X-BASE: the first terrestrial carbon and water flux products from an extended data-driven scaling framework, FLUXCOM-X

Jacob A Nelson^{1,*}, Sophia Walther^{1,*}, Fabian Gans¹, Basil Kraft¹, Ulrich Weber¹, Kimberly Novick², Nina Buchmann³, Mirco Migliavacca⁴, Georg Wohlfahrt⁵, Ladislav Šigut⁶, Andreas Ibrom⁷, Dario Papale^{8,9}, Mathias Göckede¹, Gregory Duveiller¹, Alexander Knohl^{10,11}, Lukas Hörtnagl³, Russell L. Scott¹², Weijie Zhang¹, Zayd Mahmoud Hamdi¹, Markus Reichstein^{1,13}, Sergio Aranda-Barranco^{14,15}, Jonas Ardö¹⁶, Maarten Op de Beeck^{17,18}, Dave Billesbach¹⁹, David Bowling²⁰, Rosvel Bracho²¹, Christian Brümmer²², Gustau Camps-Valls²³, Shiping Chen²⁴, Jamie Rose Cleverly²⁵, Ankur Desai²⁶, Gang Dong²⁷, Tarek S. El-Madany¹, Eugenie Susanne Euskirchen²⁸, Iris Feigenwinter³, Marta Galvagno²⁹, Giacomo Al. Gerosa³⁰, Bert Gielen³¹, Ignacio Goded⁴, Sarah Goslee³², Christopher Michael Gough³³, Bernard Heinesch³⁴, Kazuhito Ichii³⁵, Marcin Antoni Jackowicz-Korczynski^{36,37}, Anne Klosterhalfen³⁸, Sara Knox^{39,40}, Hideki Kobayashi⁴¹, Kukka-Maaria Kohonen³, Mika Korkiakoski⁴², Ivan Mammarella⁴³, Mana Gharun⁴⁴, Riccardo Marzuoli³⁰, Roser Matamala^{45,46,47}, Stefan Metzger^{48,49}, Leonardo Montagnani⁵⁰, Giacomo Nicolini^{9,58}, Thomas O'Halloran^{51,52}, Jean-Marc Ourcival⁵³, Matthias Peichl⁵⁴, Elise Pendall⁵⁵, Borja Ruiz Reverter⁵⁶, Marilyn Roland⁵⁷, Simone Sabbatini^{9,58}, Torsten Sachs⁵⁹, Marius Schmidt⁶⁰, Christopher R Schwalm⁶¹, Ankit Shekhar³, Richard Silberstein⁶², Maria Lucia Silveira⁶³, Donatella Spano^{64,9}, Torbern Tagesson^{16,65}, Gianluca Tramontana⁶⁶, Carlo Trotta⁹, Fabio Turco³, Timo Vesala^{67,68}, Caroline Vincke⁶⁹, Domenico Vitale⁷⁰, Enrique R. Vivoni^{71,72}, Yi Wang³, William Woodgate^{73,74}, Enrico A. Yepez⁷⁵, Junhui Zhang^{76,77}, Donatella Zona⁷⁸, and Martin Jung¹

- *These authors contributed equally to this work.
- ¹Max-Planck-Institute for Biogeochemistry, Germany
- ²O'Neill School of Public and Environmental Affairs, Indiana University Bloomington (USA)
- ³Department of Environmental Systems Science, ETH Zurich, 8092 Zurich, Switzerland
- ⁴European Commission, Joint Research Centre, Ispra (Varese), Italy
- ⁵Universität Innsbruck, Institut für Ökologie, Sternwartestr. 15, 6020 Innsbruck, AUSTRIA
- ⁶Global Change Research Institute CAS, Belidla 986/4a, CZ-60300 Brno, Czech Republic ˇ
- ⁷Department of Environment and Resource Engineering, Technical University of Denmark (DTU), Bygningstorvet 115, 2800 Kgs. Lyngby, Denmark
- ⁸Research Institute on Terrestrial Ecosystems (IRET), National Research Council (CNR), 00010 Montelibretti (Roma), Italy ⁹CMCC Foundation - Euro-Mediterranean Center on Climate Change, Italy
- 10 University of Goettingen, Bioclimatology, Faculty of Forest Sciences, 37077 Göttingen, Germany.
- ¹¹University of Goettingen, Centre of Biodiversity and Sustainable Land Use (CBL), 37077 Göttingen, Germany
- ¹²Southwest Watershed Research Center, USDA-ARS, Tucson, AZ
- ¹³German Centre for Integrative Biodiversity Research (iDiv) Halle–Jena–Leipzig, Leipzig, Germany
- ¹⁴Department of Ecology, University of Granada, Granada, Spain
- ¹⁵Andalusian Institute for Earth System Research (CEAMA-IISTA), University of Granada, Granada, Spain
- ¹⁶Department of Physical Geography and Ecosystem Science, Lund University, Sölvegatan 12 223 62 Lund, Sweden
- ¹⁷Research Group Plants and Ecosystems, Department of Biology, University of Antwerp
- ¹⁸ICOS / Ecosystem Thematic Centre
- ¹⁹University of Nebraska-Lincoln, School of Natural Resources (Retired)

²⁰School of Biological Sciences, University of Utah ²¹ School of Forest, Fisheries, and Geomatics Sciences University of Florida, Gainesville, FL,32611, USA ²²Thünen Institute of Climate-Smart Agriculture, Braunschweig, Germany ²³Image Processing Laboratory (IPL), Universitat de València, Spain 24 State Key Laboratory of Vegetation and Environmental Change, Institute of Botany, Chinese Academy of Sciences, Beijing 100093, P. R. China ²⁵College of Science and Engineering, James Cook University, Cairns, Queensland, Australia ²⁶Dept of Atmospheric and Oceanic Sciences, University of Wisconsin-Madison, Madison, WI 53706 USA ²⁷Shanxi University, China ²⁸University of Alaska Fairbanks, Institute of Arctic Biology, Fairbanks, AK 99775, USA ²⁹Environmental Protection Agency of Aosta Valley, Climate Change Unit, (ARPA Valle d'Aosta), Italy 30 Dept. of Mathematics and Physics, Catholic University of the Sacred Heart, Brescia (Italy) ³¹ Plants and Ecosystems (PLECO), Department of Biology, University of Antwerp, B-2610 Wilrijk, Belgium ³²Pasture Systems and Watershed Management Research Unit, USDA-ARS, University Park, PA, USA ³³Virginia Commonwealth University, Department of Biology ³⁴Terra Teaching and Research Center, University of Liège – Gembloux Agro-Bio Tech, 5030 Gembloux, Belgium. ³⁵Center for Environmental Remote Sensing, Chiba University, Japan ³⁶Department of Ecoscience, Aarhus University, Frederiksborgvej 399, Roskilde 4000, Denmark ³⁷Department of Physical Geography and Ecosystem Science, Lund University, Sölvegatan 12, 223 62 Lund. Sweden ³⁸Bioclimatology, University of Goettingen, 37077 Goettingen, Germany ³⁹Department of Geography, McGill University, Montreal, Canada ⁴⁰Department of Geography, The University of British Columbia, Vancouver, Canada ⁴¹Research Institute for Global Change, Japan Agency for Marine-Earth Science and Technology ⁴²Finnish Meteorological Institute, Climate System Research Unit, P.O. Box 503, 00101 Helsinki, Finland ⁴³Institute of Atmospheric and Earth System Research / Physics, University of Helsinki, Helsinki, Finland ⁴⁴Institute of Landscape Ecology, University of Münster, Münster, Germany ⁴⁵Environmental Science Division, Argonne National Laboratory, Lemont, IL, USA ⁴⁶University of Chicago Consortium for Advanced Science & Engineering (CASE), Chicago, IL, USA ⁴⁷Northwestern Argonne Institute of Science and Engineering, Evanston, IL, USA ⁴⁸National Ecological Observatory Network, Battelle, 1685 38th Street, 80301 Boulder, CO, USA ⁴⁹Department of Atmospheric and Oceanic Sciences, University of Wisconsin-Madison, 1225 W Dayton St, 53711 Madison, WI, USA ⁵⁰Free University of Bolzano, Faculty of Agricultural, Environmental and Food Sciences - Universitätsplatz 1 - Piazza Università, 1 39100 Bozen-Bolzano ⁵¹Belle W. Baruch Institute of Coastal Ecology and Forest Science, Clemson University, Georgetown, SC, United States ⁵²Forestry and Environmental Conservation Department, Clemson University, Clemson, SC, United States ⁵³CEFE, Univ Montpellier, CNRS, EPHE, IRD, Montpellier, France ⁵⁴Department of Forest Ecology and Management, Swedish University of Agricultural Sciences, Skogsmarksgränd 17, SE-901 83, Umeå, Sweden ⁵⁵Hawkesbury Institute for the Environment, Western Sydney University, Penrith Australia 2751 ⁵⁶Departamento de Química e Física, Universidade Federal da Paraíba - Campus II, 58397-000 Areia, Paraíba, Brazil ⁵⁷Plants and Ecosystems, Department of Biology, University of Antwerp, 2610 Wilrijk, Belgium ⁵⁸University of Tuscia, Department for Innovation in Biological, Agro-food and Forest Systems (DIBAF) ⁵⁹GFZ German Research Centre for Geosciences, Potsdam, Germany 60 Forschungszentrum Jülich, Institute of Bio-and Geosciences: Agrosphere (IBG-3), 52428 Jülich, Germany ⁶¹Woodwell Climate Research Center: FALMOUTH, MA, US ⁶²School of Science, Edith Cowan University, Australia ⁶³University of Florida, Range Cattle Research and Education Center. 3401 Experiment Station, Ona, FL, USA 33865. ⁶⁴Department of Agriculture Sciences, University of Sassari, Italy

