics of the accuracy of predictions of carbon and energy fluxes made by the ensemble median estimate based on RS and RS+METEO. For RMSE and BIAS, the reference units are gCm⁻²d⁻¹ and MJm⁻²d⁻¹, in the case of carbon fluxes (GPP, TER and NEE) and energy fluxes (H, LE and Rn) respectively.

Flux	RS					RS+M	IETEO			
	MEF	RMSE	Р	ROV	BIAS	MEF	RMSE	ρ	ROV	BIAS
GPP _R	0.71	1.56	0.85	0.69	-0.02	0.70	1.59	0.84	0.73	0.09
GPP_L	0.71	1.53	0.84	0.68	-0.02	0.71	1.54	0.84	0.74	0.09
TER_R	0.64	1.14	0.80	0.61	-0.01	0.64	1.15	0.80	0.69	0.09
TER_L	0.60	1.18	0.77	0.56	-0.01	0.63	1.14	0.79	0.66	0.08
NEE	0.46	1.24	0.68	0.39	0.04	0.43	1.28	0.65	0.40	-0.02
Н	0.79	1.36	0.89	0.71	-0.02	0.79	1.37	0.89	0.75	0.02
LE	0.76	1.37	0.87	0.71	-0.07	0.75	1.39	0.87	0.73	-0.01
Rn	0.92	1.51	0.96	0.90	-0.01	0.91	1.55	0.96	0.93	0.08

Table 4: Mean values of the determination coefficient (R^2) by the pair-wise comparison of the models output and their residuals. We compared different ML and same drivers (RS and RS+METEO respectively) or the same ML and different drivers (RS vs RS+METEO). Numbers in brackets are the standard deviation of R^2 . All correlations are statistically significant (p < 0.001).

		- hartaaraan		b	etween		
	Correlation	among mode	l s output S	Correlation among models residuals			
Fluxes		20.145750	RS vs		DC. 145750	RS vs	
	RS	RS+METEO	RS+METEO	RS	RS+METEO	RS+METEO	
GPP _R	0.95 (0.02)	0.95 (0.02)	0.89 (0.02)	0.88 (0.04)	0.87 (0.04)	0.74 (0.04)	
GPP_L	0.95 (0.02)	0.94 (0.02)	0.88 (0.02)	0.88 (0.04)	0.86 (0.04)	0.72 (0.04)	
TER _R	0.91 (0.03)	0.94 (0.03)	0.86 (0.04)	0.86 (0.05)	0.88 (0.05)	0.75 (0.06)	
TER_L	0.92 (0.03)	0.93 (0.03)	0.85 (0.03)	0.89 (0.04)	0.88 (0.05)	0.77 (0.05)	
NEE	0.84 (0.06)	0.84 (0.07)	0.75 (0.08)	0.88 (0.05)	0.87 (0.06)	0.80 (0.06)	
н	0.94 (0.02)	0.96 (0.02)	0.93 (0.03)	0.80 (0.06)	0.87 (0.05)	0.76 (0.08)	
LE	0.94 (0.02)	0.96 (0.01)	0.90 (0.02)	0.83 (0.05)	0.88 (0.04)	0.73 (0.04)	
Rn	0.98 (0.01)	0.99 (0.00)	0.97 (0.01)	0.79 (0.08)	0.86 (0.03)	0.71 (0.12)	

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between **Table 5**: R² and RMSE for the comparison among sites, mean seasonal cycle and anomalies. The last two columns show the consistency between the median estimates of the two setups. For RMSE, the reference units are gCm⁻²d⁻¹ and MJm⁻²d⁻¹, in the case of carbon fluxes (GPP, TER and NEE) and energy fluxes (H, LE and Rn) respectively.

	RS v	s. OBS	RS+MET	EO vs. OBS	RS vs. R	S+METEO					
Fluxes	R^2	RMSE	R^2	RMSE	R ²	RMSE					
Across-sites											
GPP _R	0.78	0.80	0.77	0.82	0.95	0.34					
GPP_L	0.78	0.77	0.79	0.75	0.94	0.36					
TER_R	0.68	0.73	0.61	0.81	0.92	0.32					
TER_L	0.72	0.60	0.71	0.61	0.92	0.27					
NEE	0.48	0.61	0.46	0.61	0.83	0.22					
Н	0.81	0.68	0.81	0.68	0.97	0.25					
LE	0.79	0.74	0.75	0.80	0.93	0.33					
Rn	0.80	0.93	0.79	0.96	0.96	0.38					
		M	ean Seaso	nal Cycle							
GPP _R	0.76	1.03	0.77	1.02	0.93	0.48					
GPP_L	0.77	1.00	0.77	0.99	0.93	0.50					
TER_R	0.71	0.62	0.71	0.62	0.92	0.29					
TER_L	0.67	0.64	0.68	0.63	0.92	0.29					
NEE	0.61	0.83	0.59	0.84	0.93	0.24					
Н	0.86	0.89	0.86	0.87	0.97	0.36					
LE	0.87	0.79	0.87	0.79	0.95	0.45					
Rn	0.98	0.74	0.98	0.74	0.99	0.43					
			Anoma	lies							
GPP _R	0.18	0.67	0.12	0.68	0.38	0.32					

