

Considerations on eddy-covariance data from FLUXNET in model-data fusion and data-assimilation

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1. Introduction

The first continuous observations of carbon fluxes at the ecosystem level were performed in the early '90s [e.g. Wofsy *et al.*, 1993]. The eddy covariance method used in this study is the first method that allows continuous, direct and non destructive high frequency measurements of biosphere-atmosphere exchanges of carbon, water and energy at an ecosystem scale [Baldocchi, 2003]. These observations encompass ecologically relevant temporal – ranging from hours to years – and spatial scales – spanning from hectares to several squared kilometres.

The emergence of eddy-covariance measurements constitutes an instrumental source of information for the development of ecosystem models entailing principles of biochemistry and biophysics. Model-data integration exercises at ecosystem level are usually constrained by carbon, water and/or energy flux observations, and cover two different types of problems: optimization of model parameters driven by environmental and meteorological inputs; and/or deconvolution, by determining model inputs or refining model states given its outputs [Wang *et al.*, 2009]. Model optimization approaches are followed for a wide range of model complexity, from simple and strongly empirical model structures [e.g. Richardson *et al.*, 2006] to detailed process models [e.g. Santaren *et al.*, 2007]. In this regard, the development of highly-fitted data-driven algorithms based in machine learning principles embodies a significant potential for upscaling exercises, given the data availability from local to regional and global domains and the representativeness of the measurement network.

In the present outline we first introduce the general principles of the eddy-covariance technique and address data limitations and processing needs. The principal research focuses and issues in model-data integration exercises are identified and the emergence of diagnostic fields from data-driven approaches discussed. We finalize with issues of representativeness of the present network and cautionary remarks on the usage of eddy-covariance data for model evaluation. We should emphasize that the main objective of the current paper is to highlight certain issues in the characteristics of the eddy-covariance datasets in the context of model-data fusion and refer to relevant literature.

2. Principles of eddy-covariance measurements

In the eddy-covariance (EC) technique, the exchange of CO₂ between the atmosphere and the vegetation is assessed by measuring the covariance between the instantaneous vertical wind velocity and the CO₂ mixing ratio on top of the canopy at high frequency (10 to 20 Hz). It stands on the conservation equation of a scalar (c), assuming that its transport is mostly mediated by vertical

turbulent fluxes (F_c) and the lateral gradients and molecular diffusion are negligible [e.g. *Aubinet et al.*, 2000]. The extraction of measures of net ecosystem production (NEP) through this technique is only possible by conducting measurements of F_c in the canopy-atmosphere interface [*Baldocchi*, 2003]; as well as by approximating a storage term (S_c), that takes into consideration the CO_2 that can be accumulated under the canopy under low turbulence conditions, measured with vertical profiles of CO_2 concentration in the canopy [*Aubinet et al.*, 2001; *Aubinet et al.*, 2002] ($\text{NEP}=F_c+S_c$). Such is valid in ideal conditions, when in case of low turbulence the CO_2 is only accumulated increasing the storage.

From such assumptions, the local conditions are instrumental for EC measurements, which are most reliable over flat and homogenous terrain, and under well developed turbulence and steady concentration conditions [*Aubinet et al.*, 2000]. The violation of the EC method assumptions may originate from horizontal heterogeneity and/or low turbulence conditions with the occurrence of advective air flows, which may yield unreliable net ecosystem flux estimates, given the difficulty in approximating the additional components (horizontal and vertical advection). The effects of air flows that transport air to and away from the control volume are strongly determined by the spatial distribution of source and sink regions around the EC towers [e.g. *Aubinet et al.*, 2005; *Feigenwinter et al.*, 2004], hence the importance of an homogeneous footprint. But the most significant issue is the association of advection with low turbulence conditions, mainly in nocturnal periods, which may lead to significant underestimates of night-time respiratory fluxes and general overestimations of carbon sink conditions.