⁶⁵Department of Geosciences and Natural Resource Management, University of Copenhagen, Øster Voldgade 10, DK-1350 Copenhagen, Denmark

⁶⁶Terrasystem srl

 67 Institute for Atmospheric and Earth System Research/Physics, Faculty of Science, University of Helsinki, Helsinki, 00014, Finland

⁶⁸Institute for Atmospheric and Earth System Research/Forest Sciences, Faculty of Agriculture and Forestry, University of Helsinki, Helsinki, 00014, Finland

 69 UCLouvain - Earth and Life Institute (ELI) Croix du Sud, 2 bte L7.05.24 (de Serres B249) 2013 1348 Louvain-la-Neuve 70 Department of Methods and Models for Economics, Territory and Finance (MEMOTEF), Sapienza University of Rome, Via del Castro Laurenziano, 9, 00161, Rome,Italy

⁷¹School of Sustainable Engineering and the Built Environment, Arizona State University, Tempe, AZ, USA 85287-8704

⁷²Center for Hydrologic Innovations, Arizona State University, Tempe, AZ, USA 85287-8704

 73 School of the Environment, The University of Queensland, 4072, Australia

⁷⁴CSIRO, Space and Astronomy, Kensington, 6151, WA, Australia

⁷⁵Instituto Tecnológico de Sonora, 5 de Febrero 818 Sur, Col. Centro, Cd. Obregon, Sonora, México, 85000

⁷⁶School of life sciences, University of Qufu normal university, Qufu 273165, Shandong, China

⁷⁷Institute of Applied Ecology, Chinese Academy of Sciences, Shenyang 110016, China

⁷⁸Department Biology, San Diego State University, San Diego, CA 92182, USA

Correspondence: Jacob A Nelson (jnelson@bgc-jena.mpg.de) and Sophia Walther (sophia.walther@bgc-jena.mpg.de)

Abstract. Mapping in-situ eddy covariance measurements of terrestrial land-atmosphere fluxes to the globe is a key method for diagnosing the Earth system from a data-driven perspective. We describe the first global products (called X-BASE) from a newly implemented up-scaling framework, FLUXCOM-X_a representing an advancement from the previous generation of FLUXCOM products in terms of flexibility and technical capabilities. The X-BASE products comprise of estimates of CO_2

- 5 net ecosystem exchange (NEE), gross primary productivity (GPP) as well as evapotranspiration (ET) and, for the first time, a novel fully data-driven global transpiration product (ET_T) , at high spatial (0.05°) and temporal (hourly) resolution. X-BASE estimates the global NEE at -5.75 \pm 0.33 $PgC \cdot yr^{-1}$ for the period 2001-2020, showing a much higher consistency with independent atmospheric carbon cycle constraints compared to the previous versions of FLUXCOM. The improvement of global NEE was likely only possible thanks to the international effort to increase the precision and consistency of eddy
- 10 covariance collection and processing pipelines, as well as to the extension of the measurements to more site-years resulting in a wider coverage of bio-climatic conditions. However, X-BASE global net ecosystem exchange shows a very low inter-annual variability, which is common to state-of-the-art data-driven flux products and remains a scientific challenge. With 125 ± 2.1 $PgC \cdot yr^{-1}$ for the same period, X-BASE GPP is slightly higher than previous FLUXCOM estimates, mostly in temperate and boreal areas. X-BASE evapotranspiration amounts to $74.7x10^3 \pm 0.9x10^3$ km³ globally for the years 2001-2020, but
- 15 exceeds precipitation in many dry areas likely indicating overestimation in these regions. On average 57% of evapotranspiration are estimated to be transpiration, in good agreement with isotope-based approaches, but higher than estimates from many land surface models. Despite considerable improvements to the previous up-scaling products, many further opportunities for development exist. Pathways of exploration include methodological choices in the selection and processing of eddy-covariance and satellite observations, their ingestion into the framework, and the configuration of machine learning methods. For this,

20 the new FLUXCOM-X framework was specifically designed to have the necessary flexibility to experiment, diagnose, and converge to more accurate global flux estimates.

1 Introduction

Energy, water, and carbon exchange between terrestrial surfaces and the atmosphere are key components of the Earth system and impact ecosystems, ecosystem services, weather, climate, and water availability. The exchange (or flux) can be directly

- 25 observed using eddy covariance (EC) measurement systems [\(Baldocchi, 2019\)](#page-42-0) which are installed on towers overlooking the ecosystem of interest. The EC stations typically represent an area of a few hundred square meters to a square kilometer. One key advantage of the EC methodology is the ability to provide near continuous measurements with some records now exceeding 20 years [\(Pastorello et al., 2020\)](#page-50-0), allowing for examination of flux variations from the order of thirty minutes to decades. EC systems also provide a unique perspective on the magnitude, temporal variability, and environmental sensitivity
- 30 of ecosystem CO_2 uptake, water use, and local climate regulation [\(Baldocchi, 2019;](#page-42-0) [Musavi et al., 2017;](#page-49-0) [Bao et al., 2022\)](#page-42-1). However, while many of the most pressing scientific knowledge gaps surrounding the delicate land carbon balance and the water cycle require spatially and temporally resolved flux patterns at continental to global scales, EC observations are confined to individual locations in space and limited periods in time [\(Kumar et al., 2016;](#page-47-0) [Papale et al., 2015\)](#page-50-1). Methodologies to transcend the gap between local and global scales are needed to ultimately support societal relevant activities of building greenhouse
- 35 gas monitoring systems, taking informed climate and land management actions, and verifying the effectiveness of mitigation strategies [\(Baldocchi and Penuelas, 2019;](#page-42-2) [Bonan et al., 2011;](#page-43-0) [Novick et al., 2022\)](#page-49-1).

