

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

3

4 G. Tramontana¹, M. Jung², G. Camps-Valls³, K. Ichii^{4,5}, B. Raduly^{1,6}, M. Reichstein², C. R.
5 Schwalm⁷, M. A. Arain⁸, A. Cescatti⁹, G. Kiely¹⁰, L. Merbold¹¹, P. Serrano-Ortiz¹², S.
6 Sickert¹³, S. Wolf¹⁴ and D. Papale¹.

7

8 ¹Department for Innovation in Biological, Agro-food and Forest systems (DIBAF), Univeristy of Tuscia,
9 Viterbo, 01100, Italy,

10 ²Max Planck Institute for Biogeochemistry, Jena, 07745, Germany;

11 ³Image Processing Laboratory (IPL), Paterna (València), 46980, Spain.

12 ⁴Department of Environmental Geochemical Cycle Research, Japan Agency for Marine-Earth Science and
13 Technology, Yokohama, 236-0001, Japan.

14 ⁵Center for Global Environmental Research, National Institute for Environmental Studies, Tsukuba, 305-
15 8506, Japan.

16 ⁶Department of Bioengineering Sapientia Hungarian University of Transylvania, Miercurea Ciuc, 530104,
17 Romania.

18 ⁷Woods Hole Research Center, Falmouth MA, 02540, USA.

19 ⁸School of Geography and Earth Sciences, McMaster University, Hamilton (Ontario), L8S4L8, Canada

20 ⁹Institute European Commission, Joint Research Centre, Institute for Environment and Sustainability, Ispra,
21 Ispra, 21027, Italy

22 ¹⁰Civil & Environmental Engineering and Environmental Research Institute, University College, Cork, T12
23 YN60, Ireland.

24 ¹¹Department of Environmental Systems Science, Institute of Agricultural Sciences, ETH Zurich, Zurich,
25 8092, Switzerland.

26 ¹²Department of Ecology, University of Granada, Granada, 18071, Spain.

27 ¹³Computer Vision Group, Friedrich Schiller University Jena, 07743 Jena, Germany

28 ¹⁴Department of Environmental Systems Science, ETH Zurich, Zurich, 8092, Switzerland.

30 **Abstract**

31

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

52

53 *Keywords:* Machine learning, carbon fluxes, energy fluxes, FLUXNET, remote sensing,

54 FLUXCOM

55

56

57 **1. Introduction**

58

59 Improving our knowledge of the carbon, water, and energy exchanges between
60 terrestrial ecosystems and the atmosphere is essential to better understand and model
61 the Earth's climate system (IPCC, 2007; Reich, 2010). In situ observations of these exchanges
62 are obtained by the eddy covariance technique, which directly measures turbulent fluxes
63 between ecosystems and the atmosphere (Aubinet et al., 2012; Baldocchi et al., 2014).
64 The large-scale measurement network, FLUXNET integrates site observations of these
65 fluxes globally and provides detailed time series of carbon and energy fluxes across
66 biomes and climates (Baldocchi et al., 2008). However, eddy-covariance measurements
67 are site-level observations, and spatial upscaling is required to estimate these fluxes at
68 regional to global scales.

69 The increasing number of eddy covariance sites across the globe has encouraged the
70 application of data-driven models by machine learning (ML) methods such as Artificial
71 Neural Networks (ANNs, Papale et al., 2003), Random Forest (RF, Tramontana et al.,
72 2015), Model Trees (MTE, Jung et al., 2009; Xiao et al., 2008, 2010) or Support Vector
73 Regression (SVR, Yang et al., 2006, 2007) to estimate surface-atmosphere fluxes from site
74 level to regional or global scales (e.g. Beer et al., 2010, Jung et al., 2010, 2011; Kondo et
75 al., 2015; Schwalm et al., 2010; Yang et al., 2007; Xiao et al., 2008, 2010). The ML
76 upscaled outputs are also increasingly used to evaluate land surface models (e.g., Anav et
77 al., 2013; Bonan et al., 2011; Ichii et al., 2009; Piao et al., 2013).

78 The key characteristic of data-driven models compared the process-based ones are the
79 the fact former's intrinsic observational nature, and that functional relationships are not

80 prescribed but rather emerge from ~~the~~ patterns found in the measurements. In this
81 context, data-driven models extract multivariate functional relationships between the in -
82 situ measured fluxes of the network and explanatory variables in an empirical way. The
83 explanatory variables are generally ~~coming~~ ^{originate} from satellite remote sensing, providing
84 information on vegetation state (e.g., vegetation indices) and other land surface
85 properties (e.g., surface temperature), along with continuous measurements of
86 meteorological variables at flux towers.

87 While ML-based upscaling provides a systematic approach to move from point-based flux
88 estimates to spatially explicit gridded fields, various sources of uncertainty exist. For
89 example, individual ML methods ~~might~~ ^{can} have different responses especially when these
90 models are applied beyond the conditions ~~sampled~~ ^{represented} by the training dataset (Jung et al.,
91 2009; Papale et al., 2015). The information content of the driving input variables may not
92 be sufficient to capture the variability of the fluxes in all conditions (Tramontana et al.,
93 2015). Moreover, remotely sensed and meteorological gridded datasets are affected by
94 uncertainties themselves. Remote sensing data contain noise, biases and gaps, and can
95 be perturbed by atmospheric effects or by the presence of snow. Meteorological gridded
96 datasets are known to contain product specific biases (Garnaud et al., 2014; Tramontana
97 et al., 2015; Zhao et al., 2012).

98 Thorough experiments using multiple data-driven models and explanatory variables are
99 an essential step to identify and assess limitations and sources of uncertainty in the
100 empirical upscaling approach. In this study, we present and evaluate an ensemble of ML
101 based empirical models to predict carbon and energy fluxes across FLUXNET sites. The
102 ~~participating~~ ^{included in this study} models were selected in the context of the FLUXCOM initiative, forming the
103 basis of subsequent global flux products. We perform^{ed} a consistent cross-validation for
104 two complementary experimental setups using: (1) eight days average fluxes based on

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

114

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

121

122

123 **2. Material and methods**

124

125 **2.1 Data**

126

127

128 **2.1.1 Eddy covariance study sites**

129

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

134

135

136 **2.1.2 Observation-based carbon and energy fluxes**

137 **HERE!!!**

138 All flux measurements were post-processed using standardized procedures of quality
139 control and gap-filled following Reichstein et al. (2005) and Papale et al. (2006). Estimates
140 of GPP and TER were derived from half-hourly NEE measurements using two independent
141 flux partitioning methods: (1) following Reichstein et al. (2005), where the temperature
142 sensitivity of ecosystem respiration is initially estimated from night-time NEE data and
143 then extrapolated to daytime to estimate TER and GPP, by subtracting NEE (negatively
144 signed for the carbon uptake) from TER; (2) following Lasslop et al. (2010), where daytime
145 NEE data is used to constrain a hyperbolic light response curve to directly estimate GPP
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 .

149 The half-hourly data were aggregated to daily values and screened according to multiple
150 quality criteria, as follow:

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);

153 2) we identified and removed obviously erroneous periods due to non-flagged instrument
154 or flux partitioning failures based on visual interpretation;

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

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

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

168

169

170 **2.1.2 Remote sensing data**

171

172 We collected data coming from Moderate Resolution Imaging Spectroradiometer
173 (MODIS) which provides data at a spatial resolution of 1km or better (Justice et al., 2002).

174 We used the cutout surroundings of 3x3 km pixels centered on the towers. We collected
175 and processed the following MODIS products: MOD11A2 Land Surface Temperature (LST;
176 Wan et al., 2002), MOD13A2 Vegetation Index (Normalized Difference Vegetation Index
177 (NDVI) and Enhanced Vegetation Index (EVI); Huete et al., 2002), MOD15A2 Leaf Area
178 Index (LAI) and Fraction of Absorbed Photosynthetic Active Radiation (FPAR; Myneni et
179 al., 2002), and MCD43A2 and MCD43A4 Bidirectional Reflectance Distribution Function

180 (BRDF) corrected surface reflectances (Schaaf et al., 2002). The BRDF-corrected surface
181 reflectance data were further processed to calculate the Normalized Difference Water
182 Index (NDWI) (Gao, 1996) and the Land Surface Water Index (LSWI) (Xiao et al., 2002).
183 These data were obtained from <http://daac.ornl.gov/MODIS/>.
184 The remote sensing data were further processed to improve data quality and data gaps
185 were filled to create continuous time-series data, and to minimize non-land surface
186 signals. We adopted the following processing scheme: we identified good quality pixels
187 by the using the quality assurance/quality criteria (QA/QC) included in the MODIS
188 product. If more than 25% of pixels had good quality at the time of snapshot, the average
189 of good quality pixels were assigned as the actual value. Otherwise, the data at the time
190 snapshot were marked as blank (no data). Then, we created the mean seasonal variations
191 from 2000-2012 using only good pixels data and the data gaps in the processed data were
192 filled using the mean seasonal variation. Only MOD13 is provided with 16 days
193 composite, and eight days data were created by assigning the 16 days composite value to
194 the corresponding two eight days periods.

195

196

197 **2.1.3 Meteorological data**

198

199 The in situ measured air temperature (T_{air}), global radiation (R_g), VPD, and precipitation
200 were used after data screening according to the criteria 1) and 2) as for the measured
201 fluxes (see Sect. 2.1.2). We also used long-term time series of these variables from ERA-
202 Interim for the period 1989-2010 (Dee et al., 2011), which were bias-corrected for each
203 site based on the overlapping period of in situ measurements (see [http://www.bgc-
204 jena.mpg.de/~MDIwork/meteo/](http://www.bgc-jena.mpg.de/~MDIwork/meteo/)). These long-term meteorological data are primarily

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

210

211

212 **2.2 Participating ML methods**

213

214 We chose 11 ML algorithms for regression from four broad families: tree-based methods,
215 regression splines, neural networks, kernel methods. Moreover a comprehensive review
216 of ML algorithms in biophysical parameter estimation can be found in Verrelst et al.
217 (2015).