The advective fluxes are very difficult to measure as demonstrated also in the ADVEX campaign [e.g. *Aubinet et al.*, 2010; *Feigenwinter et al.*, 2008]. Currently, the most used method to take into account these components is to filter out the measurements that are assumed to be affected by large advective fluxes [e.g. *Papale et al.*, 2006]. The largely used technique is the u_* -filtering method, where a threshold in the turbulence conditions (represented by u_* , the friction velocity) is fixed and all the data acquired under a given u_* threshold are removed and gapfilled. Several methods are proposed to calculate the threshold value [*Gu et al.*, 2005; *Reichstein et al.*, 2005]. Varying u_* thresholds may imply changes in the magnitudes of local sink/source conditions, which suggests a cautious determination of such values that can become a significant source of uncertainty in EC data. Additionally, further remarks on the violation of EC measurements render limits to the utilization of the u_* filtering technique [*Aubinet*, 2008]. In general, several aspects related to the quantification of the different terms of the conservation equation are currently under active research [*Aubinet*, 2008; *Feigenwinter et al.*, 2008].

3. Error characteristics in eddy-covariance data

The characterization of error sources and distribution of EC data is an essential step for model-data integration approaches. The errors can be divided in: i) random errors that result from the instrumental observation noise, from the stochastic properties of turbulence and/or from changes in the EC tower footprint; ii) systematic errors, as a consequence of calibration issues or a constant failure of sampling high or low frequency components of the co-spectrum; and iii) selective systematic biases, caused by low turbulence fluxes during night-time periods, yielding systematic underestimation of nocturnal respiratory fluxes [*Moncrieff et al.*, 1996]. The random error of half hourly EC measurements of carbon and water fluxes has been shown to have small auto and cross correlation, and a standard deviation that scales with the magnitude of the fluxes [*Lasslop et al.*, 2008], showing a LaPlacian distribution [e.g. *Hollinger and Richardson*, 2005]. Yet, the distribution of the random error becomes

more Gaussian after a normalization procedure that consisted in the division of each observation by its expected standard deviation [Lasslop *et al.*, 2008], revealing the superimposition of Gaussian distributions with varying standard deviation (Figure 1). The distribution of random errors can vary across sites, due to different filtering and differences in the processing of the high frequency data. Given the appropriateness of least squares estimators for normal distributed random errors and minimization of absolute deviations for Laplacian distributions, the definition of the error distribution is essential in model-data integration approaches. To account for the non-constant standard deviation of the random errors the standard deviation of each observation can be derived and included in the cost function [Lasslop *et al.*, 2008]. While the debate on the properties of the random error distribution continues – and given the strong inter-site variability – it is advisable to consider methods robust to outliers or violations of the assumed distribution [e.g. least trimmed squares regression Stromberg, 1997]. In this regard, the consideration of temporally averaged fluxes, from half hourly to daily or coarser resolutions, reduces the random error to absolute magnitudes below 5% [Baldocchi, 2003], and approximates its distribution to Gaussian [Richardson *et al.*, 2008].