Coordinated and consolidated data collections from EC networks are invaluable for the mapping of in-situ fluxes to regional [a](#page-53-0)nd global scales. For example, EC measurements aid both the parameterization [\(Huang et al., 2021\)](#page-46-0) and the validation [\(Turner](#page-53-0) [et al., 2006;](#page-53-0) [Heinsch et al., 2006\)](#page-46-1) of mechanistic models of ecosystem productivity and land surface processes. The latter

- 40 generate widely used reference data sets for terrestrial carbon cycle applications [\(Zhao and Running, 2010;](#page-54-0) [Ukkola et al.,](#page-53-1) [2022\)](#page-53-1). A complementary approach to modeling terrestrial fluxes at continental and global scales is of empirical nature and links observations of explanatory variables at the EC stations, particularly meteorological and remote sensing data, to the EC fluxes via machine learning models. This up-scaling concept does not prescribe any mechanistic formulations and assumes that the EC observations cover all complexities of ecosystem functioning. Based on a trained machine learning model and globally 45 gridded input data of the explanatory variables, EC fluxes can be mapped to the global scale.
	- First implementations of this flux up-scaling concept emerged in the early 2000s. They focused on net ecosystem exchange of CO_2 (NEE) and utilized the growing EC networks in Europe [\(Papale and Valentini, 2003\)](#page-49-2) and North America [\(Xiao et al.,](#page-54-1) [2008\)](#page-54-1). The release of the FLUXNET La Thuile Synthesis Dataset of harmonized EC data in 2007, as well as methodological improvements in the training of the machine learning models [\(Jung et al., 2009\)](#page-47-1), led to the first global products of terrestrial
- 50 CO_2 and water fluxes at a monthly time step and in 0.5° grids in 2011 [\(Jung et al., 2011\)](#page-47-2). While good agreement of flux estimates derived from complementary process-based models with the up-scaled global gross photosynthetic $CO₂$ uptake (gross primary productivity, GPP) and energy fluxes demonstrated the potential of the approach, important inconsistencies remained,

[i](#page-55-0)n particular regarding the globally integrated NEE and its year-to-year variability [\(Jung et al., 2020,](#page-47-3) [2019,](#page-47-4) [2011;](#page-47-2) [Zscheis](#page-55-0)[chler et al., 2017\)](#page-55-0). A critical component of data-driven methods, including the flux up-scaling methodologies described here,

- 55 is understanding the related uncertainties. The multi-stage process of going from the actual measured values of high frequency (10-20 Hz) measurements of w indthree-dimensional wind components, temperature, humidity, and CO_2 water vapor and CO_2 concentration to the standard half-hourly, gap-filled, long-term data records from synthesis datasets such as FLUXNET have [m](#page-52-0)ultiple associated potential biases and uncertainties. The well documented issues of gap-filling [\(Vekuri et al., 2023;](#page-53-2) [Soloway](#page-52-0) [et al., 2017;](#page-52-0) [Papale et al., 2006\)](#page-50-2), instrumentation errors [\(Zhang et al., 2023;](#page-54-2) [Fratini et al., 2014;](#page-45-0) [Vitale et al., 2020;](#page-53-3) [Rannik](#page-51-0)
- 60 [et al., 2016\)](#page-51-0), and energy balance non-closure [\(Mauder et al., 2020;](#page-48-0) [Leuning et al., 2012;](#page-48-1) [Stoy et al., 2013;](#page-52-1) [McGloin et al.,](#page-48-2) [2018;](#page-48-2) [Franssen et al., 2010\)](#page-45-1) will likely have an effect on the resulting gridded global datasets.

In an effort to better understand the uncertainties associated with mapping of EC fluxes to larger scales, the FLUXCOM intercomparison initiative built an ensemble of flux estimates as a type of factorial experiment [\(Tramontana et al., 2016;](#page-53-4) [Jung et al.,](#page-47-4) [2019,](#page-47-4) [2020\)](#page-47-3). The ensemble consisted of multiple machine learning algorithms, meteorological forcing data, and combinations

- 65 of predictor variables resulting in 120 individual up-scaled estimates per flux. These were summarized in two overall ensemble configurations, which differed in the set of predictors and spatial-temporal resolution. Apart from creating a large ensemble, the FLUXCOM evaluation included a consistent site-level cross-validation analysis as well as cross-consistency checks with terrestrial flux estimates from independent approaches, such as complementary modeling concepts or observational surrogates. From a methodological point of view, the key lessons learned from FLUXCOM were that: (1) the overall approach seems
- 70 to be primarily limited by the input information given to the machine learning algorithms rather than to the ability of the algorithm to extract the information; (2) the largest qualitative differences among flux products were related to the set of the predictor variables rather than to the choice of the machine learning method or meteorological forcing; (3) the cross-consistency checks with global independent data are essential for supplementing site-level cross-validation; and (4) the largest qualitative discrepancy with independent data was a very high (strongly negative) tropical NEE that was shared among all ensemble
- 75 members.

Next to the systematic inter-comparisons in FLUXCOM, the empirical up-scaling concept has been implemented for a series of regional and global scale applications, each of them adopting disparate and individual methodological choices (e.g. [Ichii et al., 2017;](#page-46-2) [Yao et al., 2018;](#page-54-3) [Joiner and Yoshida, 2020;](#page-47-5) [Virkkala et al., 2021;](#page-53-5) [Dannenberg et al., 2023;](#page-44-0) [Burton et al.,](#page-43-1) [2023;](#page-43-1) [Zhu et al., 2024\)](#page-55-1). These potentially important choices relate to data treatment (quality control, gap-filling, processing 80 pathways), ingestion (sampling, as well as matching EC and space-born observations), and methodological configurations

(machine learning methods and their training configuration, choice of predictor variables, resolution). The disparity of the set-ups and implementations of the empirical up-scaling approach impedes any direct comparisons among products and valid conclusions as to where potential differences originate from. Hence, flexibility to explore the large methodological space, as well as the ability to diagnose and evaluate global products in parallel to site-level cross-validation, are required to understand 85 the importance of individual methodological choices and to make progress in empirical up-scaling of EC fluxes.

We are developing a modeling framework that allows experimenting with many of these methodological choices. We coin this extended up-scaling environment FLUXCOM-X. Compared to the FLUXCOM inter-comparison initiative and the products produced therein, it follows the same overall principles. The key innovation of FLUXCOM-X is that it represents a flexibly adjustable up-scaling environment to systematically explore different methodological avenues. Lessons learned from

- 90 FLUXCOM and other up-scaling exercises further imply striving for enhancing the information content of the training data with aspects related to coverage and quality of EC measurements as well as complementarity, completeness, and quality of predictor variables. The flexibility of the way FLUXCOM-X is implemented will considerably reduce the latency with which innovations in the related fields of machine learning and spacebased Earth observations as well as novel EC data can find their way to empirical flux up-scaling. This in turn allows faster progress towards more accurate and fit-for-the-purpose global
- 95 biogenic flux estimates. Here, we introduce and evaluate the initial "basic" set of products from this flexible framework, which we refer to as FLUXCOM-X-B[A](#page-30-0)SE products (or X-BASE for short, see section Appendix A for an overview on the naming conventions).