218

219 Tree based methods

220 These methods construct hierarchical binary decision trees. The inner nodes of the tree
221 hold decision rules according to explanatory variables (e.g. less/greater than X_1),
222 recursively splitting the data into subspaces. The leaf nodes at the end of the decision
223 tree contain models for the response variable. Because a single tree is generally not
224 effective enough to cope with strong non-linear multivariate relationships, ensembles of
225 trees are often used. We applied two different tree ensemble methods: (1) Random
226 Forests (RF) which combines regression trees grown from different bootstrap samples
227 and randomly selected features at each split node (Breiman, 2001; Ho, 1998); and (2)
228 Model Tree Ensembles (MTE) which combine model trees (Jung et al., 2009). The main
229 difference between regression and model trees is the prediction model in the leaf node: a

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

235

236 Regression splines

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

241

242 Neural networks

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

254

255 Kernel methods

256 Kernel methods (Shawe-Taylor and Cristianini, 2004) owe their name to the use of kernel
257 functions, which measures similarities between input data examples. Among the
258 available kernel methods we used: (1) support vector regression (SVR) (Vapnik et al.,
259 1997), (2) kernel ridge regression (KRR) (Shawe-Taylor and Cristianini, 2004), and (3)
260 Gaussian process regression (GPR) (Rasmussen, 2006; Verrelst et al., 2012). The SVR
261 defines a linear prediction model over mapped samples to a much higher dimensional
262 space, which is non-linearly related to the original input (Verrelst et al., 2012, Yang et al.,
263 2007). The KRR is considered as the kernel version of the regularized least squares linear
264 regression (Shawe-Taylor and Cristianini, 2004, Verrelst et al., 2012). The GPR is a
265 probabilistic approximation to nonparametric kernel-based regression, and both a
266 predictive mean (point-wise estimates) and predictive variance (error bars for the
267 predictions) can be derived. We also used a hybrid approach combining RF with simple
268 decision stumps in the inner nodes and GPR for prediction in the leaf nodes (Fröhlich et
269 al., 2012).

270

271

272 **2.3 Experimental design**

273

274

275 **2.3.1. Experiment setups**

276

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

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

296

297

298 **2.3.2. Variable selection**

299

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

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

313 For each setup we selected a small subset of variables best suited to predict the target
314 fluxes using a variable selection search algorithm. Variable selection is an important
315 component in the spatial upscaling because the accuracy of predictions improves and the
316 computational costs of the global predictions are minimized. We used the Guided Hybrid
317 Genetic Algorithm (GHGA) published by Jung and Zscheischler (2013), which was
318 designed for variable selection problems with many candidate predictor variables and
319 computationally expensive cost functions. The GHGA requires the training of a regression
320 algorithm (here RF) to estimate the cost associated with selected variable subsets (see S5
321 for details).

322 Instead of doing a computationally demanding variable selection for each individual flux,
323 variable selection runs were performed for the RS and RS+METEO setups and separately
324 for carbon and energy fluxes. This procedure has the advantage that the resulting global
325 products originate from a consistent set of predictor variables. The selected variables for
326 the prediction of carbon and energy fluxes are listed in Table 2.

327

328

329 **2.3.3. Model training**

330

331 The capability of ML methods to spatially extrapolate carbon and energy fluxes was
332 evaluated by a 10-fold cross-validation strategy. The training datasets were stratified into
333 10-folds, each one roughly containing 10% of the data. Entire sites were assigned to each
334 fold (Jung et al., 2011). The target values for each fold were predicted based on the
335 training using the remaining nine folds. Due to computational expense of the RS+METEO
336 setup, only one method representing each “family” – multiple regressions, RF, MARS,
337 ANN and KRR – was trained.

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

342

343

344 **2.3.4. Model evaluation**

345

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

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

355 Pearson's linear correlation coefficient (ρ), the coefficient of determination (R^2) and the
356 ratio of variance (ROV).

357 MEF (Nash and Sutcliffe, 1970), if the capability of a model to estimate a target variables is
358 better than a reference model. If the reference model is the mean value of the target,
359 MEF can be calculated as:

360

$$361 \quad MEF = 1 - \frac{\sum_{i=1}^n (x_i - y_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (1)$$

362

363 where x_i and y_i were the predicted and the observed values respectively and \bar{y} is the
364 mean value of the observations (here the reference model). MEF can vary between -inf to
365 1; if $MEF > 0$ the predictive skill of the model is better than the mean ($MEF = 1$ for the
366 ideal model), if $MEF=0$ the predictive skill of the model is equivalent to the mean, finally if
367 $MEF < 0$, the predictive skill of the mean value of the target is better than the model.

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

369

$$370 \quad RMSE = \sqrt{\frac{\sum_{i=1}^n (x_i - y_i)^2}{n}} \quad (2)$$

371

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

373

$$374 \quad BIAS = \frac{\sum_{i=1}^n (x_i - y_i)}{n} \quad (3)$$

375

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

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

382

$$383 \quad \rho = \frac{\sigma_{xy}}{\sigma_x \sigma_y} \quad (4)$$

384

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

387 We evaluated the overall predictive skill of the models, evaluating the consistency among
388 trained ML approaches and across the experimental setup. Then we evaluated the
389 capability of the regression models to predict site-specific mean fluxes, mean seasonal
390 cycle (MSC), and anomalies (Jung et al., 2011). The MSC per site was calculated using the
391 averaged values for each eight days period across all available years, but only when at
392 least two values (i.e., years) for each eight days period were available. To assess the
393 mean values of the study sites, we calculated the mean of the MSC if at least 50% of the
394 46 eight daily values were present, whereas the weekly anomalies were calculated as the
395 deviation of a flux value from the MSC. Finally, the mean site value was removed from
396 the MSC to disentangle the seasonal variation from the mean, thus making the MSC and
397 mean complementary.

398 We also analyzed the performance for the different Köppen climate zone and IGBP plant
399 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.

402

403

404 **3. Results and Discussions**

405

406

407 **3.1 Overview**

408

409 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 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.

416

417

418 **3.2 Predictive skill of carbon and energy fluxes**

419

420 Predictive skill of the ensemble median estimate clustered into tiers whereby energy
421 fluxes are uniformly better predicted than carbon fluxes: $R_n > H/LE/GPP > TER > NEE$
422 (Table 3). The highest skill levels as exhibited by net radiation shows near perfect
423 agreement; R_n displays a model efficiency (MEF) of 0.91-0.92 and a correlation of 0.96.
424 The decline in skill for the second tier fluxes is ca. 15% to 20%; MEF 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 The overall skill profile in this study confirms previous upscaling efforts (Jung et al., 2011;
435 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 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 and canopy properties, which were strongly related to GPP, were well represented by the

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

457

458

459 **3.3 Are the flux predictions consistent between RS and RS+METEO?**

460

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

474

475

476 **3.4 How different are the predictions of the various ML algorithms?**

477

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

495

496

497 **3.5 How does the performance differ among capturing the across-sites, seasonal and**
498 **the deviations from the mean seasonal cycle variability?**

499

500 Decomposing FLUXNET data into across-sites variability, mean seasonal cycle, and
501 interannual variability components (Sect. 2.3.4) revealed clear gradients in predictive skill
502 (Table 5 and Fig. 2). Across-sites variability was in general well-captured by the ML (R^2
503 range: 0.61 to 0.81 except for NEE) and the best predicted pattern for GPP and TER. This
504 suggests that ML are suitable to reproduce the spatial pattern of mean annual fluxes.
505 The variability in the mean seasonal cycle (at weekly time scale) was also uniformly well
506 predicted (R^2 between 0.67-0.77 for GPP and TER, and between 0.86-0.98 for the energy
507 fluxes) and the best predicted pattern for energy fluxes in particular for LE and Rn.
508 The importance of seasonality in carbon and energy annual fluxes is known (Joiner et al.,
509 2014; Jung et al., 2011; Merbold et al., 2009; Wolf et al., 2011) and biases in its dynamic
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
512 parameters controlling seasonality are prescribed, reducing the possibility of biases.
513 In contrast, interannual variability is generally poorly captured by all the ML approaches
514 used with only H and Rn showing an R^2 greater than 0.4. This low predictive skill holds
515 regardless of whether weekly, monthly (Jung et al., 2011), or annual time steps are used
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
518 and target variables that plays a major role when small differences (like in the interannual
519 variability) are predicted. The slightly better performances when sensible heat flux is
520 estimated could be due to the lower uncertainty in this flux respect to the others (only
521 one sensor used, the sonic anemometer, in contrast 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
523 used as driver. In any case, predicting interannual variability remains one of the largest
524 challenges in the context of empirical upscaling.

525 NEE is confirmed to be the most difficult and consequently poorest predicted flux (Table
526 3). NEE shows considerably lower skill relative to the other fluxes for across-sites
527 variability ($R^2 = 0.46$), the mean seasonal cycle ($R^2 = 0.59$), and interannual variability ($R^2 =$
528 0.13 , TER_L is lowest at 0.10).

529

530

531 **3.6 How does the performance differ among climate zones or ecosystem types?**

532

533 Using climate zone and plant functional type (PFT) to disaggregate ML methods
534 performances we find that in general energy fluxes are better predicted than carbon
535 fluxes among the different climate zone and PFTs (Fig. 3 and Appendix C). The median R^2
536 between simulation and observation for carbon fluxes (excluding NEE) is greater than 0.6
537 for more than 75% of the PFT and climate zone, while in the energy fluxes an R^2 greater
538 than 0.7 is found for more than the 85% of the PFT and climate zone (in all sites for R_n).

539 NEE is again consistently poorly predicted (low R^2 and high relative RMSE; Fig. 3), apart
540 from deciduous broadleaf forests (DBF) and MF where a marginal improvement is
541 evident. The better performance in these two vegetation types could be related to the
542 higher seasonal variance of NEE in comparison with the other PFTs that is a pattern more
543 consistent with the seasonal variance of the used drivers.