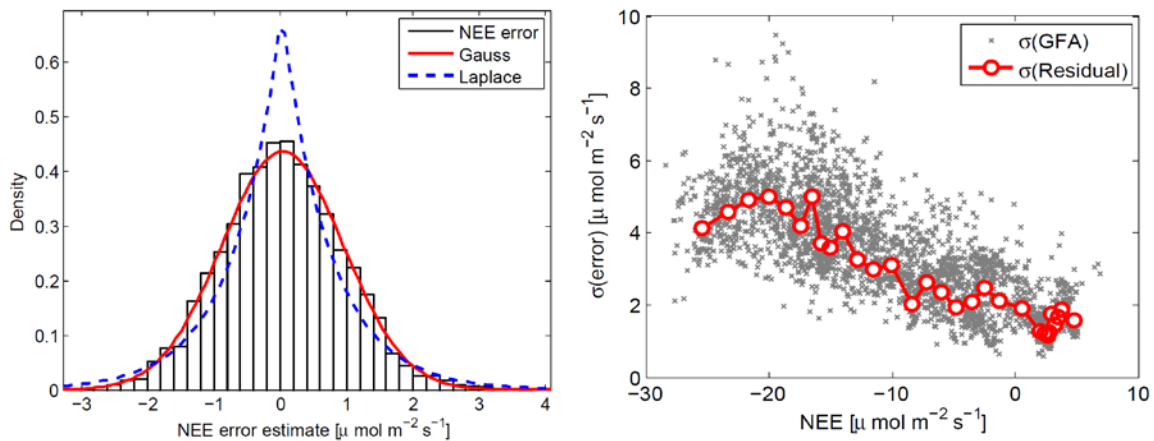


Figure 1: Distributions of net ecosystem exchange ($NEE = -NEP$) error estimated with the gap-filling algorithm normalized with the standard deviation of the residuals between observations with similar meteorological conditions and expected value. Data uncertainty derived from the gap-filling algorithm directly ($\sigma(GFA)$) and standard deviation of the gapfilling algorithm residuals for NEE ($\sigma(Res)$) [Lasslop *et al.*, 2008]. Data: Hainich May–September 2005 [Knohl *et al.*, 2003].

4. Treatment of eddy covariance data

The development of heuristic approaches which make use of measurements of friction velocity (u_*) to filter out observations performed under less favourable turbulence conditions represents a sensible approach to circumvent such issues [Aubinet *et al.*, 2000; Goulden *et al.*, 1996; Papale *et al.*, 2006]. These rejected measurements, plus the missing observations due to malfunctions of the measurement system, result in gaps in the EC datasets time series that can span from 20% to 60% of the half hourly fluxes [Moffat *et al.*, 2007]. Consequently, the development of gap-filling methods received particular attention. In general, these methods contribute little to biases in the annual sums of net ecosystem fluxes ($< 25\text{gC}\cdot\text{m}^{-2}\cdot\text{yr}^{-1}$), corroborating the application of robust approaches to complete the observational datasets [Moffat *et al.*, 2007]. Most gap-filling methods embed an explicit partitioning of NEP into assimilatory (gross primary production, GPP) and respiratory (ecosystem respiration, Reco) fluxes [Desai *et al.*, 2008; Moffat *et al.*, 2007]. Despite the methodological differences in flux-partitioning approaches, these are invariantly supported by ancillary observations of meteorological variables. One commonly used approach makes use of night-time fluxes – when photosynthetic

processes are absent – to build empirical models of Reco; by extrapolating the Reco model to day-time periods, GPP time-series are then estimated as the residuals between NEP and Reco ($GPP = NEP - Reco$) [e.g. *Reichstein et al.*, 2005]. In complement to these “night-time methods”, “day-time methods” develop on the parameterization of semi-empirical models of NEP (e.g. light-response curves) to perform the partitioning of NEP fluxes, like hyperbolic light response curves [e.g. *Lasslop et al.*, 2010]. But the diversity of algorithms expands from the construction of look up tables, to highly parameterized ecophysiological models and neural network approaches [for further details please see *Desai et al.*, 2008; *Moffat et al.*, 2007]. An accurate evaluation of such algorithms would require additional measurements of individual fluxes, which lends a cautionary perspective on the use of partitioned fluxes. In particular diurnal cycles have proven to be uncertain and diverging between different approaches. However, the inter-site variability of GPP and Reco fluxes is consistent between methods, implying the general coherent spatial distribution of the partitioned fluxes [*Desai et al.*, 2008] (Figure 2). By contributing to more accurate representation of ecosystem fluxes and disentangling assimilatory and respiratory fluxes, gap-filling and flux-partitioning techniques support ecosystem diagnostics as well as model-data integration approaches, for models operated at coarser temporal scales (daily and above).

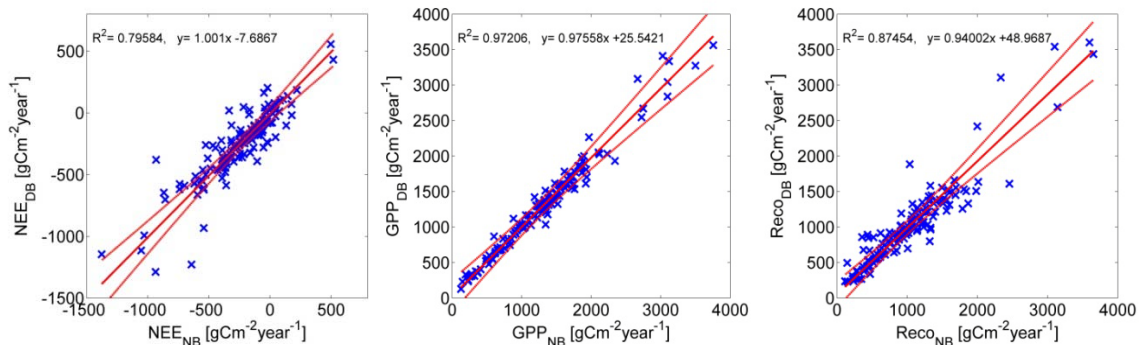


Figure 2: Flux partition results for night-time (NB) and day-time (DB) based estimates following *Reichstein et al.* [2005] and *Lasslop et al.* [2010], respectively. Values report mean yearly fluxes for a set of eddy-covariance sites.