X-BASE products were comparably generated to the original FLUXCOM ensemble using qualitatively similar predictor variables, i.e. remotely sensed vegetation indices and land surface temperatures from the Moderate Resolution Imaging Spec-

- 100 troradiometer (MODIS) along with meteorological variables. In contrast to FLUXCOM, the remotely sensed and the meteorological predictors are combined in the X-BASE products, and the subdaily variability is resolved. We furthermore made efforts to provide more and improved information to the machine learning models by enhancing coverage and quality of the training data, and by further developing the processing of satellite predictor variables [\(Walther and Besnard et al., 2022\)](#page-54-4). In this manuscript, we show results for X-BASE NEE, GPP, evapotranspiration (ET), and for the first time transpiration (ET_T),
- 105 for the period 2001-2020 at 0.05° spatial and hourly temporal resolution. We are focusing here on the evaluation and crossconsistency checks of X-BASE with previous FLUXCOM products and independent data streams. Our specific objectives are:
	- 1. to describe the production of X-BASE products;
	- 2. to evaluate the X-BASE setup using site-level cross-validation;
- 110 3. to assess qualitative differences of global patterns compared to previous FLUXCOM products with reference to independent flux estimates where possible; and

4. to synthesize lessons learned from this basic exercise to guide future FLUXCOM-X developments.

X-BASE products are freely available and serve as a baseline for future FLUXCOM-X developments (see data availability statement). Any future product releases originating from FLUXCOM-X will follow the naming convention X-[specific name].

115 2 Data and Methods

The following section gives an overview on the essential methodological implementations and data choices adopted in the generation of X-BASE products.

2.1 Eddy Covariance Data

Eddy covariance data consisted of 294 sites from around the world though skewed towards higher representation from tem-

- 120 perate forests from North America and Europe. All EC data were collected, processed, analyzed for quality by the station teams, before being processed using state-of-the-art approaches in the ONEFLUX data processing pipeline [\(Pastorello et al.,](#page-50-0) [2020\)](#page-50-0). ONEFLUX provides consistent quality checks, gap-filling, and carbon flux partitioning. The data included was collected between 2001-2020 and available with a CC BY 4.0 license. Based on this criterion, data for each site came from one of five different sources based on most recent availability: FLUXNET 2015 [\(Pastorello et al., 2020\)](#page-50-0), ICOS Drought 2018
- 125 [\(Team and Centre, 2020\)](#page-52-2), ICOS Warm Winter 2020 [\(Team and Centre, 2022\)](#page-53-6), or the most recent Ameriflux or ICOS release as of December 2022. Table [1](#page-6-0) lists all sites included as well as the associated digital object identifier specific to the associated release.

Table 1: Citation data for the 294 sites used in the X-BASE products.

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Meteorological data measured at each site consisted of incoming shortwave radiation, air temperature and vapor pressure deficit, of which all data were gap-filled using the Marginal Distribution Sampling method [\(Reichstein et al., 2005\)](#page-51-17), as well 130 as the computed potential shortwave incoming radiation (top of atmosphere theoretical maximum radiation) for every hour. Carbon dioxide flux data consisted of gap-filled net ecosystem exchange (NEE, variable ustar threshold 50th percentile i.e., NEE_VUT_50) and the corresponding gross primary productivity $(GPP$, nighttime partitioning method after [Reichstein et al.](#page-51-17)

[\(2005\)](#page-51-17)). Water flux data consisted of evapotranspiration (ET) , no energy balance correction) which was converted from the

latent energy and transpiration estimates based on the Transpiration Estimation Algorithm (TEA, [Nelson et al.](#page-49-10) [\(2018\)](#page-49-10); [Nelson](#page-49-11) 135 [\(2021\)](#page-49-11)). The TEA algorithm estimates transpiration based on the relationship between GPP and ET under conditions where surface and soil evaporation are expected to be minimal and accounting for residual non-transpiration evaporation. Note that estimates of GPP and transpiration are not direct measurements but instead based on statistical relationships localized to each station and time period and thus contain their own assumption and uncertainties. All data were aggregated to a common hourly time resolution, an overview of which can be found in Table [2.](#page-10-0)

Table 2: Fluxes to be predicted and predictor variables used in X-BASE. The units of the fluxes correspond to the native hourly resolution. Upon temporal aggregation as in some analyses in the presented results, the units may change.

predictor variables

air temperature \circ C

140 Data from the EC dataset that ultimately were used for training the models varied between ~12-14 million site-hours depending on the target variable (i.e. GPP , NEE , ET , or ET_T). Training of the machine learning algorithms was only conducted on hours where all input variables passed quality control. The quality control procedure consisted of two levels, with the first being each hour must have at least one value of good quality measured or gap-filled with confidence (i.e. at least one half hour was either 0 or 1 based on the OneFLUX _QC flags). Second, a set of consistency tests were performed on each used variable 145 to check the consistency both among variables and across sites. As the consistency flags were based on daily aggregates of the meteorological and flux data, entire days were removed if the test indicated inconsistencies among related variables. The consistency flag also checked the relationship between variables across sites, ensuring that the relationships found across the data are coherent. A detailed explanation of these consistency flags can be found in [Jung et al.](#page-47-16) [\(2024\)](#page-47-16).

2.2 Global Meteorology

150 For the generation of global flux maps we used hourly meteorological data from ERA5 global reanalysis products at 0.25° [\(Hersbach et al., 2020\)](#page-46-23). Variables included air temperature at 2m height, incoming shortwave radiation at the surface, as well as vapour pressure deficit (computed from relative humidity, air temperature, and surface pressure). Units were converted to correspond to the site level measurements which were used for training the machine learning model, and the data were re-gridded to a 0.05° resolution using bilinear interpolation for every hour.

155 2.3 Satellite Earth Observation

The X-BASE products are based on measurements of the MODerate Imaging Spectroradiometer (MODIS) of surface reflectance and land surface temperature from collection 006 at daily resolution. Missing records were gap-filled consistently in both the average time series per EC station and in the global gridded data following the procedures of the FluxnetEO data version 2 [\(Walther and Besnard et al., 2022;](#page-54-4) [Walther, 2023\)](#page-54-14).

160 2.3.1 Spectral vegetation indices

At site level we used surface reflectance in the first seven MODIS spectral bands from the MCD43A4 c006 reflectance data set (500 m and daily, where each daily value is inverted from all valid observations within a 16-day window, [Schaaf and Wang](#page-52-24) [\(2015b\)](#page-52-24)). The spectral vegetation indices computed from the reflectance data were the enhanced vegetation index (EVI, [Huete](#page-46-24) [et al.](#page-46-24) [\(2002\)](#page-46-24)), the spectral reflectance of vegetation in the near-infrared (NIRv, [Badgley et al.](#page-42-29) [\(2017\)](#page-42-29)), and the normalized 165 difference water index (NDWI) with MODIS band 7 as reference [\(Gao, 1996\)](#page-45-22). We followed the procedure of the FluxnetEO data sets version 2 [\(Walther and Besnard et al., 2022\)](#page-54-4) for data acquisition from Google Earth Engine for all pixels in a cutout

- of 4x4 km² around each EC station, as well as for quality checks in terms of cloud, snow, and land cover, index values outside the defined ranges, and outliers. An iterative approach then determined both, the strictness of the inversion quality of the bidirectional reflectance distribution function (BRDF, based on the MCD43A2 data, [Schaaf and Wang](#page-52-25) [\(2015a\)](#page-52-25)) and the set of
- 170 pixels in a cutout that shall represent a given EC station. Supporting information section Appendix [B1](#page-31-0) outlines all technical details of the dynamic procedure.