544 Overall the ML methods show poor prediction capability in tropics and evergreen
545 broadleaf forests (EBF). Possible explanations are the absence of a clear seasonal cycle
546 traceable by the remote sensing signal (evergreen vegetation) and a low variance in their
547 seasonal cycle that is challenging to explained mathematically and capture with a model.
548 (Sims et al., 2008; Yebra et al., 2015; Yuan et al., 2010). In addition, the difficulty in

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

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

559

560

561 **4. Conclusions**

562

563 The ML methods presented and evaluated in this study have shown high capability to
564 predict carbon and energy fluxes, in particular the between-site variability and the
565 seasonal variations, with a general tendency of increasing performance in the following
566 order: NEE, TER, GPP, LE, H, and Rn. The relatively poor performance for NEE likely results
567 from factors that cannot be easily accounted for in ML based modelling approaches, such
568 as legacies of site history (e.g. disturbances, management, age and stocks). Future
569 progress in this direction requires the reconstruction of the relevant management and
570 disturbance history, trying to integrate information from forest inventories, high
571 resolution satellites such LANDSAT and high resolution biomass data from radar and
572 LIDAR with the aim to improve model performance. The better results obtained for the
573 energy fluxes (LE and H) in comparison to the carbon fluxes (GPP and TER) could be
574 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
576 and TER due to the use of flux partitioning methods based on NEE measurements.

577 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
580 number of eddy-covariance sites, in particular new sites in poorly represented regions
581 will likely improves the predictive skill in the future. This is particularly relevant since
582 tropical areas account for a disproportionate share of the global water and carbon cycle
583 (Beer et al., 2010).

584 The deviations from the mean seasonal cycle (weekly anomalies) are still poorly captured
585 by the ML methods. We expected the RS+METEO approach to perform better regarding
586 the prediction of anomalies as meteorological drivers were included and the noise in
587 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
589 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
591 accounted for in the predictors. Hence, the prediction of interannual anomalies remains a
592 major unresolved research topic.

593 The predictions for ecosystem fluxes across FLUXNET by different ML techniques and by
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
597 slightly larger than among different ML methods, suggesting that future activities should
598 concentrate on identifying new driver variables to further improve the performance of
599 fluxes predictions. Nevertheless, we recommend using the ensemble median estimate of

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

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

610

611

612 **Appendix A: Median performance of the methods.**

613

614 In table A1 we reported, for both setups, the median value of skill metrics (MEF, RMSE,
615 and absolute value of BIAS) realized by singular ML and their related variability such
616 estimated as the median absolute deviation (MAD) from the median multiplied per
617 1.4826 (see Jung et al., 2009 for details)

618

619

620 **Appendix B: scatterplot between the observations and the predictions by the median** 621 **ensemble of ML.**

622

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

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

628

629

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

631

632 At follow we reported the median estimate of site-by-site R^2 , RMSE, and absolute bias per
633 PFT and climate zones.

634

635

636 **Acknowledgments**

637 G. Tramontana was supported by the GEOCARBON EU FP7 project (GA 283080). D.
638 Papale, M. Jung and M. Reichstein thank the support of the BACI H2020 (GA 640176) EU
639 project. G. Camps-Valls wants to acknowledge the support by an ERC Consolidator Grant
640 with grant agreement 647423 (SEDAL). K. Ichii was supported by Environment Research
641 and Technology Development Funds (2-1401) from the Ministry of the Environment of
642 Japan and the JAXA Global Change Observation Mission (GCOM) project (#115). C. R.
643 Schwalm was supported by National Aeronautics and Space Administration (NASA) Grants
644 #NNX12AP74G, #NNX10AG01A, and #NNX11AO08A. M. A. Arain thanks the support of
645 Natural Sciences and Engineering Research Council (NSREC) of Canada. P. Serrano Ortiz
646 was partially supported by the Spanish Ministry of Economy and Competitiveness though
647 the project CGL2014-52838-C2-R(GEISpain). S. Wolf acknowledges support from a Marie
648 Curie International Outgoing Fellowship (European Commission, grant 300083). This work
649 used Eddy Covariance data acquired by the FLUXNET community and in particular by the

650 following networks: AmeriFlux (U.S. Department of Energy, Biological and Environmental
651 Research, Terrestrial Carbon Program (DE-FG02-04ER63917 and DE-FG02-04ER63911)),
652 AfriFlux, AsiaFlux, CarboAfrica, CarboEuropeIP, CarboItaly, CarboMont,ChinaFlux, Fluxnet-
653 Canada (supported by CFCAS, NSERC, BIOCAP, Environment Canada, and NRCan),
654 GreenGrass, KoFlux, LBA, NECC, OzFlux, TCOS-Siberia, USCCC. We acknowledge the
655 financial support to the eddy covariance data harmonization provided by CarboEuropeIP,
656 FAO-GTOS-TCO, iLEAPS, Max Planck Institute for Biogeochemistry, National Science
657 Foundation, University of Tuscia and US Department of Energy and the databasing and
658 technical support from Berkeley Water Center, Lawrence Berkeley National Laboratory,
659 Microsoft Research eScience, Oak Ridge National Laboratory, University of California -
660 Berkeley, University of Virginia.

661

662

663 **5. References**

664

665 Amiro, B. D., Barr, A. G., Barr, J. G., Black, T. A., Gracho, R., Brown, M., Chen, J., Clark, K. L.,
666 Davis, K. J., Desai, A. R., Dore, S., Engel, V., Fuentes, J. D., Goldstein, A. H., Goulden, M. L.,
667 Kolb, T. E., Lavigne, M. B., Law, B. E., Margolis, H. A., Martin, T., McCaughey, J. H., Misson,
668 L., Montes, Helu, M., Noormets, A., Randerson, J. T., Starr, G. and Xiao, J.: Ecosystem
669 carbon dioxide fluxes after disturbance in forests of North America. *J Geophys Res-*
670 *Biogeo*, 115, G00K02, doi:10.1029/2010JG001390, 2010.

671

672 Alonso Fernández, J.R., DíazMuñiza, C., Garcia, Nieto, P.J., de Cos, Juez, F.J, Sánchez,
673 Lasheras, F. and Roqueñic, M.N.: Forecasting the cyanotoxins presence in fresh waters: A

674 new model based on genetic algorithms combined with the MARS technique, *Ecol Eng*,
675 53, 68–78. doi:10.1016/j.ecoleng.2012.12.015, 2013.

676

677 Anav, A., Friedlingstein, P., Kidston, M., Bopp, L., Ciais, P., Cox, P., Jones, C., Jung, M.,
678 Myneni, R. and Zhu Z.: Evaluating the land and ocean components of the global carbon
679 cycle in the cmip5 earth system models, *J Climate*, 26, 6801–6843, doi:
680 <http://dx.doi.org/10.1175/JCLI-D-12-00417.1>, 2013.

681

682 Aubinet, M., Vesala, T. and Papale, D.: *Eddy Covariance: A Practical Guide to*
683 *Measurement and Data Analysis*, Springer, Dordrecht Heidelberg London New York, 460,
684 2012.

685

686 Baldocchi, D.: Breathing of the terrestrial biosphere: lessons learned from a global
687 network of carbon dioxide flux measurement systems, *Aust J Bot*, 56, 1–26,
688 <http://dx.doi.org/10.1071/BT07151>, 2008.

689

690 Baldocchi, D.: Measuring fluxes of trace gases and energy between ecosystems and the
691 atmosphere – the state and future of the eddy covariance method, *Global Change Biol*,
692 20, 3600–3609, DOI: 10.1111/gcb.12649, 2014.

693

694 Beer, C., Reichstein, M., Tomelleri, E., Ciais, P., Jung, M., Carvalhais, N., Rödenbeck, C.,
695 Arain, A., M., Baldocchi, D., Bonan, B., G., Bondeau, A., Cescatti, A., Lasslop, G., Lindroth,
696 A., Lomas, M., Luyssaert, S., Margolis, H., Oleson, W. K., Rouspard, O., Veenendaal, E.,
697 Viovy, N., Woodward, I. F. and Papale, D.: *Terrestrial Gross Carbon Dioxide Uptake: Global*

698 Distribution and Covariation with Climate, *Science*, 329, 834-838, doi:
699 10.1126/science.1184984, 2010.

700

701 Bell, T. W., Menzer, O., Troyo-Diéquez, E. and Oechel, W.: Carbon dioxide exchange over
702 multiple temporal scales in an arid shrub ecosystem near La Paz, Baja California Sur,
703 Mexico, *Global Change Biol*, 18, 2570–2582, doi:10.1111/j.1365-2486.2012.02720.x.,
704 2012.

705

706 Bonan, G. B., Lawrence, P. J., Oleson, K. W., Levis, S., Jung, M., Reichstein, M., Lawrence,
707 D. M. and Swenson, S. C.: Improving canopy processes in the Community Land Model
708 version 4 (CLM4) using global flux fields empirically inferred from FLUXNET data, *J*
709 *Geophys Res-Bioge*, 116, G02014, doi:10.1029/2010JG001593, 2011.

710

711 Breiman, L.: Random Forests, *Mach. Learn.*, 45 (1), 5–32, doi:10.1023/A:1010933404324,
712 2001.

713

714 Dee, D. P., Uppala, S. M., Simmons, A. J., Berrisford, P., Poli, P., Kobayashi, S., Andrae, U.,
715 Balmaseda, M. A., Balsamo, G., Bauer, P., Bechtold, P., Beljaars, A. C. M., van de Berg, L.,
716 Bidlot, J., Bormann, N., Delsol, C., Dragani, R., Fuentes, M., Geer, A. J., Haimberger, L.,
717 Healy, S. B., Hersbach, H., Hólm, E. V., Isaksen, L., Kållberg, P., Köhler, M., Matricardi, M.,
718 McNally, A. P., Monge-Sanz, B., M., Morcrette, J.-J., Park, B.-K., Peubey, C., de Rosnay, P.,
719 Tavolato, C., Thépaut, J.-N. and Vitart, F.: The ERA-Interim reanalysis: configuration and
720 performance of the data assimilation system, *Q.J.R. Meteorol Soc*, 137, 553–597, doi:
721 10.1002/qj.828, 2011.