GPP_L	0.16	0.67	0.11	0.68	0.37	0.31
TER_R	0.14	0.48	0.15	0.48	0.36	0.17
TER_L	0.10	0.58	0.13	0.57	0.35	0.18
NEE	0.13	0.56	0.13	0.55	0.43	0.20
Н	0.43	0.81	0.41	0.81	0.77	0.34
LE	0.21	0.78	0.21	0.77	0.46	0.32
Rn	0.57	0.81	0.54	0.83	0.84	0.41

Table A1: Accuracy of carbon and energy fluxes predicted by machine learning methods based on RS and RS+METEO dataset. The median value of methods and the variability (in brackets) estimated as the median absolute deviation (MAD) from the median multiplied per 1.4826 (as reported in Jung et al., 2009) were reported.

FLUXES		RS			RS+METEO	
	MEF	RMSE	Abs BIAS	MEF	RMSE	Abs BIAS
GPP	0.698 (±0.012)	1.604 (±0.033)	0.022 (±0.019)	0.694 (±0.012)	1.614 (±0.032)	0.073 (±0.011)
GPP_{HB}	0.700 (±0.009)	1.564 (±0.024)	0.023 (±0.024)	0.701 (±0.008)	1.561 (±0.020)	0.083 (±0.011)
TER	0.612 (±0.022)	1.183 (±0.033)	0.026 (±0.025)	0.623 (±0.005)	1.166 (±0.008)	0.089 (±0.033)
TER _{HB}	0.571 (±0.016)	1.218 (±0.023)	0.019 (±0.017)	0.609 (±0.001)	1.163 (±0.002)	0.079 (±0.017)
NEE	0.433 (±0.017)	1.270 (±0.019)	0.024 (±0.021)	0.407 (±0.029)	1.298 (±0.032)	0.014 (±0.003)
Н	0.767 (±0.015)	1.426 (±0.047)	0.014 (±0.005)	0.776 (±0.008)	1.397 (±0.025)	0.022 (±0.009)
LE	0.739 (±0.015)	1.418 (±0.042)	0.052 (±0.046)	0.734 (±0.003)	1.434 (±0.009)	0.023 (±0.008)
Rn	0.909 (±0.009)	1.589 (±0.082)	0.030 (±0.025)	0.908 (±0.008)	1.600 (±0.070)	0.073 (±0.015)

Table C1. Median site-by-site R² of the carbon fluxes per PFT and climate zones. ENF is vvergreen needle leaf forest, DBF deciduous broadleaf forest, EBF Evergreen broadleaf forest, MF mixed forest, SHR shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland, Tmp Temperate, TmpCont Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by ice.