5. Model-data fusion approaches

Most commonly, model-data fusion approaches at ecosystem level comprise inverse parameter optimization exercises by minimizing the mismatch between model estimates and EC measurements of ecosystem fluxes (carbon, water and/or energy) [*Raupach et al.*, 2005; *Wang et al.*, 2009; *Williams et al.*, 2009]. Additionally, the construction of the mismatch function, or cost function, may include information on the observational uncertainties as well as in a priori knowledge on model parameters [*Van Oijen et al.*, 2005]. Given the inverse problem complexity, an extensive set of optimization algorithms is available, from gradient search [e.g. *Byrd et al.*, 1995; *More*, 1978] to global search methods [e.g. *Metropolis et al.*, 1953]. However, the field is still under active research and newer approaches ponders mostly global search methods using genetic algorithms [e.g. *Deb et al.*, 2002], multi-objective algorithms [*Vrugt et al.*, 2003] and adaptive nested algorithms [*Vrugt and Robinson*, 2007]. The main advantage of global search methods lies on the robustness to ill-posed problems, although these are dependent on the particularities of each exercise (case study, model, observational datasets and cost function). Yet, the required amount of model evaluations by global search methods often renders impeditive of its application for more complex models [e.g. *Santaren et al.*, 2007].

Overall, *Trudinger et al.* [2007] emphasize the selection of the cost function over the panoply of optimization algorithms in a model optimization inter-comparison study.

Currently, the model-data integration exercises focus on different components of ecosystem models, such as: model structure selection [e.g. *Richardson et al.*, 2006]; the optimization of parameters controlling different ecosystem processes and components [e.g. *Knorr and Kattge*, 2005; *Santaren et al.*, 2007]; estimating the state variables [e.g. *Williams et al.*, 2005] and ecosystem initial conditions [e.g. *Braswell et al.*, 2005]; exploring the limits of model-data integration approaches themselves [Wang *et al.*, 2001]; as well as addressing ecologically relevant issues like the effects of drought on ecosystem fluxes [Reichstein *et al.*, 2003]; seasonal controls on carbon fluxes [Sacks *et al.*, 2006]. One common assumption in ecosystem modelling exercises is the consideration of initial steady-state conditions in carbon fluxes. These are prescribed by spin-up runs that circulate – and accumulate – carbon in the ecosystem pools until assimilation and release fluxes equilibrate ($NEP \approx 0$). In the context of inverse parameter optimization, the consideration of initial equilibrium conditions was shown to cause significant decrement in model performance (Figure 3), as well as to bias and increase uncertainties in parameters governing the response of assimilatory and respiratory fluxes to climate drivers [Carvalhois *et al.*, 2008b]. The following upscaling of parameters to regional scales shows that equilibrium assumptions during parameter optimization not only increase regional fluxes' uncertainties but also change its seasonal and inter-annual variability [Carvalhois *et al.*, 2008a]. In general, exercises challenging common modelling approaches emphasize the importance of model structure evaluation as integral part of model-data synthesis approaches.