Global data of BRDF-corrected surface reflectance stem from the MCD43C4 c006 data [\(Schaaf and Wang, 2015b\)](#page-52-24), available in a climate modelling grid of 0.05° with the same temporal sampling and subject to the same removal of snow and water pixels and outlier values like at site level. The BRDF quality control of the global data followed the same dynamic approach (see 175 supporting information Appendix [B1\)](#page-31-0), which maximized data availability especially in tropical regions.

2.3.2 Land surface temperature

Satellite observations of land surface temperature (LST) were based on the MODIS c006 TERRA observations which are available every day at 1 km resolution [\(Wan et al., 2015\)](#page-54-15). We selected the 1 km^2 pixel containing a specific tower and treated the two MODIS LST data streams as independent predictor variables which represent clear-sky LST at a specific time of 180 the day (namely around 10.30 AM and PM local time). Quality checks and gap-filling followed the procedure described in

FluxnetEO version 2 [\(Walther and Besnard et al., 2022\)](#page-54-4).

For the global spatialization of the flux estimates we relied on climate modelling grid LST from the MODIS TERRA data sets [\(Wan et al., 2015\)](#page-54-15) and apply consistent quality control and imputation of missing values like at site-level.

2.3.3 Land cover

185 Land cover information used the IGBP global vegetation classification. Site level classification was as reported by the principal investigators. Global data were based on the yearly-resolved MODIS MCD12C1 c006 product [\(Friedl and Sulla-Menashe,](#page-45-23) [2015\)](#page-45-23). In order to ease the transition between site and global land cover classifications, an intermediate classification scheme was utilized which translated each classification into characteristics (e.g. trees, crops, needleleaf, deciduous, etc. . .) based on whether the classification has (value=1.0), might have (value=0.5), does not have (value=0.0) a specific feature, or is unknown

190 (value=-1.0). A full description of this intermediate classification system can be found in supplementary section Appendix [B2.](#page-32-0)

2.4 Machine Learning Method

All X-BASE products are based on gradient boosted regression trees using the XGBoost library [\(Chen and Guestrin, 2016\)](#page-44-29). XGBoost is known as a robust algorithm that is able to handle a variety of variable types (numeric, boolean, categorical). Training was conducted using a two-thirds training sub-sampling ratio and a 0.05 learning rate. Hyperparameters were chosen 195 based on preliminary testing to predict eddy covariance data, and a full list of hyperparameters can be found in supplemental

section Appendix [B3.](#page-33-0) Boosting was stopped when no model improvement (based on mean squared error of validation data) was observed for ten consecutive rounds, and the best performing model was stored to generate predictions. In all cases, the model reached the stopping criteria relatively quickly, with the final number of boosting rounds between 80-230, depending on the flux.

200 2.5 Cross-validation

All cross-validation was performed using a ten-fold, leave-site-fold-out scheme, where each fold was constructed by randomly assigning each site to a fold. For each round of cross-validation, eight folds were used for training, one for validation and the remaining one as the test fold for which the actual predictions were made. The leave-site-fold-out scheme ensures that no data from the sites in the test fold were ever seen by the algorithm during training, and in turn iterated such that each site was in

- 205 the test set once. As eddy covariance sites are sometimes clustered in the same location (e.g. as different treatments) and can therefore be both physically closely located and not truly independent, sites are assigned to the same fold if they are less than 0.05° apart to reduce over-fitting. We evaluate the accuracy of the cross-validation models by computing the Nash-Sutcliffe modeling efficiency (NSE, [Nash and Sutcliffe](#page-49-12) [\(1970\)](#page-49-12)), where a negative NSE indicates a model accuracy that is worse than a mean prediction, while a value close to one indicates high model accuracy. We compute the NSE for each site and for a range 210 of temporal scales from hourly to inter-annual.
	- 2.6 Up-scaling

The final step to train a model to use in the final global prediction step was identical to the training in the cross-validation, with the exception that, because no test fold was required, we used nine of the ten folds for the training and validation was done on the remaining fold. The final trained models (one trained model for each target flux) were then used to predict fluxes

215 at the global scales using the associated globally gridded input variables that correspond to those used at site level, as outlined in Table [2.](#page-10-0)

2.7 Previous FLUXCOM and independent global flux estimates

We compare X-BASE with up-scaling results from FLUXCOM [\(Jung et al., 2019,](#page-47-4) [2020\)](#page-47-3). As mentioned earlier, FLUXCOM comprised an ensemble of up-scaling experiments that differed in the choice of machine learning method, meteorological forc-

- 220 ing data, and which were summarized in two groups of set-ups that shared the same predictor variables and spatiotemporal resolution: The "remote-sensing-only" set-up (RS) mostly used spaceborne observations of MODIS as explanatory variables and produced flux estimates every 8 days at 0.083° resolution, while the 'remote-sensing plus meteorology set-up' (RS+METEO) produced daily flux estimates at half degree resolution from meteorological predictor variables and an average seasonal cycle of satellite observations [\(Tramontana et al., 2016;](#page-53-4) [Jung et al., 2019,](#page-47-4) [2020\)](#page-47-3). Comparisons to FLUXCOM RS+METEO datasets
- 225 always refer to the ensemble over multiple machine learning methods for all realizations driven by the ERA5 meteorology [\(Hersbach et al., 2020\)](#page-46-23). RS+METEO uses average seasonal cycles of MODIS c005 observations. For the FLUXCOM RS set-up we use the ensemble over all machine learning methods. Please note that both the previous RS runs and the X-BASE runs presented here are driven by data from MODIS c006, but the processing has changed in some aspects such as quality control and gap-filling. For clarification, an overview on FLUXCOM(-X) naming conventions is given in supplemental
- 230 section Appendix [A.](#page-30-0)

For evaluating X-BASE NEE globally, in particular its seasonal cycle and for different regions, we used two different at[m](#page-43-24)ospheric inversion model products: the Orbiting Carbon Observatory-2 (OCO-2) v10 model intercomparison project [\(Byrne](#page-43-24) [et al., 2023\)](#page-43-24) and the CarboScope inversion [\(Rödenbeck et al., 2018\)](#page-51-18) version s99oc_v2022 [\(Roedenbeck and Heimann, 2022\)](#page-51-19). Estimates from the OCO-2 came from the the LNLGIS experiment which combines satellite-based column-averaged $CO₂$

235 (XCO2) retrievals and in-situ $CO₂$ measurements as observational constraints in the assimilation, and consists of 13 different [e](https://gml.noaa.gov/ccgg/OCO2_v10mip/index.php)nsemble members covering the period 2015-2020 with a monthly frequency and 1° spatial resolution [\(https://gml.noaa.gov/](https://gml.noaa.gov/ccgg/OCO2_v10mip/index.php) [ccgg/OCO2_v10mip/index.php\)](https://gml.noaa.gov/ccgg/OCO2_v10mip/index.php). The CarboScope product consisted of a single inversion output at the same spatial resolution as OCO-2, but a longer temporal period from 2001 to 2020. In each case, as the inversion products estimate net biome exchange, we subtracted from the inversions data fire emissions as estimated by the Global Fire Emissions Database, Version 4.1

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240 (Randerson et al., 2017).
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We compared temporal patterns of X-BASE GPP with the patterns in global retrievals of sun-induced chlorophyll fluorescence (SIF) from the Sentinel-5P TROPOMI instrument [\(Köhler et al., 2018\)](#page-48-29), which under most conditions approximate the variability in GPP . For the comparison we used estimates of daily mean SIF applying a correction factor to instantaneous observations [\(Zhang et al., 2018\)](#page-54-16) and averaged both X-BASE GPP and TROPOMI SIF to a temporal resolution of 16 days 245 and 0.5° spatial grids for the common period 04/2018-12/2020.