CAT	GF	P_R	GI	P _L	TE	R _R	TE	R_L	N	EE
	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO
ENF	0.87 (0.10)	0.86 (0.10)	0.85 (0.12)	0.86 (0.12)	0.81 (0.15)	0.85 (0.11)	0.75 (0.24)	0.76 (0.20)	0.50 (0.34)	0.55 (0.30)
DBF	0.89 (0.07)	0.87 (0.09)	0.87 (0.07)	0.88 (0.08)	0.81 (0.12)	0.83 (0.13)	0.76 (0.14)	0.76 (0.14)	0.72 (0.16)	0.68 (0.17)
EBF	0.50 (0.29)	0.48 (0.20)	0.48 (0.29)	0.44 (0.28)	0.34 (0.34)	0.49 (0.35)	0.15 (0.18)	0.29 (0.20)	0.26 (0.23)	0.24 (0.26)
MF	0.91 (0.06)	0.95 (0.02)	0.91 (0.03)	0.95 (0.04)	0.85 (0.10)	0.90 (0.07)	0.84 (0.10)	0.86 (0.15)	0.73 (0.10)	0.75 (0.09)
SHR	0.67 (0.30)	0.71 (0.28)	0.67 (0.36)	0.72 (0.23)	0.80 (0.13)	0.78 (0.24)	0.68 (0.18)	0.66 (0.38)	0.37 (0.38)	0.41 (0.31)
SAV	0.75 (0.13)	0.70 (0.13)	0.72 (0.05)	0.67 (0.17)	0.65 (0.07)	0.72 (0.11)	0.55 (0.16)	0.61 (0.10)	0.38 (0.20)	0.34 (0.29)
GRA	0.69 (0.27)	0.62 (0.33)	0.69 (0.25)	0.60 (0.32)	0.70 (0.25)	0.73 (0.25)	0.66 (0.20)	0.72 (0.21)	0.40 (0.29)	0.36 (0.30)
CRO	0.58 (0.41)	0.44 (0.36)	0.56 (0.41)	0.45 (0.31)	0.78 (0.17)	0.76 (0.15)	0.68 (0.22)	0.65 (0.23)	0.35 (0.46)	0.33 (0.43)
WET	0.87 (0.11)	0.91 (0.07)	0.85 (0.12)	0.87 (0.09)	0.78 (0.19)	0.83 (0.14)	0.65 (0.17)	0.74 (0.20)	0.64 (0.16)	0.61 (0.24)
Trop	0.32 (0.46)	0.40 (0.39)	0.63 (0.23)	0.31 (0.32)	0.25 (0.23)	0.34 (0.47)	0.11 (0.13)	0.26 (0.14)	0.28 (0.35)	0.21 (0.30)
SubTrop	0.64 (0.26)	0.66 (0.28)	0.65 (0.26)	0.65 (0.24)	0.64 (0.25)	0.66 (0.26)	0.52 (0.24)	0.55 (0.28)	0.39 (0.37)	0.39 (0.26)
Dry	0.47 (0.27)	0.40 (0.33)	0.50 (0.25)	0.38 (0.30)	0.62 (0.25)	0.62 (0.38)	0.55 (0.19)	0.55 (0.39)	0.21 (0.29)	0.11 (0.14)
Tmp	0.81 (0.19)	0.74 (0.24)	0.83 (0.14)	0.78 (0.22)	0.78 (0.13)	0.77 (0.18)	0.68 (0.20)	0.72 (0.17)	0.56 (0.28)	0.47 (0.34)
TmpCont	0.86 (0.09)	0.82 (0.16)	0.84 (0.11)	0.80 (0.17)	0.81 (0.12)	0.78 (0.14)	0.75 (0.17)	0.76 (0.15)	0.54 (0.42)	0.53 (0.36)
Bor	0.90 (0.07)	0.90 (0.07)	0.92 (0.06)	0.89 (0.07)	0.90 (0.05)	0.91 (0.04)	0.86 (0.08)	0.89 (0.06)	0.59 (0.31)	0.59 (0.25)
Cold	0.56 (0.57)	0.50 (0.56)	0.49 (0.62)	0.46 (0.59)	0.84 (0.20)	0.86 (0.13)	0.50 (0.38)	0.55 (0.23)	0.47 (0.56)	0.45 (0.57)

Table C2. Median site-by-site RMSE of the carbon fluxes per PFT and climate zones. ENF is svergreen needle leaf forest, DBF deciduous broadleaf forest, EBF Evergreen broadleaf
 forest, MF mixed forest, SHR shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland, Tmp Temperate, TmpCont
 Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by ice.