722

723 Frank, D., Reichstein, M., Bahn, M., Thonicke, K., Frank, D., Mahecha, M. D., Smith, P.,
724 Van Der Velde, M., Vicca, S., Babst, F., Beer, C., Buchmann, N., Canadell, J. G., Ciais, P.,
725 Cramer, W., Ibrom, A., Miglietta, F., Poulter, B., Ramming, A., Seneviratne, S. I., Walz, A.,
726 Wattenbach, M., Zavala, M. A. and Zscheischler, J.: Effects of climate extremes on the
727 terrestrial carbon cycle: concepts, processes and potential future impacts, *Global Change*
728 *Biol*, 21, 2861–2880, doi: 10.1111/gcb.12916, 2015.

729

730 Friedman, J. H.: Multivariate Adaptive Regression Splines, *Ann. Statist.*, 19, 1-67,
731 doi:10.1214/aos/1176347963, 1991.

732

733 Fröhlich, B., Rodner, E., Kemmler, M. and Denzler, J.: Large-scale gaussian process
734 classification using random decision forests, *S. Mach. Perc.*, 22 (1), 113–120, DOI
735 10.1007/s00138-012-0480-y, 2012.

736

737 Gao, B. C.: NDWI-A Normalized difference water index for remote sensing of vegetation
738 liquid water from space, *Remote Sens Environ*, 58, 257-266, doi:10.1016/S0034-
739 4257(96)00067-3, 1996.

740

741 Garnaud, C., Sushama, L. and Arorab, V. K.: The effect of driving climate data on the
742 simulated terrestrial carbon pools and fluxes over North America, *Int J Climatol*, 34, 1098-
743 1110, DOI: 10.1002/joc.3748, 2014.

744

745 Giri, C., Zhu, Z. and Reed B.: A comparative analysis of the Global Land Cover 2000 and
746 MODIS land cover data sets, *Remote Sens Environ*, 94, 123–132,
747 doi:10.1016/j.rse.2004.09.005, 2005

748

749 Gupta, H. V., Kling, H., Yilmaz, K. K. and Martinez, G. F.: Decomposition of the mean
750 squared error and NSE performance criteria: Implications for improving hydrological
751 modelling, *J Hydrol*, 20, 80-91, doi:10.1016/j.jhydrol.2009.08.003, 2009.

752

753 Haykin, S.: *Neural Networks – A Comprehensive Foundation* (2nd ed.), Prentice Hall.,
754 1999.

755

756 Ho, T. K.: The Random Subspace Method for Constructing Decision Forests, *IEEE T Pattern*
757 *Anal*, 20 (8), 832–844, doi:10.1109/34.709601, 1998.

758

759 Huete, A., Didan, K., Miura, T., Rodriguez, E. P., Gao, X. and Ferreira, L.G.: Overview of the
760 radiometric and biophysical performance of the MODIS vegetation indices, *Remote Sens*
761 *Environ*, 83, 195–213, doi:10.1016/S0034-4257(02)00096-2, 2002.

762

763 Ichii, K., Wang, W., Hashimoto, H., Yang, F., Votava, P., Michaelis, A. R. and Nemani, R. R.:
764 Refinement of rooting depths using satellite-based evapotranspiration seasonality for
765 ecosystem modeling in California, *Agr Forest Meteorol*, 149, 1907-1918,
766 doi:10.1016/j.agrformet.2009.06.019, 2009.

767

768 Ichii, K., Suzuki, T., Kato, T., Ito, A., Hajima, T., Ueyama, M., Sasai, T., Hirata, R., Saigusa,
769 N., Ohtani, Y. and Takagi, K.: Multi-model analysis of terrestrial carbon cycles in Japan:
770 limitations and implications of model calibration using eddy flux observations,
771 *Biogeosciences*, 7, 2061–2080, doi:10.5194/bg-7-2061-2010, 2010.

772

773 IPCC: Climate Change 2007: Synthesis Report. Contribution of Working Groups I, II and III
774 to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change
775 [Core Writing Team, Pachauri, R.K and Reisinger, A. (eds.)]. IPCC, Geneva, Switzerland,
776 104, 2007.

777

778 Joiner, J., Yoshida, Y., Vasilkov, A. P., Schaefer, K., Jung, M., Guanter, L., Zhang, Y., Garrity,
779 S., Middleton, E. M., Huemmrich, K. F., Guh, L. and Belelli Marchesini, L.: The seasonal
780 cycle of satellite chlorophyll fluorescence observations and its relationship to vegetation
781 phenology and ecosystem atmosphere carbon exchange, *Remote Sens Environ*, 152, 375–
782 391, <http://dx.doi.org/10.1016/j.rse.2014.06.022>, 2014.

783

784 Jung, M., and Zscheischler, J.: A Guided Hybrid Genetic Algorithm for Feature Selection
785 with Expensive Cost Functions, *Procedia Computer Science*, 18, 2337-2346, doi:
786 10.1016/j.procs.2013.05.405, 2013.

787

788 Jung, M., Verstraete, M., Gobronz, N., Reichstein, M., Papale, D., Bondeau, A., Robustelli,
789 M. and Pinty, R.: Diagnostic assessment of European gross primary production, *Global
790 Change Biol*, 14, 2349–2364, doi: 10.1111/j.1365-2486.2008.01647.x, 2008.

791

792 Jung, M., Reichstein, M. and Bondeau, A.: Towards global empirical upscaling of FLUXNET
793 Eddy Covariance observations: validation of a model tree ensemble approach using a
794 biosphere model, *Biogeosciences*, 6, 2001-2013, doi:10.5194/bg-6-2001-2009, 2009.

795

796 Jung, M., Reichstein, M., Ciais, P., Seneviratne, S. I., Sheffield, J., Goulden, M. L., Bonan,
797 G., Cescatti, A., Chen, J., de Jeu, R., Dolman, A. J., Eugster, W., Gerten, D., Gianelle, D.,

798 Gobron, N., Heinke, J., Kimball, J., Law, B. E., Montagnani, L., Mu, Q., Mueller, B., Oleson,
799 K., Papale, D., Richardson, A. D., Rouspard, O., Running, S., Tomelleri, E., Viovy, N.,
800 Weber, U., Williams, C., Wood, E., Zaehle, S. and Zhang, K.: Recent decline in the global
801 land evapotranspiration trend due to limited moisture supply, *Nature Letter*, 467, 951-
802 953, doi:10.1038/nature09396, 2010.

803

804 Jung, M., Reichstein, M., Margolis, H. A., Cescatti, A., Richardson, A. D., Arain, M. A.,
805 Arneth, A., Bernhofer, C., Bonal, D., Chen, J., Gianelle, D., Gobron, N., Kiely, G., Kutsch,
806 W., Lasslop, G., Law, B. E., Lindroth, A., Merbold, L., Montagnani, L., Moors, E. J., Papale,
807 D., Sottocornola, M., Vaccari, F. and Williams, C.: Global patterns of land-atmosphere
808 fluxes of carbon dioxide, latent heat, and sensible heat derived from eddy covariance,
809 satellite, and meteorological observations, *Journal of geophys res-Biogeo*, 116, G00J07,
810 doi:10.1029/2010JG001566, 2011.

811

812 Justice, C. O., Townshend, J. R. G., Vermote, E. F., Masuoka, E., Wolfe, R. E., Saleous, N.,
813 Roy, D. P. and Morisette, J. T.: An overview of MODIS Land data processing and product
814 status, *Remote Sens Environ*, 83, 3–15, doi:10.1016/S0034-4257(02)00084-6, 2002.

815

816 Kondo, M., Ichii, K., Takagi, H. and Sasakawa, M.: Comparison of the data-driven top-
817 down and bottom-up global terrestrial CO₂ exchanges: GOSAT CO₂ inversion and
818 empirical eddy flux upscaling, *Journal of geophys res-Biogeo*, 120, 1226–1245,
819 doi:10.1002/2014JG002866, 2015.

820

821 Lasslop, G., Reichstein, M., Papale, D., Richardson, A. D., Arneth, A., Barr, A., Stoy, P. and
822 Wohlfahrt, G.: Separation of net ecosystem exchange into assimilation and respiration

823 using a light response curve approach: critical issues and global evaluation, *Global Change*
824 *Biol*, 16, 187-208, doi:10.1111/j.1365-2486.2009.02041.x, 2010.

825

826 Merbold, L., Ardö, J., Arneth, A., Scholes, R. J., Nouvellon, Y., de Grandcourt, A., Archibald,
827 S., Bonnefond, J. M., Boulain, N., Brueggemann, N., Bruemmer, C., Cappelaere, B.,
828 Ceschia, E., El-Khidir, H. A. M., El-Tahir, B. A., Falk, U., Lloyd, J., Kergoat, L., Le Dantec, V.,
829 Mougin, E., Muchinda, M., Mukelabai, M. M., Ramier, D., Roupsard, O., Timouk, F.,
830 Veenendaal, E. M. and Kutsch, W. L.: Precipitation as driver of carbon fluxes in 11 African
831 ecosystems, *Biogeosciences*, 6, 1027–1041, doi:10.5194/bg-6-1027-2009, 2009, 2009.

832

833 Myneni, R.B., Hoffman, S., Knyazikhin, Y., Privette, J.L., Glassy, J., Tian, Y., Wang, Y., Song,
834 X., Zhang, Y., Smith, G.R., Lotsch, A., Friedl, M., Morisette, J.T., Votava, P., Nemani, R.R.,
835 and Running, S.W.: Global products of vegetation leaf area and fraction absorbed PAR
836 from year one of MODIS data, *Remote Sens Environ*, 83, 214–231, doi:10.1016/S0034-
837 4257(02)00074-3, 2002.

838

839 Nash, J. E. and Sutcliffe J. V.: River flow forecasting through conceptual models part I: A
840 discussion of principles, *Journal Hydrol*, 10, 282–290, doi:10.1016/0022-1694(70)90255-6,
841 1970.