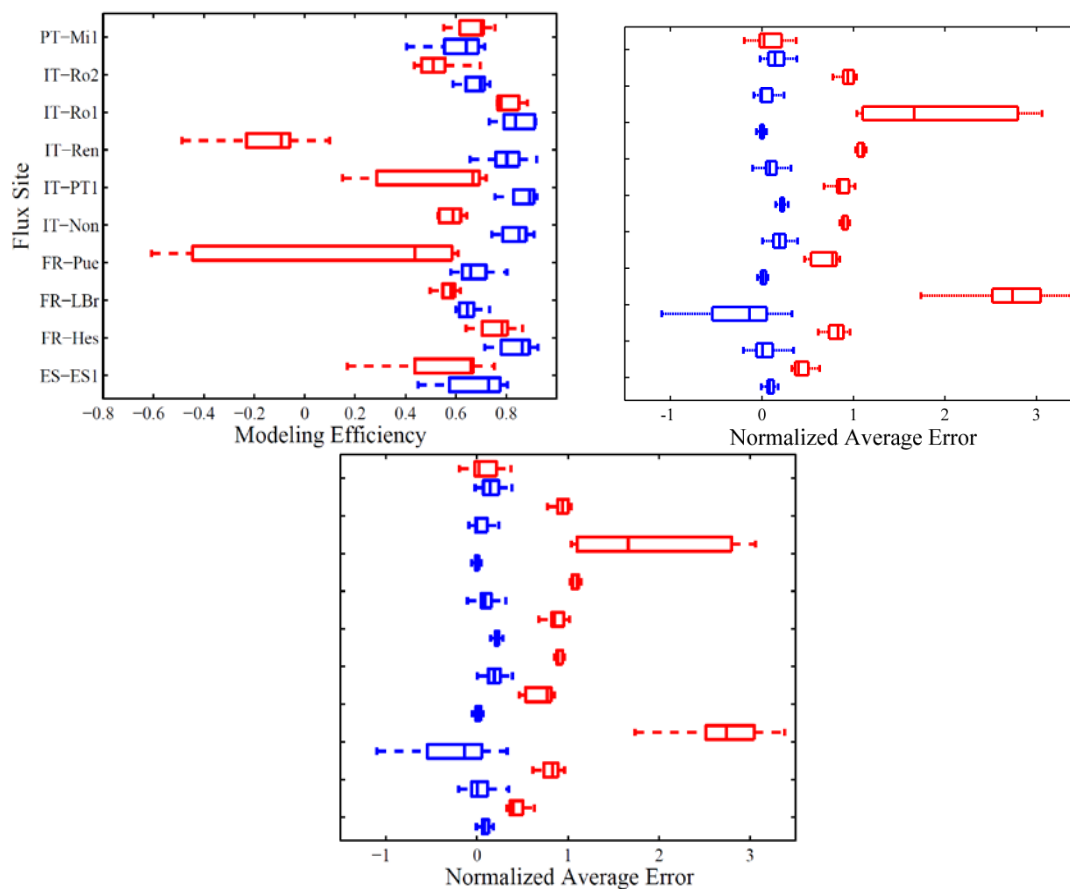


Figure 3: Model performance of simulations under forced steady-state assumptions (red) are significantly poorer than under relaxed initial equilibrium conditions (blue) [Carvalhois *et al.*, 2008b; adapted from Williams *et al.*, 2009].

Yet, the differentiation between varying model representations is not always possible through the evaluation of the modelling outputs, configuring a clear example of equifinality [Franks *et al.*, 1997]. The inability to differentiate modelling structures hampers the distinction of working hypotheses, limiting our ability to clarify particular dynamics and controls of ecosystem function [Franks *et al.*, 1997; Reichstein *et al.*, 2003]. In addition, different parameterizations may reveal insignificant changes in model performance in a model-data integration perspective although lending significant uncertainty to prognostic exercises [Fox *et al.*, 2009; Tang and Zhuang, 2008]. Generally, the main factors that yield equifinality include the observational datasets, which may reveal a limited range of environmental and response conditions and/or due to data uncertainties [e.g. Sorooshian and Gupta, 1983], as well as the statistical measures used in the model evaluation [Medlyn *et al.*, 2005]. But ultimately, the uncertainties in any component of a model-data integration exercise may contribute to such issue [Luo *et al.*, 2009]. Different measures to circumvent equifinality comprise the integration of prior information on the system's properties [e.g. Omlin and Reichert, 1999; Van Oijen *et al.*, 2005]; as well as introducing additional constraints in the cost function (multiple constraints approaches), which tends to narrow the parameter spaces that can simultaneously describe several system processes [e.g. Carvalhais *et al.*, 2010, in press; Reichstein *et al.*, 2003]. However, under conditions of equifinality, a proper quantification of uncertainty in diagnostic [Beven and Freer, 2001] and prognostic simulations [Tang and Zhuang, 2008] should consider the full set of valid model representations in ensemble model runs.