CAT	GPP _R (g	Cm ⁻² d ⁻ 1)	GPP _L (g	Cm ⁻² d ⁻ 1)	TER _R (g	Cm ⁻² d ⁻ 1)	TER _L (go	Cm ⁻² d ⁻ 1)	NEE (go	Cm ⁻² d ⁻ 1)
	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO
ENF	1.05 (0.60)	1.12 (0.60)	1.04 (0.59)	1.14 (0.66)	0.82 (0.50)	0.80 (0.52)	0.87 (0.60)	0.91 (0.68)	0.87 (0.51)	0.86 (0.53)
DBF	1.21 (0.78)	1.35 (0.59)	1.17 (0.68)	1.36 (0.62)	0.68 (0.26)	0.76 (0.33)	0.76 (0.33)	0.93 (0.44)	1.28 (0.39)	1.28 (0.39)
EBF	1.70 (0.55)	1.64 (0.85)	1.65 (0.70)	1.46 (0.51)	1.23 (0.69)	1.48 (0.85)	1.88 (1.23)	1.71 (0.73)	1.15 (0.48)	1.15 (0.45)
MF	0.87 (0.17)	0.76 (0.45)	0.89 (0.27)	0.97 (0.56)	0.65 (0.18)	0.73 (0.42)	0.79 (0.14)	0.79 (0.18)	0.91 (0.47)	0.81 (0.29)
SHR	0.73 (0.47)	0.78 (0.46)	0.69 (0.44)	0.77 (0.37)	0.50 (0.33)	0.70 (0.41)	0.50 (0.34)	0.55 (0.36)	0.57 (0.31)	0.52 (0.15)
SAV	0.83 (0.44)	0.81 (0.18)	0.87 (0.45)	0.84 (0.18)	0.80 (0.53)	0.68 (0.41)	0.86 (0.55)	0.77 (0.38)	0.71 (0.36)	0.69 (0.31)
GRA	1.22 (0.64)	1.22 (0.60)	1.18 (0.68)	1.20 (0.62)	1.00 (0.48)	1.01 (0.54)	0.99 (0.58)	0.95 (0.52)	0.76 (0.61)	0.85 (0.49)
CRO	1.69 (1.38)	2.30 (1.02)	1.57 (1.42)	2.24 (1.10)	0.87 (0.46)	0.90 (0.57)	0.80 (0.51)	0.98 (0.57)	1.42 (0.90)	1.44 (0.70)
WET	1.04 (0.95)	0.93 (0.77)	1.03 (0.96)	0.78 (0.53)	1.04 (0.87)	0.98 (0.82)	1.07 (0.51)	1.02 (0.51)	0.46 (0.19)	0.64 (0.26)
Trop	1.93 (0.46)	1.74 (1.01)	2.24 (0.62)	1.56 (0.78)	2.07 (0.69)	1.55 (0.87)	2.47 (0.74)	2.05 (0.43)	1.28 (0.29)	1.17 (0.46)
SubTrop	1.37 (0.55)	1.40 (0.61)	1.37 (0.56)	1.38 (0.57)	1.03 (0.46)	1.00 (0.41)	1.08 (0.36)	1.11 (0.40)	1.13 (0.63)	1.15 (0.62)
Dry	0.60 (0.24)	0.78 (0.36)	0.63 (0.16)	0.74 (0.30)	0.49 (0.10)	0.54 (0.20)	0.58 (0.26)	0.67 (0.32)	0.41 (0.13)	0.46 (0.15)
Tmp	1.73 (1.02)	1.82 (0.99)	1.73 (0.98)	1.71 (1.03)	1.09 (0.54)	1.17 (0.67)	1.24 (0.57)	1.31 (0.59)	1.43 (0.59)	1.40 (0.61)
TmpCont	1.01 (0.42)	1.29 (0.59)	1.00 (0.45)	1.26 (0.57)	0.71 (0.30)	0.75 (0.38)	0.74 (0.31)	0.79 (0.34)	0.95 (0.39)	1.02 (0.43)
Bor	0.66 (0.27)	0.70 (0.36)	0.66 (0.27)	0.67 (0.33)	0.48 (0.27)	0.47 (0.27)	0.48 (0.16)	0.45 (0.21)	0.50 (0.32)	0.48 (0.22)
Cold	0.44 (0.04)	0.58 (0.42)	0.51 (0.24)	0.46 (0.32)	0.41 (0.06)	0.23 (0.06)	0.57 (0.16)	0.29 (0.12)	0.51 (0.21)	0.54 (0.35)

Table C3. Median site-by-site absolute bias of the carbon fluxes per PFT and climate zones. ENF is evergreen needle leaf forest, DBF deciduous broadleaf forest, EBF Evergreen
 broadleaf forest, MF mixed forest, SHR shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland, Tmp Temperate,
 TmpCont Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by ice.