X-BASE ET and ET_T were cross-compared with transpiration estimates from the Global Land Evaporation Amsterdam Model (GLEAM) v3.6a [\(Martens et al., 2017;](#page-48-30) [Miralles et al., 2011\)](#page-49-13). GLEAM also utilizes satellite and reanalysis data sets [b](#page-51-21)ut in a more physically constrained way, relying on semi-empirical models such as the Priestley and Taylor [\(Priestley and](#page-51-21) [Taylor, 1972\)](#page-51-21) and Gash models [\(Gash, 1979\)](#page-45-24). Further comparisons were made to precipitation data from GPCC [\(Schneider](#page-52-26) 250 [et al., 2022\)](#page-52-26).

2.8 Units across scales and conversion

Given the broad range of spatial and temporal scales reported here, we utilized different units depending on each use case. All base measurements and predictions are at hourly timescale and in units of $\mu molCO_2 \cdot m^{-2} \cdot s^{-1}$ for carbon fluxes and $mm \cdot hr^{-1}$ for water fluxes (as reported in Table [2\)](#page-10-0). In the case of carbon fluxes, all timescales which are not sub-daily are 255 reported in grams carbon per unit time and area. Globally integrated values are reported in Pg carbon or km^2 water and are aggregated using a common land area estimate per grid cell.

3 Results

3.1 Cross-validation and data space

- One important innovation in FLUXCOM-X compared to the previous FLUXCOM ensemble was the training data base, which 260 was larger due to an incease in both number of sites and years. Furthermore, the EC methodology has changed considerably in many aspects ranging from collection and processing to quality filtering in the last 15 years. We show here one illustrative example of the changes in the environmental space that is represented in the training samples for daily NEE : between daily VPD and daily incoming shortwave radiation the distribution of training samples was considerably broader in X-BASE compared to the RS+METEO ensemble (Fig. [1\)](#page-16-0). Furthermore, the number of unique sites contributing to a certain VPD-radiation 265 bin has increased (Fig. [C1\)](#page-34-0), i.e. the number of ecosystems sampled in each climatic condition has also increased. The increases were seen particularly at the margins of the distribution, i.e. for days with high VPD along the full radiation spectrum, and
- vice versa for days with high radiation conditions along the full VPD spectrum. Remarkably, the number of sites contributing training samples for high VPD *and* high radiation were observed much more frequently (Fig. [1\)](#page-16-0) and at more sites (Fig. [C1\)](#page-34-0) compared to RS+METEO - providing more and more varied information for dry conditions. Overall for NEE, the number of 270 sampled site-days increased over three-fold (552878 to 183216 for X-BASE and RS+METEO respectively), note however that X-BASE is modeled at hourly instead of daily resolution and thus the number of sampled site-days should not be considered a

metric of how well the feature space is sampled.

The results from the ten-fold cross validation showed an overall high performance with most fluxes and scales of variability having an NSE above 0.6 (Fig. [2\)](#page-16-1). In terms of scales of variability across all fluxes, the monthly mean diel cycle ("diel") and the 275 daily median seasonal cycle ("seasonal") were very regular patterns that the trained models reproduced best. Also, among-site changes ("spatial", except for NEE) and monthly aggregated fluxes ("monthly") were reliably predicted. Deviations from the median daily seasonality ("anom") were only moderately reliable with NSE between 0.25 and 0.5. The XGBoost models did not succeed in accurately reproducing inter-annual changes ("i.a.v.") of all fluxes and between-site patterns in NEE . Consistently across all scales, the net fluxes which are directly calculated (i.e., ET and even more so NEE) showed lower performance 280 than their respective modelled gross fluxes (i.e., GPP and ET_T). Note that the cross validation results from Fig. [2](#page-16-1) cannot

be quantitatively compared to previous cross validation results in FLUXCOM as the training data are not the same. However, qualitatively the accuracy gradient among fluxes, as well as along scales of variability, corresponded to patterns identified in

Figure 1. Cross-validation sampling in meteorological space: Number of site-days contributing to sampling for NEE for the previous FLUXCOM RS+METEO ensemble (left) compared to the sampling of FLUXCOM-X-BASE (right) in environmental space of daily aggregated incoming shortwave radiation and VPD. Color corresponds to number of site days per bin in log scale. Only bins with at least twenty site-days are shown.

Figure 2. FLUXCOM-X-BASE site-level accuracy of predicted fluxes in ten-fold leave-site-fold-out cross-validation in terms of NSE computed per site for a range of scales of variability. Scales of variability include the hourly timescale ("hourly"), daily ("daily") and monthly ("monthly") aggregated fluxes, as well as between-site changes ("spatial"), monthly mean diel cycle ("diel"), daily median seasonal cycle ("seasonal"), deviations from the median daily seasonality ("anom."), and inter-annual variability ("i.a.v."). Boxes denote the range from the 25th to the 75th percentile of sites, whiskers extend 1.5 times the interquartile range from the 25th and 75th percentile of NSE across sites.

FLUXCOM and in comparable empirical modeling activities [\(Jung et al., 2011;](#page-47-2) [Tramontana et al., 2016;](#page-53-4) [Virkkala et al., 2021;](#page-53-5) [Dannenberg et al., 2023\)](#page-44-0).

Figure 3. Resolution improvements for the X-BASE products compared to RS and RS+METEO: Average NEE for an 8-day period in Europe in 2010 as estimated from the RS, RS+METEO and X-BASE set-ups (top panel), as well as snapshots of temporal trajectories of NEE in pixels closest to selected EC station locations (A:UK-Tad, B: DE-Hai, C: ES-LM1, D: FR-Pue). Negative values of NEE denote a $CO₂$ flux from the atmosphere to the land.

285 3.2 Global flux estimates

One asset of FLUXCOM-X is flexibility in the spatiotemporal resolution of the flux estimates. We are producing X-BASE products at 0.05° spatial and hourly temporal resolution globally. Figure [3](#page-17-0) illustrates the increase in spatial and temporal detail in X-BASE compared to RS $(0.083^{\circ}, 8$ -daily) and RS+METEO $(0.5^{\circ}, 4)$ using the example of NEE.

3.2.1 Net Ecosystem Exchange (NEE)

290 The X-BASE product estimates the global terrestrial NEE to be -5.75 \pm 0.33 $PgC \cdot yr^{-1}$ (2001-2020), with hotspots of strong $CO₂$ flux into the ecosystems in the tropical regions, and temperate regions of North America and Europe (Fig. [4\)](#page-18-0). In contrast to both RS and RS+METEO, India and some regions in central Sahel show prominent patterns of a mean CO_2 flux from the ecosystems to the atmosphere in X-BASE, corresponding mostly to crop designated areas (Fig. [C2\)](#page-35-0). However, X-BASE global terrestrial NEE (-5.63 $PgC \cdot yr^{-1}$) agrees well with the inversion estimates of OCO-2 (-4.12 $PgC \cdot yr^{-1}$) and CarboScope 295 $(-3.46 PgC \cdot yr^{-1})$ over the common period (2015-2020). Here, GFED 4.1 [\(Randerson et al., 2017\)](#page-51-20) emission estimates have been used to correct the inversion estimates for fire emissions.