842

843 Papale, D. and Valentini, R.: A new assessment of European forests carbon exchanges by
844 eddy fluxes and artificial neural network spatialization, *Global Change Biol*, 9, 525–535,
845 doi: 10.1046/j.1365-2486.2003.00609.x, 2003.

846

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

851

852 Papale, D., Black, T. A., Carvalhais, N., Cescatti, A., Chen, J., Jung, M., Kiely, G., Lasslop, G.,
853 Mahecha, D. M., Margolis, H., Merbold, L., Montagnani, L., Moors, E., Olesen, J. E.,
854 Reichstein, M., Tramontana, G., van Gorsel, E., Wohlfahrt, G. and Ráduly, B.: Effect of
855 spatial sampling from European flux towers for estimating carbon and water fluxes with
856 artificial neural networks, *Journal of geophys res-Biogeo*, 120, 1941-1957,doi:
857 10.1002/2015JG00299, 2015.

858

859 Paruelo, J. M., Piñero, G., Oyonarte, C., Alcaraz, D., Cabello, J. and Escribano, P.: Temporal
860 and spatial patterns of ecosystem functioning in protected arid areas in southeastern
861 Spain, *Appl Veg Sci*, 8, 93–102, doi: [http://dx.doi.org/10.1658/1402-](http://dx.doi.org/10.1658/1402-2001(2005)008[0093:TASPOE]2.0.CO;2)
862 [2001\(2005\)008\[0093:TASPOE\]2.0.CO;2](http://dx.doi.org/10.1658/1402-2001(2005)008[0093:TASPOE]2.0.CO;2), 2005.

863

864 Piao, S., Sitch, S., Ciais, P., Friedlingstein, P., Peylin, P., Wang, X., Ahlström, A., Anav, A.,
865 Canadell, J. G., Cong, N., Huntingford, C., Jung, M., Levis, S., Levy, P. E., Li, J., Lin, X.,
866 Lomas, M. R., Lu, M., Luo, Y., Ma, Y., Myneni, R. B., Poulter, B., Sun, Z., Wang, T., Viovy,
867 N., Zaehle, S. and Zeng, N.: Evaluation of terrestrial carbon cycle models for their
868 response to climate variability and to CO₂ trends, *Glob Change Biol.*, 19, 2117–2132,
869 doi:10.1111/gcb.12187, 2013.

870

871 Rasmussen C. E. and Williams C. K. I.: Gaussian Processes for Machine Learning, the MIT
872 Press, ISBN 026218253X, 2006.

873

874 Reichstein, M., Falge, E., Baldocchi, D., Papale, D., Aubinet, M., Berbigier, P., Bernhofer,
875 C., Buchmann, N., Gilmanov, T., Granier, A., Grünwald, T., Havránková, K., Ilvesniemi, H.,
876 Janous, D., Knohl, A., Laurila, T., Lohila, A., Loustau, D., Matteucci, G., Meyers, T.,
877 Miglietta, F., Ourcival, J.-M., Pumpanen, J., Rambal, S., Rotenberg, E., Sanz, M., Tenhunen,
878 J., Seufert, G., Vaccari, F., Vesala, T., Yakir, D., and Valentini R.: On the separation of net
879 ecosystem exchange into assimilation and ecosystem respiration: Review and improved
880 algorithm, *Global Change Biol*, 11, 1424–1439, doi:10.1111/j.1365-2486.2005.001002.x,
881 2005.

882

883 Reich, P. B.: The carbon dioxide exchange, *Science*, 329, 774-775,
884 <http://dx.doi.org/10.1126/science.1194353>, 2010.

885

886 Schwalm C. R., Williams C. A., Schaefer K., Anderson R., Arain M. A., Baker I., Barr A.,
887 Black T. A., Chen G., Chen J. M., Ciais P., Davis K. J., Desai A., Dietze M., Dragoni D., Fischer
888 M. L., Flanagan L. B., Grant R., Gu L., Hollinger D., Izaurralde R. C., Kucharik C., Lafleur P.,
889 Law B. E., Li L., Li Z., Liu S., Lokupitiya E., Luo Y., Ma S., Margolis H., Matamala R.,
890 McCaughey H., Monson R. K., Oechel W. C., Peng C., Poulter B., Price D. T., Riciutto D. M.,
891 Riley W., Sahoo A. K., Sprintsin M., Sun J., TI. H., Tonitto C., Verbeeck H., Verma S. B.: A
892 model-data intercomparison of CO₂ exchange across North America: Results from the
893 North American Carbon Program site synthesis, *Journal of geophys res-Biogeo*, 115,
894 G00H05, doi:10.1029/2009JG001229, 2010.

895

896 Schaaf, C. B., Gao, F., Strahler, A. H., Lucht, W., Li, X., Tsang, T., Strugnell, N. C., Zhang, X.,
897 Jin, Y., Muller, J-P., Lewis, P., Barnsley, M., Hobson, P., Disney, M., Roberts, G.,
898 Dunderdale, M., Doll, C., d'Entremont, R. P., Hu, B., Liang, S., Privette, J. L. and Roy, D.:
899 First operational BRDF, albedo nadir reflectance products from MODIS, *Remote Sens*
900 *Environ*, 83, 135–148, doi:10.1016/S0034-4257(02)00091-3, 2002.

901

902 Shawe-Taylor, J. and Cristianini, N.: *Kernel Methods for Pattern Analysis*, Cambridge
903 University Press, 2004.

904

905 Shirmohammadi, R., Ghorbani, B., Hamed, M., Hamed, M. H., and Romeo, L. M.:
906 Optimization of mixed refrigerant systems in low temperature applications by means of
907 group method of data handling (GMDH), *Journal of Natural Gas Science and Engineering*,
908 26, 303-312, doi:10.1016/j.jngse.2015.06.028, 2015.

909

910 Sims, D. A., Rahman, A. F., Cordova, V. D., El-Masri, B. Z., Baldocchi, D. D., Bolstad, P. V.,
911 Flanagan, L. B., Goldstein, A. H., Hollinger, D. Y., Misson, L., Monson, R. K., Oechel, W. C.,
912 Schmid, H. P., Wofsy, S. C. and Xu, L.: A new model of gross primary productivity for
913 North American ecosystems based solely on the enhanced vegetation index and land
914 surface temperature from MODIS, *Remote Sens Environ*, 12, 1633–1646,
915 doi:10.1016/j.rse.2007.08.004, 2008.

916

917 Thornton, P. E., Law, B. E., Gholz, H. L., Clark, K. L., Falge, E., Ellsworth, D. S., Goldstein, A.
918 H., Monson, R. K., Hollinger, D., Falk, M., Chen, J., Sparks, J. P.: Modeling and measuring
919 the effects of disturbance history and climate on carbon and water budgets in evergreen

920 needleleaf forests, *Agr Forest Meteorol*, 113, 185-222, doi:10.1016/S0168-
921 1923(02)00108-9, 2002.

922

923 Tramontana, G., Ichii, K., Camps-Valls, G., Tomelleri, E. and Papale, D.: Uncertainty
924 analysis of gross primary production upscaling using Random Forests, remote sensing and
925 eddy covariance data, *Remote Sens Environ*, 168, 360–373,
926 doi:10.1016/j.rse.2015.07.015, 2015.

927

928 Ungaro, F., Calzolari, C. and Busoni, E: Development of pedotransfer functions using a
929 group method of data handling for the soil of the Pianura Padano–Veneta region of North
930 Italy: water retention properties, *Geoderma*, 124, 293–317,
931 doi:10.1016/j.geoderma.2004.05.007, 2005.

932

933 Valentini, R., Arneeth, A., Bombelli, A., Castaldi, S., Cazzolla Gatti, R., Chevallier, F., Ciais, P.,
934 Grieco, E., Hartmann, J., Henry, M., Houghton, R. A., Jung, M., Kutsch, W. L., Malhi, Y.,
935 Mayorga, E., Merbold, L., Murray-Tortarolo, G., Papale, D., Peylin, P., Poulter, B.,
936 Raymond, P. A., Santini, M., Sitch, S., Vaglio Laurin, G., van der Werf, G. R., Williams, C. A.
937 and Scholes, R. J.: A full greenhouse gases budget of Africa: synthesis, uncertainties, and
938 vulnerabilities, *Biogeosciences*, 11, 381-407, doi:10.5194/bg-11-381-2014., 2014.

939

940 Vapnik, V., Golowich, S. and Smola, A.: Support vector method for function
941 approximation, regression estimation, and signal processing, *Adv Neur In*, 9, 281–287,
942 1997.

943

944 Verrelst, J., Muñoz, J., Alonso, L., Delegido, J., Rivera, J., Camps-Valls, G., and Moreno, J.:
945 Machine learning regression algorithms for biophysical parameter retrieval:
946 Opportunities for Sentinel-2 and -3, *Remote Sens Environ*, 118, 127–139, 2012
947
948 Verrelst, J., Camps-Valls, G., Muñoz, J., Rivera, J. P., Veroustraete, F., Clevers, J. P. G. W.
949 and Moreno, J.: Optical remote sensing and the retrieval of terrestrial vegetation bio-
950 geophysical properties – A review, *ISPRS J Photogramm*,
951 doi:10.1016/j.isprsjprs.2015.05.005, 108, 273-290, 2015
952
953 Wan, Z., Zhang, Y., Zhang, Q. and Li, Z. L.: Validation of the land-surface temperature
954 products retrieved from Terra Moderate Resolution Imaging Spectroradiometer data,
955 *Remote Sens Environ*, 83, 163–180, doi: 10.1016/S0034-4257(02)00093-7, 2002.
956
957 Wolf, S., Eugster, W., Potvin, C. and Buchmann, N.: Strong seasonal variations in net
958 ecosystem CO₂ exchange of a tropical pasture and afforestation in Panama, *Agr Forest*
959 *Meteorol*, 151, 1139-1151, doi:10.1016/j.agrformet.2011.04.002, 2011.
960
961 Xiao, J., Zhuang, Q., Baldocchi, D. D., Law, B. E., Richardson, A. D., Chen, J., Oren, R., Starr,
962 G., Noormets, A., Ma, S., Verma, S. B., Wharton, S., Wofsy, S. C., Bolstad, P. V., Burns, S.
963 P., Cook, D. R., Curtis, P. S., Drake, B. G., Falk, M., Fischer, M. L., Foster, D. R., Gu, L.,
964 Hadley, J. L., Hollinger, D. Y., Katul, G. G., Litvak, M., Martin, T. A., Matamala, R., McNulty,
965 S., Meyers, T. P., Monson, R. K., Munger, J. W., Oechel, W. C., Paw U, K. T., Schmid, H. P.,
966 Scott, R. L., Sun, G., Suyker, A. E., Torn, M. S.: Estimation of net ecosystem carbon
967 exchange for the conterminous United States by combining MODIS and AmeriFlux data,
968 *Agr Forest Meteorol*, 148, 1827-1847, doi:10.1016/j.agrformet.2008.06.015, 2008.