CAT	GPP _R (g	Cm ⁻² d ⁻ 1)	GPP _L (g	Cm ⁻² d ⁻ 1)	TER _R (g	Cm ⁻² d ⁻ 1)	TER _L (go	Cm ⁻² d ⁻ 1)	NEE (go	Cm ⁻² d ⁻ 1)
	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO
ENF	0.53 (0.46)	0.54 (0.56)	0.45 (0.42)	0.48 (0.50)	0.47 (0.47)	0.50 (0.54)	0.42 (0.40)	0.41 (0.43)	0.39 (0.44)	0.32 (0.36)
DBF	0.43 (0.38)	0.56 (0.59)	0.42 (0.36)	0.50 (0.52)	0.29 (0.32)	0.35 (0.35)	0.39 (0.33)	0.42 (0.34)	0.60 (0.28)	0.55 (0.30)
EBF	0.82 (0.91)	0.77 (0.50)	0.75 (0.81)	0.76 (0.48)	0.88 (0.98)	0.84 (0.72)	0.76 (0.81)	0.93 (0.65)	0.36 (0.45)	0.46 (0.44)
MF	0.47 (0.20)	0.34 (0.38)	0.38 (0.29)	0.57 (0.29)	0.39 (0.28)	0.41 (0.13)	0.37 (0.15)	0.30 (0.35)	0.34 (0.49)	0.32 (0.36)
SHR	0.38 (0.37)	0.54 (0.49)	0.38 (0.44)	0.39 (0.47)	0.36 (0.38)	0.50 (0.43)	0.31 (0.40)	0.32 (0.23)	0.27 (0.27)	0.28 (0.24)
SAV	0.42 (0.40)	0.36 (0.21)	0.35 (0.40)	0.23 (0.15)	0.43 (0.41)	0.35 (0.23)	0.42 (0.37)	0.31 (0.10)	0.23 (0.21)	0.19 (0.10)
GRA	0.60 (0.59)	0.48 (0.49)	0.60 (0.56)	0.52 (0.55)	0.38 (0.29)	0.36 (0.37)	0.44 (0.39)	0.38 (0.38)	0.17 (0.20)	0.31 (0.31)
CRO	0.47 (0.37)	0.66 (0.44)	0.36 (0.33)	0.56 (0.47)	0.29 (0.32)	0.25 (0.22)	0.29 (0.32)	0.30 (0.29)	0.41 (0.31)	0.56 (0.55)
WET	0.54 (0.64)	0.28 (0.41)	0.55 (0.62)	0.29 (0.25)	0.72 (0.35)	0.48 (0.52)	0.69 (0.29)	0.50 (0.51)	0.24 (0.19)	0.30 (0.25)
Trop	1.66 (1.31)	0.67 (0.79)	1.71 (1.23)	0.77 (0.86)	1.73 (0.88)	1.16 (1.19)	1.94 (0.81)	1.21 (0.67)	0.52 (0.57)	0.38 (0.55)
SubTrop	0.54 (0.45)	0.55 (0.43)	0.50 (0.38)	0.52 (0.55)	0.46 (0.44)	0.53 (0.47)	0.47 (0.35)	0.42 (0.37)	0.34 (0.44)	0.37 (0.34)
Dry	0.31 (0.20)	0.33 (0.26)	0.33 (0.38)	0.36 (0.29)	0.24 (0.21)	0.32 (0.35)	0.34 (0.21)	0.43 (0.26)	0.14 (0.08)	0.22 (0.14)
Tmp	0.72 (0.55)	0.77 (0.71)	0.66 (0.59)	0.63 (0.56)	0.50 (0.46)	0.47 (0.50)	0.51 (0.55)	0.41 (0.45)	0.46 (0.43)	0.51 (0.41)
TmpCont	0.45 (0.35)	0.60 (0.52)	0.39 (0.35)	0.57 (0.47)	0.37 (0.28)	0.29 (0.25)	0.37 (0.33)	0.38 (0.37)	0.35 (0.40)	0.55 (0.55)
Bor	0.36 (0.30)	0.32 (0.34)	0.32 (0.24)	0.27 (0.31)	0.32 (0.40)	0.32 (0.33)	0.31 (0.35)	0.26 (0.32)	0.27 (0.26)	0.23 (0.26)
Cold	0.07 (0.00)	0.08 (0.09)	0.08 (0.12)	0.15 (0.06)	0.34 (0.04)	0.12 (0.06)	0.34 (0.06)	0.15 (0.01)	0.37 (0.15)	0.27 (0.27)

Table C4. Median site-by-site R² of the energy fluxes per PFT and climate zones. ENF is evergreen needle leaf forest, DBF deciduous broadleaf forest, EBF Evergreen broadleaf forest, MF mixed forest, SHR shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland, Tmp Temperate, TmpCont Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by ice.

CAT	I	Н	L	E	Rn		
	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO	
ENF	0.87 (0.10)	0.86 (0.10)	0.83 (0.10)	0.84 (0.11)	0.97 (0.02)	0.97 (0.02)	
DBF	0.76 (0.18)	0.74 (0.12)	0.87 (0.05)	0.87 (0.07)	0.97 (0.01)	0.97 (0.02)	
EBF	0.85 (0.13)	0.82 (0.17)	0.56 (0.30)	0.52 (0.42)	0.95 (0.05)	0.96 (0.03)	
MF	0.85 (0.06)	0.82 (0.10)	0.91 (0.07)	0.89 (0.06)	0.97 (0.02)	0.96 (0.02)	
SHR	0.83 (0.15)	0.83 (0.17)	0.73 (0.29)	0.77 (0.23)	0.98 (0.01)	0.97 (0.01)	
SAV	0.74 (0.25)	0.77 (0.26)	0.85 (0.06)	0.78 (0.11)	0.86 (0.05)	0.88 (0.10)	
GRA	0.72 (0.22)	0.71 (0.22)	0.85 (0.11)	0.83 (0.16)	0.96 (0.02)	0.96 (0.02)	
CRO	0.70 (0.16)	0.66 (0.18)	0.79 (0.14)	0.80 (0.14)	0.97 (0.02)	0.96 (0.02)	
WET	0.81 (0.06)	0.78 (0.14)	0.86 (0.10)	0.84 (0.06)	0.94 (0.02)	0.92 (0.06)	
Trop	0.52 (0.18)	0.60 (0.32)	0.56 (0.38)	0.50 (0.44)	0.86 (0.14)	0.89 (0.13)	
SubTrop	0.81 (0.18)	0.82 (0.18)	0.78 (0.13)	0.80 (0.13)	0.96 (0.03)	0.96 (0.02)	
Dry	0.87 (0.07)	0.86 (0.13)	0.80 (0.07)	0.79 (0.14)	0.90 (0.06)	0.93 (0.05)	
Tmp	0.78 (0.14)	0.78 (0.13)	0.86 (0.11)	0.83 (0.13)	0.97 (0.02)	0.96 (0.02)	
TmpCont	0.72 (0.18)	0.69 (0.18)	0.83 (0.08)	0.84 (0.09)	0.97 (0.02)	0.96 (0.02)	
Bor	0.90 (0.07)	0.89 (0.08)	0.92 (0.05)	0.92 (0.03)	0.98 (0.01)	0.97 (0.02)	
Cold	0.83 (0.12)	0.57 (0.19)	0.83 (0.08)	0.82 (0.07)	0.94 (0.03)	0.85 (0.13)	