6. Potential of diagnostic fields for model evaluation

Fitting machine learning algorithms to observations of ecosystem fluxes tends to provide the best empirical fit to measurement datasets possible with any ecosystem model forced with the same drivers [Abramowitz, 2005]. The possibility of training such algorithms with variables observed at ecosystem level but also available on wider spatial (and temporal) domains, such as climatic datasets or remote sensing products, sets floor for the applications of such algorithms in upscaling exercises [e.g. Jung *et al.*, 2009; Papale and Valentini, 2003; Reichstein *et al.*, 2007]. Primarily, these approaches serve as site level benchmarks [Abramowitz *et al.*, 2006], but the benchmark could be extended to spatially explicit diagnostic fields [Jung *et al.*, 2009]. Upon a significant representativeness of the network of EC measurements, these diagnostic fields could be considered as an empirical reference against which results from more mechanistic model approaches would be benchmarked (Figure 4). Mismatches in the spatial-temporal domains between the different approaches could highlight local limitations and/or corroborate modelling scenarios. However, these diagnostic fields are time-independent estimates that generally do not embed internal representations of ecosystem dynamics or states (e.g. soil water or ecosystem carbon pools). Unless the effects of such dynamics are captured via remotely sensed states used as inputs, these may not be accurately represented (e.g. lag-effects due to water storage changes or physiological damage). Hence, the vulnerability outside training and testing regions depends on the relevance of such dynamics in driving the diagnostic variables. Larger uncertainties stem from extrapolating to environmental domains that are not, or are poorly, sampled by the FLUXNET data set. Here, substantial errors occur if the response of the land surface-atmosphere exchange to explanatory environmental variables differs substantially to nearby sampled domains. Data-driven models are limited by the quality of the data used. Therefore, an appropriate uncertainty characterization is required towards proper data integration in the training exercises and the identification and removal of erroneous measurements from the training data set.

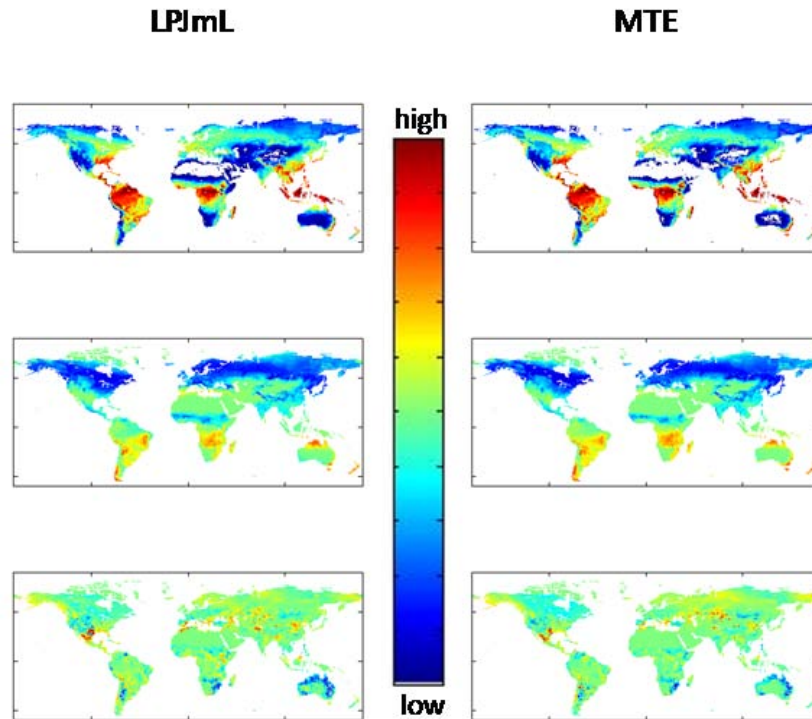


Figure 4: Global comparison between the GPP results of a dynamic global vegetation model [LPJmL, Bondeau et al., 2007] and a machine learning algorithm [MTE, Jung et al., 2009] trained with local simulations of GPP fluxes for 178 locations of FLUXNET sites. Results show strong similarities between mean annual GPP fields (top row), as well as between the first component of the principal component analysis for the seasonal cycle (middle row) and of the inter-annual variability (bottom row) [Jung et al., 2009].