969

970 Xiao, J., Zhuang, Q., Law, B. E., Chen, J., Baldocchi, D. D., Cook, D. R., Oren, R., Richardson,
971 A. D., Wharton, S., Ma, S., Martin, T. A., Verma, S. B., Suyker, A. E., Scott, R. L., Monson, R.
972 K., Litvak, M., Hollinger, D. Y., Sun, G., Davis, K. J., Bolstad, P. V., Burns, S. P., Curtis, P. S.,
973 Drake, B. G., Falk, M., Fischer, M. L., Foster, D. R., Gu, L., Hadley, J. L., Katul, G. G.,
974 Matamala, R., McNulty, S., Meyers, T., P., Munger, J. W., Noormets, A., Oechel, W. C.,
975 Paw, K. T., Schmid, H. P., Starr, G. Torn, M. S. and Wofsy, S. C.: A continuous measure of
976 gross primary production for the conterminous United States derived from MODIS and
977 AmeriFlux data, *Remote Sens Environ*, 114, 576–591, doi: 10.1016/j.rse.2009.10.013,
978 2010.

979

980 Xiao, X., Boles, S., Liu, J. Y., Zhuang, D. F. and Liu, M. L.: Characterization of forest types in
981 Northeastern China, using multi-temporal SPOT-4 VEGETATION sensor data, *Remote Sens*
982 *Environ*, 82, 335–348, doi:10.1016/S0034-4257(02)00051-2, 2002.

983

984 Yang, F., White, M. A., Michaelis, A. R., Ichii, K., Hashimoto, H., Votava, P., Zhu, A. X. and
985 Nemani, R. R.: Prediction of continental-scale evapotranspiration by combining MODIS
986 and AmeriFlux data through support Vector machine, *IEEE T. Geosci Remote*, 44, 3452-
987 3461, doi: 10.1109/TGRS.2006.876297, 2006.

988

989 Yang, F., Ichii, K., White, M. A., Hashimoto, H., Michaelis, A. R., Votava, P., Zhu, A-X.,
990 Huete, A., Running, S. W., and Nemani, R. R.: Developing a continental-scale measure of
991 gross primary production by combining MODIS and AmeriFlux data through Support
992 Vector Machine approach, *Remote Sens Environ*, 110, 109–122,
993 doi:10.1016/j.rse.2007.02.016, 2007.

994

995 Yebra, M., Van Dijk, A. I. J. M., Leuning, R. and Guerschman, J. P.: Global vegetation gross
996 primary production estimation using satellite-derived light-use efficiency and canopy
997 conductance, *Remote Sens Environ*, 163, 206–216, doi:10.1016/j.rse.2015.03.016, 2015.

998

999 Yuan, W., Liu, S., Yu, G., Bonnefond, J-M., Chen, J., Davis, K., Desai, A. R., Goldstein, A. H.,
1000 Gianelle, D., Rossi, F., Suyker, A. E. and Verma, S. B.: Global estimates of
1001 evapotranspiration and gross primary production based on MODIS and global
1002 meteorology data, *Remote Sens Environ*, 114, 1416–1431, doi:10.1016/j.rse.2010.01.022,
1003 2010.

1004

1005 Zhao, Y., Ciais, P., Pylin, P., Viovy, N., Longdoz, B., Bonnefond, J. M., Rambal, S., Klumpp,
1006 K., Oliosio, A., Cellier, P., Maigna, F., Eglin, T. and Calvet, J. C.: How errors on
1007 meteorological variables impact simulated ecosystem fluxes: a case study for six French
1008 sites, *Biogeosciences*, 9, 2537-2564, doi:10.5194/bg-9-2537-2012, 2012.

1009 **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	Arctic	5
Shrubland	12		
Mixed forest	11		
Savannah	10		

1010 **Table 2.** Selected predictors for both setup for carbon fluxes (GPP, TER and NEE) and energy
 1011 fluxes (H, LE and Rn). List of acronyms: Enhanced Vegetation Index (EVI), fraction of
 1012 photosynthetically active radiation absorbed by a canopy (fPAR), Leaf Area Index (LAI), daytime
 1013 Land Surface Temperature (LST_{Day}) and nighttime Land Surface Temperature (LST_{Night}), Middle
 1014 Infrared Reflectance (band 7) (MIR⁽¹⁾), Normalized Difference Vegetation Index (NDVI),
 1015 Normalized Difference Water Index (NDWI), Plant Functional Type (PFT), incoming global
 1016 Radiation (Rg), top of atmosphere potential Radiation (Rpot), Index of Water Availability (IWA),
 1017 Relative humidity (Rh), Water Availability Index lower (WAI_L), and upper (WAI_U) (for details see
 1018 supplementary material, Sect. S3), Mean Seasonal Cycle (MSC). Interaction between A and B is
 1019 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 & interannual	NDWI	Rg	
	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 6	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)	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.

1021 **Table 3.** Statistics of the accuracy of predictions of carbon and energy fluxes made by the
 1022 ensemble median estimate based on RS and RS+METEO. For RMSE and BIAS, the reference units are
 1023 $\text{gCm}^{-2}\text{d}^{-1}$ and $\text{MJm}^{-2}\text{d}^{-1}$, in the case of carbon fluxes (GPP, TER and NEE) and energy fluxes (H, LE and Rn)
 1024 respectively.

Flux	RS				RS+METEO					
	MEF	RMSE	P	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
H	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

1025

1026 **Table 4:** Mean values of the determination coefficient (R^2) by the pair-wise comparison of the
 1027 models output and their residuals. We compared different ML and same drivers (RS and
 1028 RS+METEO respectively) or the same ML and different drivers (RS vs RS+METEO). Numbers in
 1029 brackets are the standard deviation of R^2 . All correlations are statistically significant ($p <$
 1030 0.001).

Fluxes	Correlation among models output			Correlation among models residuals		
	RS	RS+METEO	RS vs RS+METEO	RS	RS+METEO	RS vs 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)
H	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)

1031

1032 **Table 5:** R^2 and RMSE for the comparison among sites, mean seasonal cycle and anomalies. The
 1033 last two columns show the consistency between the median estimates of the two setups. For
 1034 RMSE, the reference units are $\text{gCm}^{-2}\text{d}^{-1}$ and $\text{MJm}^{-2}\text{d}^{-1}$, in the case of carbon fluxes (GPP, TER and
 1035 NEE) and energy fluxes (H, LE and Rn) respectively.

Fluxes	RS vs. OBS		RS+METEO vs. OBS		RS vs. RS+METEO	
	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
H	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
Mean Seasonal 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
H	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
Anomalies						
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
H	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

1036

1037 **Table A1:** Accuracy of carbon and energy fluxes predicted by machine learning methods based on
 1038 RS and RS+METEO dataset. The median value of methods and the variability (in brackets)
 1039 estimated as the median absolute deviation (MAD) from the median multiplied per 1.4826 (as
 1040 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)
H	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)

1041

1042 **Table C1.** Median site-by-site R^2 of the carbon fluxes per PFT and climate zones. ENF is vvergreen needle leaf forest, DBF deciduous broadleaf forest, EBF Evergreen broadleaf
 1043 forest, MF mixed forest, SHR shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland, Tmp Temperate, TmpCont
 1044 Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by ice.

CAT	GPP _R		GPP _L		TER _R		TER _L		NEE	
	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)

1045

1046 **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
 1047 forest, MF mixed forest, SHR shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland, Tmp Temperate, TmpCont
 1048 Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by ice.

CAT	GPP _R (gCm ⁻² d ⁻¹)		GPP _L (gCm ⁻² d ⁻¹)		TER _R (gCm ⁻² d ⁻¹)		TER _L (gCm ⁻² d ⁻¹)		NEE (gCm ⁻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)

1049

1050 **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
 1051 broadleaf forest, MF mixed forest, SHR shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland, Tmp Temperate,
 1052 TmpCont Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by ice.

CAT	GPP _R (gCm ⁻² d ⁻¹)		GPP _L (gCm ⁻² d ⁻¹)		TER _R (gCm ⁻² d ⁻¹)		TER _L (gCm ⁻² d ⁻¹)		NEE (gCm ⁻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)

1053

1054 **Table C4.** Median site-by-site R^2 of the energy fluxes per PFT and climate zones. ENF is evergreen needle
 1055 leaf forest, DBF deciduous broadleaf forest, EBF Evergreen broadleaf forest, MF mixed forest, SHR
 1056 shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical,
 1057 Dry Dryland, Tmp Temperate, TmpCont Temperate-continental, Bor Boreal, Cold cold environment or
 1058 Iceland covered by ice.

CAT	H		LE		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)

1059

1060 **Table C5.** Median site-by-site RMSE of the energy fluxes per PFT and climate zones. ENF is evergreen needle
 1061 leaf forest, DBF deciduous broadleaf forest, EBF Evergreen broadleaf forest, MF mixed forest, SHR
 1062 shrubland, SAV Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical,
 1063 Dry Dryland, Tmp Temperate, TmpCont Temperate-continental, Bor Boreal, Cold cold environment or
 1064 Iceland covered by ice.