Comparison with OCO-2 and CarboScope inversions also indicates a substantial improvement of the global mean seasonal cycle of NEE (Fig. [5\)](#page-19-0) in X-BASE compared to RS and RS+METEO. The systematic bias present in RS and RS+METEO has essentially disappeared in X-BASE. The shape, and in particular the amplitude, of the global NEE seasonal cycle of X-BASE

Figure 4. Comparison of annually integrated NEE from X-BASE, RS+METEO with ERA5 forcing and RS averaged over the period 2001-2020. The difference maps show the difference of the averages over 2001-2020.

300 is more consistent with the inversions. The larger and more realistic seasonal cycle amplitude of global NEE in X-BASE originates primarily from improved and increased amplitudes in boreal regions. Interestingly, X-BASE suggests slightly larger NEE seasonal cycle amplitudes in temperate regions compared to the inversions. In seasonally dry regions, the timing of maximum uptake is consistent between X-BASE and inversions, while the peak of maximum net release is larger and delayed in the inversions. In Australia, the peak of $CO₂$ release to the atmosphere at the end of the year present in both inversions is not 305 evident in X-BASE, which instead shows a relatively consistent $CO₂$ flux to the atmosphere throughout the year. In tropical regions, the patterns of seasonal variations are qualitatively consistent between X-BASE and the previous RS and RS+METEO products. The seasonal patterns in tropical regions are relatively weak overall and seem inconsistent both between the inversions and X-BASE as well as among the inversions.

As seen in Figure [5,](#page-19-0) the X-BASE product shows the same large underestimation of globally integrated NEE inter-annual 310 variance as the previous RS and RS+METEO products. In terms of temporal trends, the X-BASE products show almost no

change in annual NEE in time, which is in contrast to the RS+METEO (slight positive trend) and RS (slight negative trend) and more consistent with the CarboScope inversions (Table [C2\)](#page-37-0). However, as inter-annual variability was poorly reproduced even in the cross validation (Fig. [2\)](#page-16-1), trends in the X-BASE products should be taken with caution and interpreted with careful scrutiny.

Figure 5. Seasonal and inter-annual variability of global NEE. Comparison of mean seasonal cycles (calculated over the common time period, 2015-2020) and inter-annual variability (2001-2020) of NEE estimated from CARBOSCOPE and OCO2 inversions as well as FLUXCOM-X-BASE and FLUXCOM RS+METEO and RS outputs. All products were integrated with a common mask that removes sparsely vegetated arid regions not predicted by RS and RS+METEO.

Figure 6. Comparison of annually integrated GPP from X-BASE, RS+METEO with ERA5 forcing and RS averaged over the period 2001-2020. The difference maps show the difference of the averages over 2001-2020.

315 3.2.2 Gross Primary Productivity (GPP)

X-BASE estimates the globally integrated GPP at 124.7 \pm 2.1 PgC · yr⁻¹ on average in the time period 2001-2020. Globally integrated GPP over vegetated areas (RS and RS+METEO do not have estimates for non-vegetated areas) was approximately equal for X-BASE (121.9 \pm 2.1 $PgC \cdot yr^{-1}$) and RS+METEO (121.6 \pm 0.4 $PgC \cdot yr^{-1}$) but considerably higher than RS (113.2 \pm 1.8 $P g C \cdot yr^{-1}$) over the same period. In terms of regional patterns, X-BASE GPP consistently exceeds both 320 RS+METEO and RS in temperate, boreal, and most subtropical ecosystems, but is lower in sparsely vegetated (semi-)arid regions like southwestern North America as well as southeast Asian croplands (Fig. [6\)](#page-20-0). This qualitatively consistent pattern is only broken in the humid tropics, where X-BASE GPP is higher than RS, but lower than RS+METEO.

Comparing the estimated trend over the last two decades, X-BASE GPP has a clear increasing linear trend of 0.34 PqC yr^{-2} which is slightly higher than the trend in RS (0.25 $PgC \cdot yr^{-2}$, Table [C2\)](#page-37-0). In contrast, the RS+METEO product shows 325 nearly no trend in annual GPP . The increases in both the X-BASE and RS products may be related to increases in surface greenness coming from variability in the remote sensing forcing data which are inter-annually dynamic in both products, whereas the remote sensing data were not inter-annually dynamic in the RS+METEO product which instead used only the mean seasonal cycle of the remote sensing data. The magnitude of between-year changes in globally integrated X-BASE GPP is 0.575 $PgC \cdot yr^{-1}$ over the years 2001-2020, which is about twice as large as RS+METEO (0.248 $PgC \cdot yr^{-1}$), but only half

330 the magnitude estimates in the RS set-up (1.02 $PgC \cdot yr^{-1}$, Table [C2\)](#page-37-0).

We further compared the temporal trajectory in GPP estimates against TROPOMI SIF as an independent proxy for GPP dynamics (Fig. [7\)](#page-22-0) at a temporal resolution of 16 days. The temporal variability of X-BASE GPP strongly agrees with that in TROPOMI SIF, with squared Spearman correlation values (denoted as R^2) of the time series above 0.85 across most of the vegetated land surface (Fig. [7](#page-22-0) top left). The only exceptions are regions with no or very small variability in both GPP and SIF

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- 335 such as in either evergreen tropical ecosystems in South America, Africa and southeast Asia, or sparsely to non-vegetated areas due to aridity (e.g. Mexican, and African deserts) or cold conditions (e.g. Canadian and Siberian subpolar regions). In inner Australia, despite being sparsely vegetated, variability between years is expected in GPP due to precipitation increases during La Niña years, which is however not reflected in the squared correlations. R^2 for the deviations from the average seasonality (again computed with a temporal resolution of 16 days) show the same qualitative spatial patterns (Fig. [7](#page-22-0) top right), but are 340 overall lower with R^2 values between 0.55 and 0.8. Anomalies of X-BASE GPP and SIF agree best in eastern European
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temperate forests as well as grassy and shrub ecosystems in eastern South America.

Comparison of the level of agreement of SIF and X-BASE with that of SIF and RS and RS+METEO, respectively, illustrates that X-BASE and RS GPP estimates have comparable consistency both for the time series (global area weighted mean R^2 values of 0.72 and 0.73, respectively) and anomalies (global mean R^2 values of 0.64 and 0.66, respectively). In contrast, the R^2

- 345 between RS+METEO and SIF is lower in both cases (R^2 values of 0.66 for the time series and 0.58 for anomalies). X-BASE GPP shows a higher agreement with SIF than RS both in terms of the actual trajectory and anomalies in evergreen tropical forests with no or only a very short dry season in the Amazon and Africa, as well as in fully humid parts of southeast Asia (Fig. [7](#page-22-0) middle panel). Improvements in X-BASE GPP compared to RS are also consistent in the very continental and polar tundra areas in eastern Siberia, northern Canada and Alaska. Conversely, in arid steppe climates globally, X-BASE GPP variability
- 350 agrees less with SIF than does RS GPP . X-BASE GPP variability is consistently and widespread much more similar to the variability in TROPOMI SIF than RS-METEO GPP . Increases in R^2 for X-BASE compared to RS+METEO are most pronounced in arid to semi-arid ecosystems (large parts of the Caatinga and Gran Chaco regions on South America, steppe regions in Mexico, southern and eastern Africa, Australia and central Siberia) as well as in global crop regions, especially for the deviations from the seasonality (albeit the magnitude of R^2 change is quite variable between regions, Fig. [7](#page-22-0) bottom).