7. The global representativeness of FLUXNET

The present distribution of the global network of EC measurements results from the integration of regional networks with diverse sources of funding, including sites from Fluxnet-Canada, AmeriFlux, LBA, CARBOEUROPE, CarboAfrica, TCOS-Siberia, USCCC, AsiaFlux, KoFlux and OzFlux. FLUXNET emerges from the general realization of the need for data storage and processing towards data quality control and harmonization of a global dataset. Additionally, FLUXNET gathers far more information concerning the characterization of the ecosystem properties in the instrumented sites (www.fluxdata.org). But ultimately, the global distribution aims at, but still falls short on, a wide representativeness of the world's ecosystems within the different climate regimes [Baldocchi, 2008], which is comprehensible given its genesis. Consequently, the better representativeness of European and North-American regions ecosystems contrasts the clear subsampling in tropical equatorial and tundra regions (Figure 5). Nevertheless, the network has significantly grown in the last 10 years and represents a unique source of information which importantly contributed for research in biochemistry and biophysics at ecosystem scales.

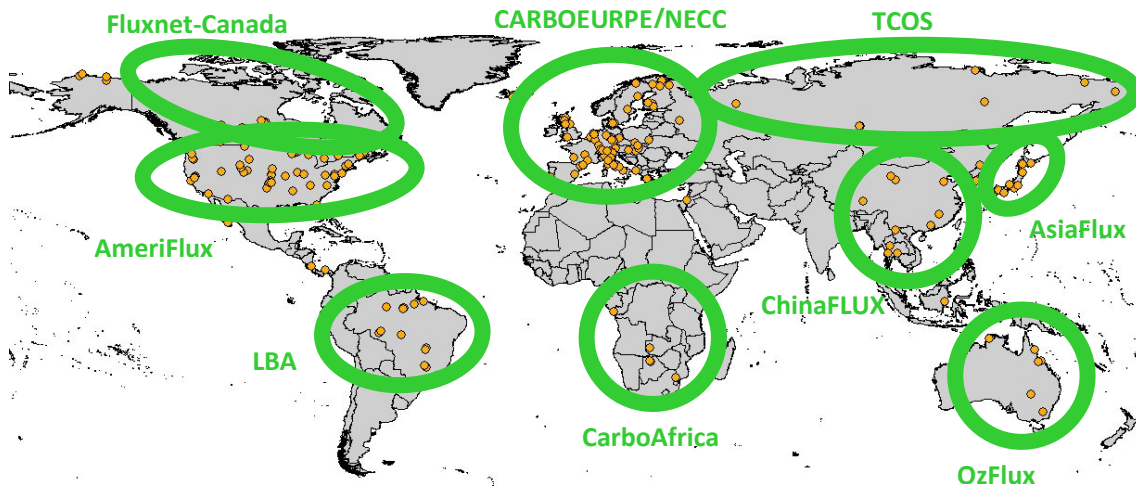


Figure 5: Global distribution of the difference EC networks

8. Concluding remarks

The measurements of ecosystem fluxes based on the EC technique constitute a unique source of continuous information on land surface-atmosphere exchanges of carbon, water and energy. The assessment of observational errors and uncertainty is essential for an appropriate biogeochemical characterization of the ecosystems, as well as for model-data integration exercises. The current treatment of EC datasets generates additional information on gross assimilatory and respiratory fluxes, which are complementary to net ecosystem flux measurements in model evaluations. Within a modelling context, model-data integration approaches reveal a strong potential in the development of any of the modelling components. In particular, challenging general model structures, and/or assumptions, may be informative on potential biases and limitations transversal in biogeochemical modelling. Furthermore, such exercises not only render knowledge about the model but also about the dynamics underlying the observed systems, whenever model equifinality can be avoided. In parallel, the emergence of diagnostic fields generated by highly flexible statistical model structures trained at site level and upscaled to global domains represents a benchmark opportunity for more mechanistic modelling approaches. Ultimately, future establishment of instrumented sites should consider the representativeness of the FLUXNET sites and bridge current gaps in the network distribution.

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