Table C5. Median site-by-site RMSE of the energy fluxes per PFT and climate zones. ENF is evergreen needle leaf forest, DBF deciduous broadleaf forest, EBF Evergreen broadleaf forest, MF mixed forest, SHR shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland, Tmp Temperate, TmpCont Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by ice.

CAT	H (MJ	m ⁻² d ⁻¹)	LE (MJ	m ⁻² d ⁻¹)	Rn (MJm ⁻² d ⁻¹)		
	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO	
ENF	1.09 (0.25)	1.16 (0.25)	1.00 (0.56)	1.02 (0.55)	1.27 (0.68)	1.26 (0.57)	
DBF	1.30 (0.43)	1.31 (0.38)	1.22 (0.26)	1.14 (0.46)	1.11 (0.42)	1.24 (0.41)	
EBF	1.14 (0.60)	1.29 (0.76)	1.55 (0.39)	1.60 (0.46)	1.33 (0.43)	1.14 (0.56)	
MF	1.18 (0.44)	1.12 (0.42)	0.82 (0.37)	1.15 (0.54)	1.14 (0.45)	1.09 (0.43)	
SHR	1.21 (0.46)	1.14 (0.28)	1.12 (0.41)	1.11 (0.56)	1.37 (0.80)	1.01 (0.43)	
SAV	1.23 (0.25)	1.20 (0.22)	1.32 (0.56)	1.35 (0.30)	1.10 (0.33)	1.19 (0.60)	
GRA	1.14 (0.35)	1.08 (0.47)	1.09 (0.34)	1.32 (0.54)	1.48 (0.83)	1.48 (0.90)	
CRO	1.24 (0.45)	1.36 (0.33)	1.51 (0.61)	1.54 (0.35)	1.24 (0.52)	1.23 (0.26)	
WET	0.97 (0.36)	1.22 (0.60)	0.88 (0.13)	0.90 (0.18)	1.42 (0.51)	1.65 (0.71)	
Trop	0.98 (0.51)	1.19 (0.63)	1.60 (0.52)	1.62 (0.41)	1.33 (0.73)	1.03 (0.48)	
SubTrop	1.28 (0.38)	1.32 (0.46)	1.36 (0.62)	1.36 (0.53)	1.40 (0.40)	1.33 (0.49)	
Dry	1.07 (0.24)	1.05 (0.50)	1.21 (0.33)	1.27 (0.52)	1.61 (0.75)	2.02 (0.93)	
Tmp	1.18 (0.23)	1.15 (0.33)	1.18 (0.43)	1.17 (0.49)	1.10 (0.36)	1.14 (0.47)	
TmpCont	1.30 (0.42)	1.35 (0.37)	1.25 (0.41)	1.47 (0.37)	1.17 (0.65)	1.16 (0.54)	
Bor	0.98 (0.23)	1.05 (0.26)	0.70 (0.26)	0.61 (0.20)	0.88 (0.31)	1.08 (0.50)	
Cold	1.03 (0.36)	1.50 (0.55)	1.00 (0.23)	1.03 (0.45)	1.47 (0.18)	2.04 (0.19)	

Table C6. Median site-by-site absolute bias for energy fluxes. . ENF is evergreen needle leaf forest, DBF deciduous broadleaf forest, EBF Evergreen broadleaf forest, MF mixed forest, SHR shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland, Tmp Temperate, TmpCont Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by ice.