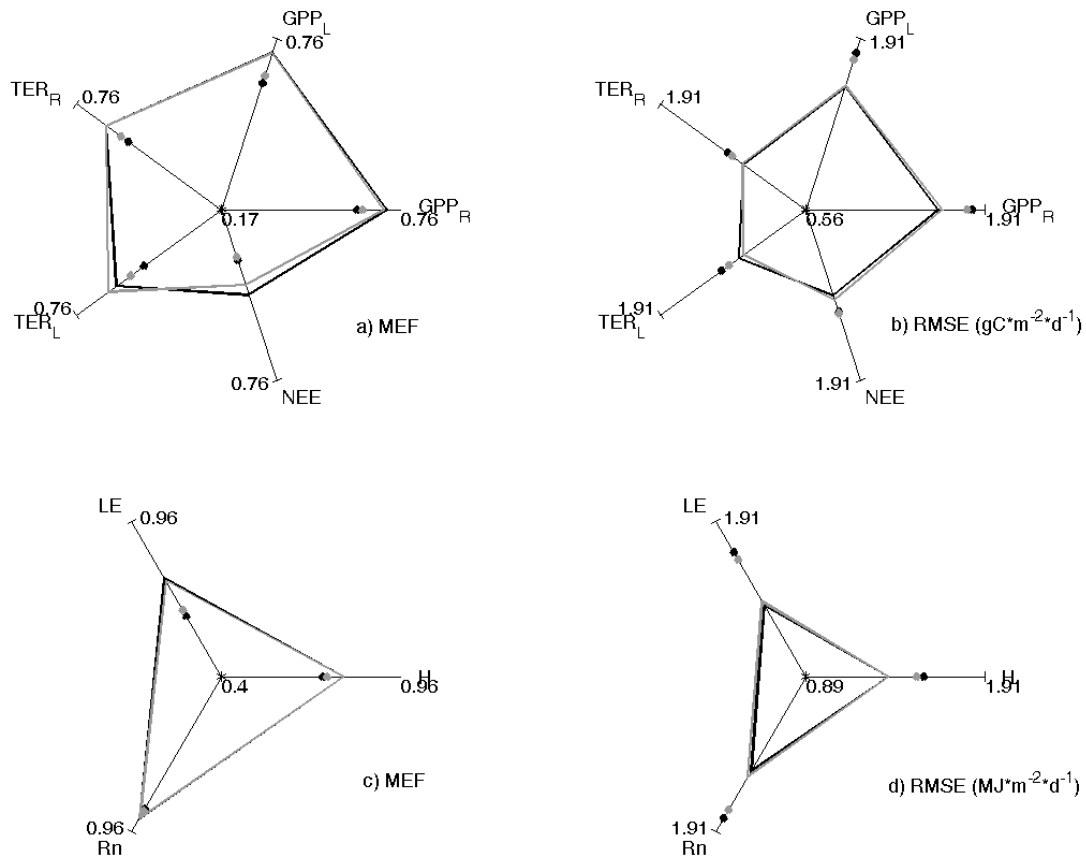
CAT	H (MJm ⁻² d ⁻¹)		LE (MJm ⁻² d ⁻¹)		Rn (MJm ⁻² d ⁻¹)	
	RS	RS+METEO	RS	RS+METEO	RS	RS+METEO
ENF	1.09 (0.25)	1.16 (0.25)	1.00 (0.56)	1.02 (0.55)	1.27 (0.68)	1.26 (0.57)
DBF	1.30 (0.43)	1.31 (0.38)	1.22 (0.26)	1.14 (0.46)	1.11 (0.42)	1.24 (0.41)
EBF	1.14 (0.60)	1.29 (0.76)	1.55 (0.39)	1.60 (0.46)	1.33 (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)

1065

1066 **Table C6.** Median site-by-site absolute bias for energy fluxes. . ENF is evergreen needle leaf forest, DBF
 1067 deciduous broadleaf forest, EBF Evergreen broadleaf forest, MF mixed forest, SHR shrubland, SAV
 1068 Savannah, GRA Grassland, CRO cropland, WET Wetland, Trop Tropical, SubTrop Subtropical, Dry Dryland,
 1069 Tmp Temperate, TmpCont Temperate-continental, Bor Boreal, Cold cold environment or Iceland covered by
 1070 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)

1071

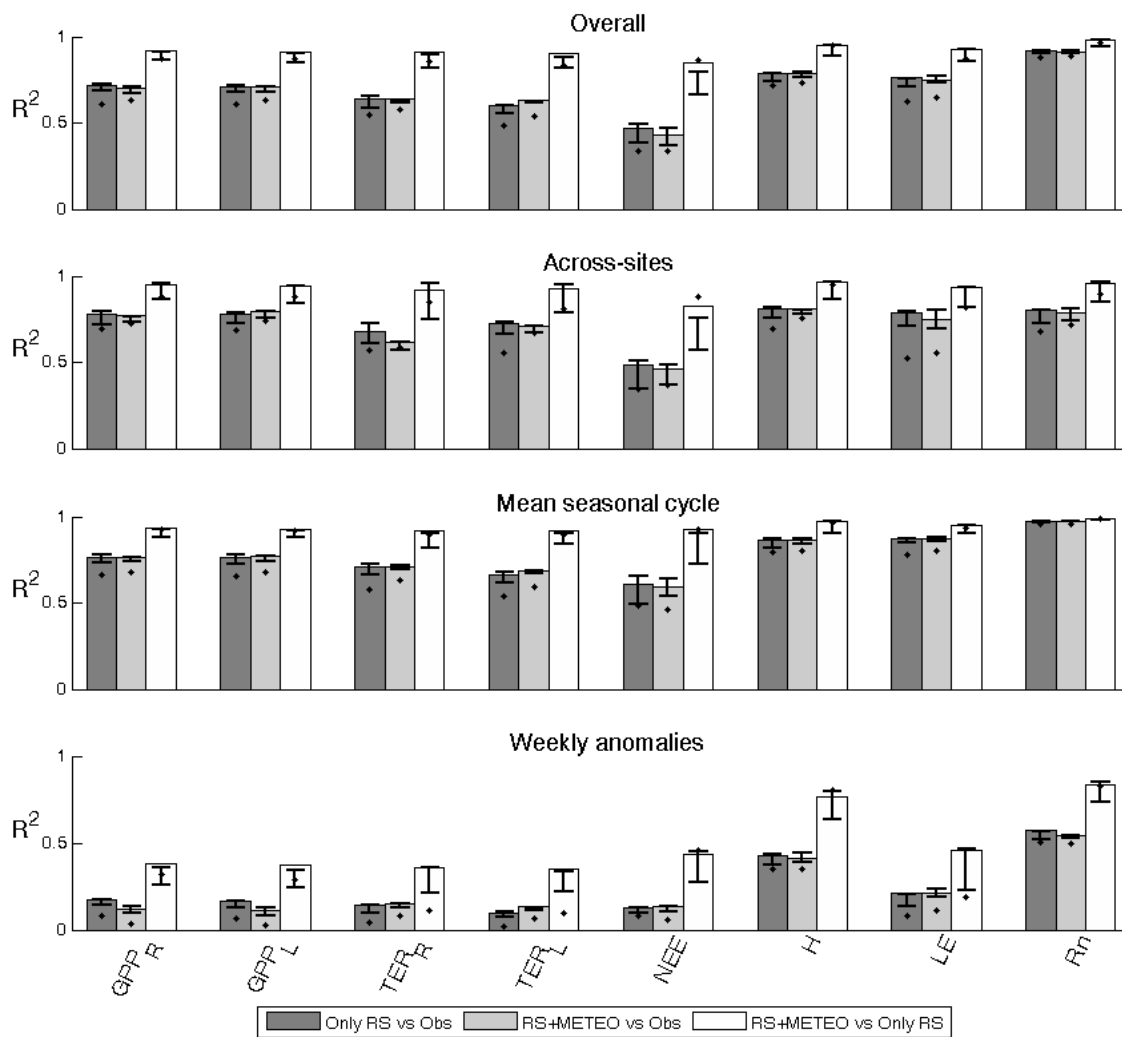


1072

1073 **Fig. 1:** Spider plot of MEF (first column) and RMSE (second column) for carbon (first row) and
 1074 energy fluxes (second row) showing the consistency of prediction made RS (Black line) and
 1075 RS+METEO (grey lines) setups. The lines are the ensemble median estimate; we also show the
 1076 performance of multiple regressions trained with RS (black point) and RS+METEO (gray points).
 1077 GPP_R and GPP_L are respectively gross primary production estimated following Reichstein et al.
 1078 (2005) and Lasslop et al. (2010), TER_R and TER_L the total ecosystem respiration estimated
 1079 following Reichstein et al. (2005) and Lasslop et al. (2010), NEE net ecosystem exchange, H the
 1080 sensible heat, LE the latent heat and Rn the net radiation.

1081

1082



1083

1084

1085

1086

1087

1088

1089

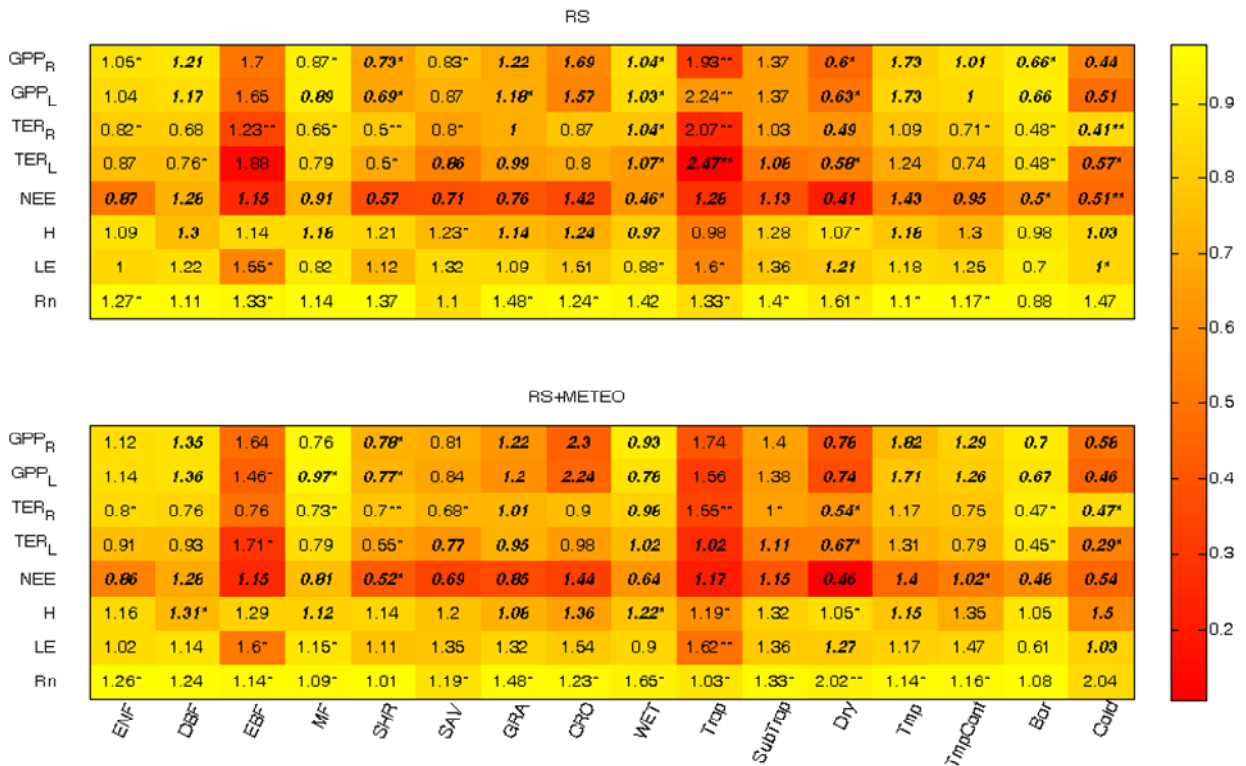
1090

1091

1092

1093

Fig. 2: Coefficients of determination (R^2) 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 R^2 when the comparisons are made among the singular ML. The comparison of output by the multiple regressions is also shown (black points).



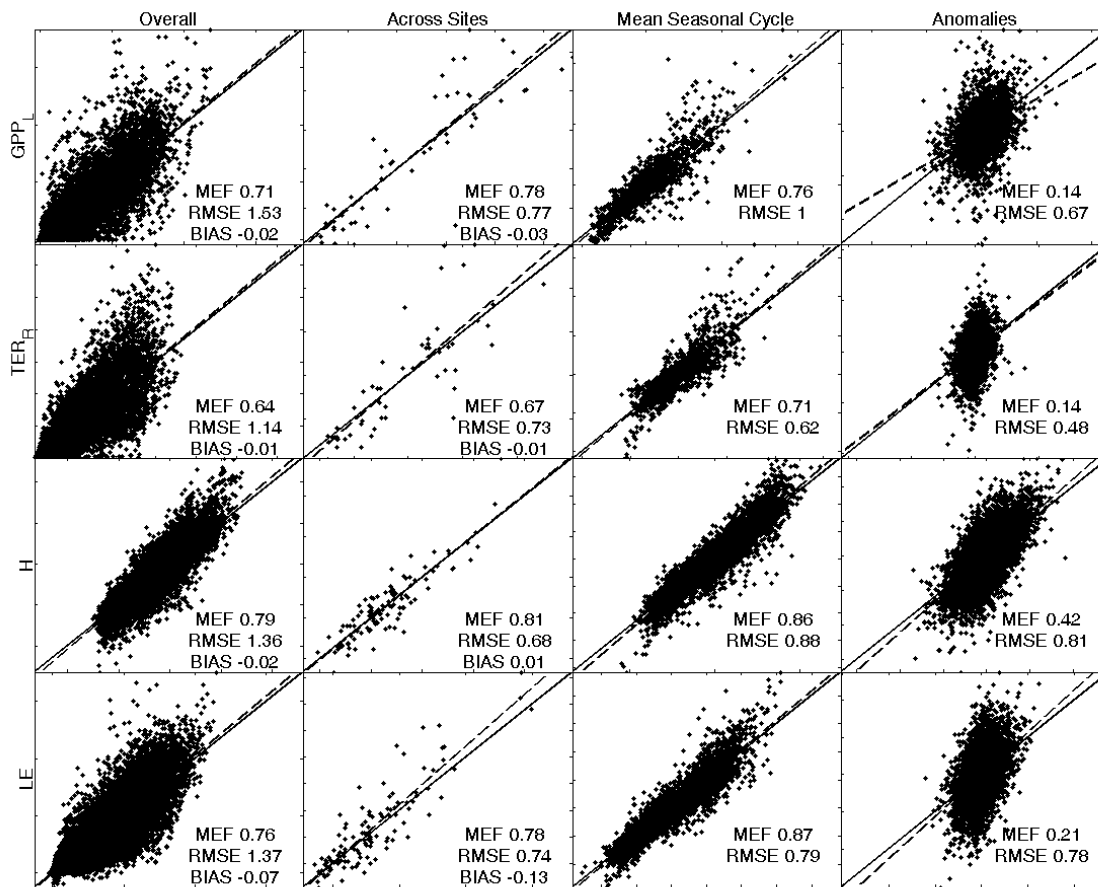
1094

1095 **Fig. 3:** Performance of FLUXCOM median estimates per climate zone and plant functional type
 1096 (PFT). The colored matrices show the median values of R^2 (red pixels for low R^2 , yellow pixels for
 1097 high R^2). Number indicate the RMSE (units of carbon fluxes are $\text{gCm}^{-2}\text{d}^{-1}$ and $\text{MJm}^{-2}\text{d}^{-1}$ in the case
 1098 of energy fluxes). Oblique and bold font are used when the relative RMSE (normalized for the
 1099 mean observed fluxes per PFT and climate zone) is greater than 0.5. The symbols '**' after RMSE
 1100 are used when the weight of bias (estimated as the ratio between the square of median absolute
 1101 bias and the MSE) is greater than 0.5, instead '*' are used if the weight of bias is between 0.25
 1102 than 0.5. No symbols are used if the weight of bias is lesser than 0.25.

1103

1104

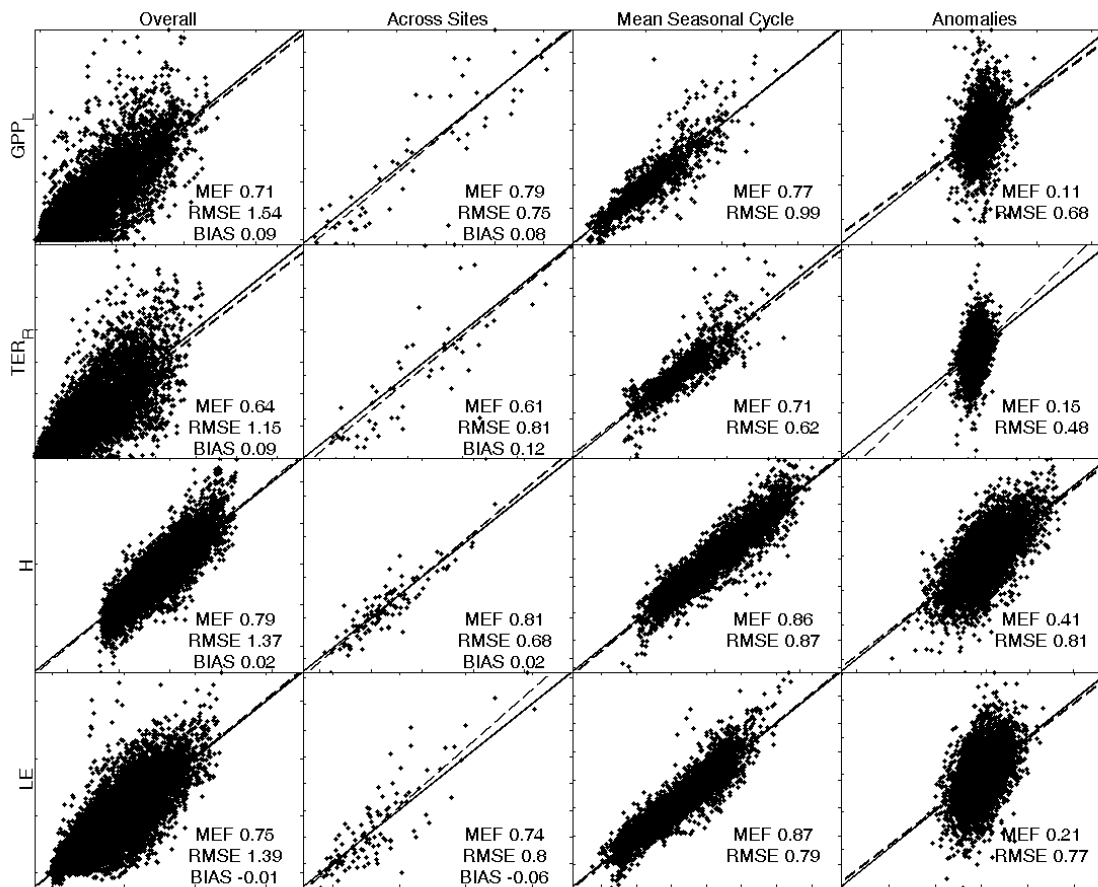
1105



1106

1107 **Fig. B1.** Scatterplots of observed data by eddy covariance (y-axis) and the median ensemble of
 1108 modeled fluxes by RS setup (x-axis). The panels from left to right are the eight days predictions,
 1109 across sites variability, mean seasonal cycle and weekly anomalies. The fluxes considered here are
 1110 GPP_L (first row), TER_R (second row), H (third row) and LE (fourth row).

1111



1112

1113 **Fig. B2.** As Fig. B1 but the predictions (x-axis) were obtained by the RS+METEO setup.