CAT	H (MJm ⁻² d ⁻¹)		LE (MJm ⁻² d ⁻¹)		Rn (MJm ⁻² d ⁻¹)	
	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO
ENF	0.44 (0.40)	0.40 (0.33)	0.42 (0.41)	0.44 (0.49)	0.78 (0.63)	0.64 (0.61)
DBF	0.60 (0.35)	0.66 (0.35)	0.57 (0.56)	0.49 (0.50)	0.38 (0.28)	0.61 (0.49)
EBF	0.38 (0.48)	0.55 (0.46)	0.97 (0.79)	0.88 (0.70)	0.88 (0.51)	0.62 (0.43)
MF	0.48 (0.40)	0.26 (0.31)	0.34 (0.40)	0.64 (0.52)	0.56 (0.45)	0.56 (0.57)
SHR	0.34 (0.43)	0.47 (0.52)	0.41 (0.41)	0.50 (0.43)	0.62 (0.76)	0.44 (0.52)
SAV	0.68 (0.35)	0.56 (0.15)	0.63 (0.80)	0.40 (0.15)	0.27 (0.22)	0.63 (0.55)
GRA	0.51 (0.39)	0.40 (0.24)	0.38 (0.38)	0.57 (0.50)	0.97 (0.81)	0.81 (1.03)
CRO	0.23 (0.21)	0.24 (0.24)	0.36 (0.38)	0.41 (0.50)	0.66 (0.58)	0.68 (0.39)
WET	0.47 (0.51)	0.67 (0.37)	0.54 (0.41)	0.38 (0.21)	0.34 (0.34)	0.83 (0.78)
Trop	0.37 (0.51)	0.67 (0.47)	0.97 (0.79)	1.24 (0.82)	0.94 (1.10)	0.63 (0.60)
SubTrop	0.58 (0.59)	0.50 (0.39)	0.62 (0.58)	0.58 (0.56)	0.83 (0.71)	0.70 (0.55)
Dry	0.68 (0.62)	0.55 (0.56)	0.21 (0.14)	0.30 (0.26)	1.06 (0.55)	1.61 (0.91)
Tmp	0.38 (0.23)	0.34 (0.31)	0.49 (0.46)	0.56 (0.54)	0.65 (0.49)	0.68 (0.58)
TmpCont	0.49 (0.41)	0.40 (0.46)	0.44 (0.51)	0.53 (0.50)	0.69 (0.72)	0.61 (0.58)
Bor	0.33 (0.32)	0.38 (0.24)	0.22 (0.16)	0.23 (0.24)	0.38 (0.27)	0.50 (0.47)
Cold	0.43 (0.46)	0.71 (0.11)	0.56 (0.31)	0.39 (0.18)	0.30 (0.29)	0.86 (0.58)

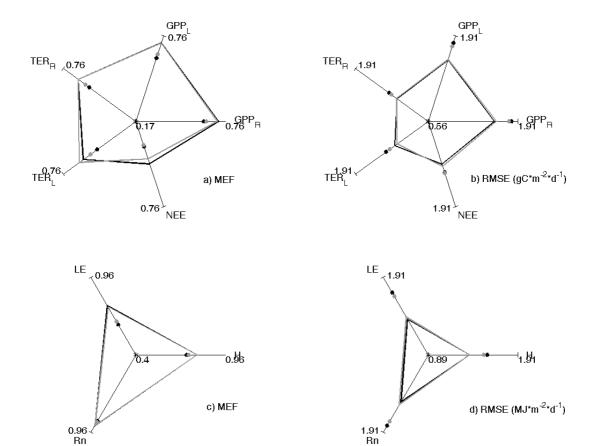


Fig. 1: Spider plot of MEF (first column) and RMSE (second column) for carbon (first row) and energy fluxes (second row) showing the consistency of prediction made RS (Black line) and RS+METEO (grey lines) setups. The lines are the ensemble median estimate; we also show the performance of multiple regressions trained with RS (black point) and RS+METEO (gray points). GPP_R and GPP_L are respectively gross primary production estimated following Reichstein et al. (2005) and Lasslop et al. (2010), TER_R and TER_L the total ecosystem respiration estimated following Reichstein et al. (2005) and Lasslop et al. (2010), NEE net ecosystem exchange, H the sensible heat, LE the latent heat and Rn the net radiation.

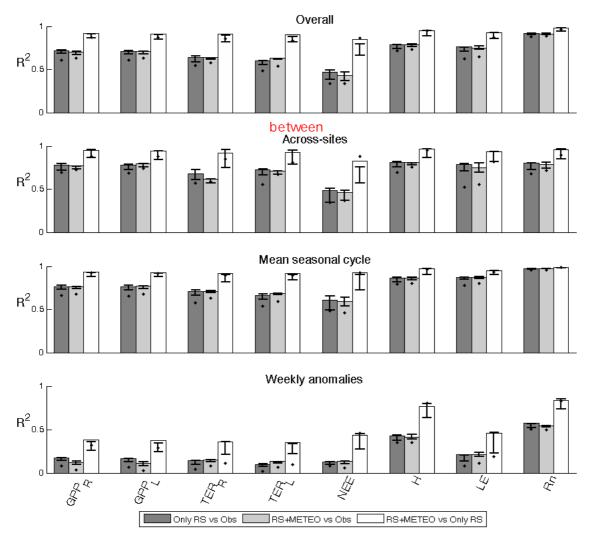


Fig. 2: Coefficients of determination (R²) from the comparison of overall time series, across-sites, mean seasonal cycle, and the anomalies, in particular: the determination coefficients between predictions by the ensemble median estimate of RS setup and observation (dark grey bars), between predictions by the ensemble median estimate of RS+METEO setup and observation (light grey bars), and between the two ensembles median estimate (white bars). Whiskers are the higher and lower R² when the comparisons are made among the singular ML. The comparison of output by the multiple regressions is also shown (black points).



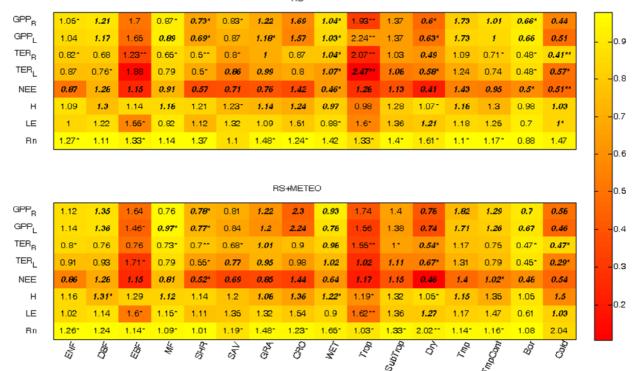


Fig. 3: Performance of FLUXCOM median estimates per climate zone and plant functional type 1096 (PFT). The colored matrices show the median values of R² (red pixels for low R², yellow pixels for 1097 high R²). Number indicate the RMSE (units of carbon fluxes are gCm⁻²d⁻¹ and MJm⁻²d⁻¹ in the case

high R²). Number indicate the RMSE (units of carbon fluxes are gCm⁻²d⁻¹ and MJm⁻²d⁻¹ in the case of energy fluxes). Oblique and bold font are used when the relative RMSE (normalized for the mean observed fluxes per PFT and climate zone) is greater than 0.5. The symbols '**' after RMSE are used when the weight of bias (estimated as the ratio between the square of median absolute

bias and the MSE) is greater than 0.5, instead '*' are used if the weight of bias is between 0.25

than 0.5. No symbols are used if the weight of bias is lesser than 0.25.

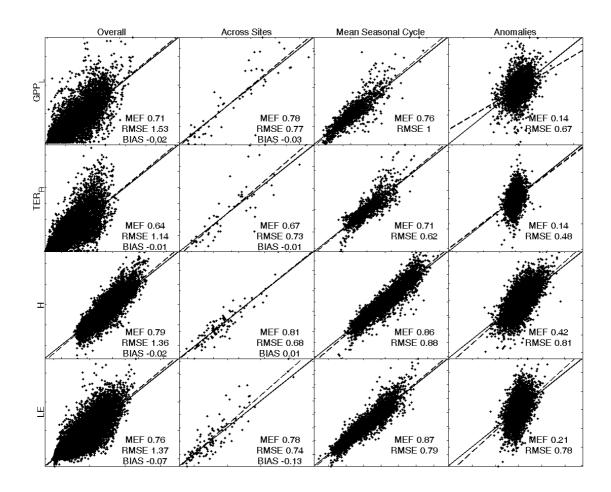


Fig. B1. Scatterplots of observed data by eddy covariance (y-axis) and the median ensemble of modeled fluxes by RS setup (x-axis). The panels from left to right are the eight days predictions, across sites variability, mean seasonal cycle and weekly anomalies. The fluxes considered here are GPP_L (first row), TER_R (second row), H (third row) and LE (fourth row).

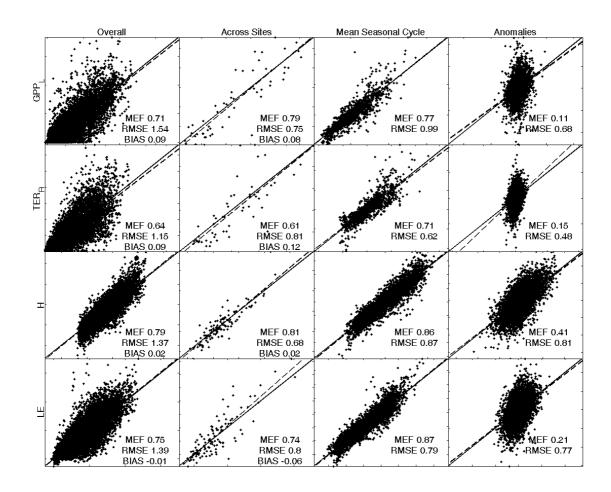


Fig. B2. As Fig. B1 but the predictions (x-axis) were obtained by the RS+METEO setup.