355 3.2.3 Water Vapor Fluxes

Globally integrated ET amounts to $74.7 \times 10^3 \pm 0.9 \times 10^3$ km³ · yr^{-1} for 2001-2020 (Table [C1\)](#page-36-0) for X-BASE, with the highest rates in the tropics (Fig. [8\)](#page-24-0). Comparing global totals for vegetated areas only (where all products give outputs) shows similar values for X-BASE (68.9x10³ ± 0.9x10³ km³·yr⁻¹), GLEAM (70.9x10³ ± 0.9x10³ km³·yr⁻¹) and RS+METEO (68.3x10³ \pm 0.3x10³ km³ · yr⁻¹) ET estimates, while the RS ET is more than 11% higher (78.5x10³ ± 0.5x10³ km³ · yr⁻¹, Table [C1\)](#page-36-0). 360 Particularly in evergreen tropical ecosystems, X-BASE estimates a considerably lower ET than both GLEAM, RS+METEO, and RS (Fig. [8\)](#page-24-0). Furthermore, in the temperate and high latitudes of the northern hemisphere, annually integrated X-BASE ET is consistently lower than the other estimates, though the magnitude of the bias is smaller than in the tropical regions. The pattern is only reversed with higher X-BASE ET in the semi-arid and arid ecosystems of the lower and middle latitudes, especially with respect to annual ET in RS+METEO and GLEAM.

Figure 7. Similarity of temporal patterns between GPP estimates and TROPOMI SIF observations: R^2 (computed as the square of the Spearman correlation) between X-BASE GPP and TROPOMI SIF [\(Köhler et al., 2018\)](#page-48-29) for the actual time series at a temporal resolution of 16 days (top left) and anomalies from the median seasonality in both variables (top right). The middle and the bottom panels relate the agreement between X-BASE GPP and TROPOMI SIF to the agreement between FLUXCOM GPP and TROPOMI SIF, where the middle panel refers to TROPOMI SIF and GPP from the RS+METEO set-up, and the bottom panel to the RS set-up. All comparisons are done for time series with a resolution of 16 days for the common time period 04/2018 to 12/2020. SIF observations have been applied a correction factor to estimate daily average SIF before aggregation. Semi-transparent areas mark pixels in which the correlation of at least one of the data sets is negative.

- 365 Comparison to precipitation estimates shows that X-BASE ET greatly exceeds precipitation inputs over large areas, indicating a strong overestimation of X-BASE ET in many arid regions with sparse vegetation (e.g. the Sahara region, Fig. [C3\)](#page-39-0). While transport of water both laterally (i.e. runoff from other areas) and from deeper groundwater could cause ET to exceed precipitation inputs in some areas, the extent of area where ET exceeds precipitation (e.g. the entire Sahara region) and the magnitude of the excess ET (over three times precipitation inputs) indicates a major bias in these areas and is likely due
- 370 to a lack of EC data in similar ecosystems. As a rough estimate, constraining the X-BASE estimates with precipitation (see supplement section Appendix [C5\)](#page-38-0) suggests about 4-6x10³ $km^3 \cdot yr^{-1}$ of water is overestimated globally.

The globally integrated ET_T amounts to $42.6x10^3 \pm 1.0x10^3$ $km^3 \cdot yr^{-1}$ (2001-2020) in X-BASE, resulting in an average ratio of transpiration to total evaporation of 57.0% \pm 0.6% (Table [C1\)](#page-36-0). In contrast to ET, the ET_T estimates from X-BASE do not commonly exceed precipitation estimates (Fig. [C3\)](#page-39-0), which could indicate that because the water vapor flux is more tightly 375 coupled with vegetation, the model is able to distinguish that no vegetation corresponds with no transpiration, which is not

- generally the case for non-transpiration evaporation. The RS and RS+METEO products did not produce ET_T estimates, so the comparison is limited to GLEAM (50.7x10³ ± 0.6x10³ $km^3 \cdot yr^{-1}$), which estimates ET_T on average 17% higher than X-BASE, with strong contributions from the evergreen tropics. Only in single semi-arid regions, such as northernmost Sahel as well as large parts of the South American Caatinga and Chaco regions is this pattern reversed (Fig. [8\)](#page-24-0).
- 380 Spatially, X-BASE-estimated ET_T/ET exceeds 50% in the majority of areas, with the highest values seen in the higher latitude regions of Europe and Asia, as well as in subtropical ecosystems (Fig. [8\)](#page-24-0). Arid regions with sparse vegetation show the lowest ET_T/ET overall, with values generally below 20%. With 71.4% \pm 0.6% over global vegetated surfaces, GLEAM attributes about 10% more of its ET to ET_T than does X-BASE (Table [C1\)](#page-36-0). Regionally, this difference can even reach up to 40%, with the only exception being boreal forests and very dry ecosystems in the Sahel, the Arabian Peninsula and central 385 Asia (Fig. [8\)](#page-24-0).

Trends in ET , ET_T and ET_T/ET are positive and exceed the trends seen in all other estimates over the years 2001-2020. Conversely, the magnitude of inter-annual changes in X-BASE ET , ET_T , and ET_T/ET is mostly less than half than the variability in GLEAM (Table [C2\)](#page-37-0). Low inter-annual changes are common to the RS and RS+METEO ET as well.

- Figure [9](#page-25-0) shows the temporal correlation at 16-daily temporal scale using GLEAM as a reference, showing overall high 390 values of squared correlation between X-BASE and GLEAM ET and ET_T (top and bottom left). Notable exceptions with low correlations are areas with low variability in ET such as the arc of deforestation, very dry areas, and tropical evergreen ecosystems in Africa. Compared to RS+METEO and RS (middle panels left column in Fig. [9\)](#page-25-0), X-BASE ET temporal patterns are more similar to GLEAM ET in many areas, and especially so in areas north of the arc of deforestation and parts of tropical evergreen areas in central Africa and souteast Asia. Conversely, X-BASE ET agrees less well with GLEAM than RS
- 395 or RS+METEO in the arc of deforestation itself, the eastern parts of the Amazon basin, as well as dry areas. The deviations from the mean annual cycle in ET and ET_T (right column) show overall lower correlations than the actual time series, with the highest agreement between GLEAM and X-BASE in large parts of the Amazon forest and central European ecosystems. X-BASE ET anomalies are much more strongly correlated with GLEAM ET than either RS or RS+METEO everywhere except for most (semi-)arid regions.

Figure 8. Comparison of evaporative flux estimates ET , ET_T and ET_T/ET from X-BASE and its difference with RS, RS+METEO, and GLEAM. ET_T is compared in the case of GLEAM, but is unavailable in the previous FLUXCOM ensembles.

Figure 9. Similarity of temporal patterns of X-BASE an GLEAM terrestrial water fluxes in comparison to those from FLUXCOM: $R²$ (computed as the square of the Pearson correlation) between X-BASE ET and GLEAM ET for the actual time series (left column) and anomalies from the median seasonality (right column). The middle panels compare the agreement between X-BASE ET and GLEAM ET to the agreement between FLUXCOM ET and GLEAM ET . The bottom panel shows the squared correlations between X-BASE and GLEAM ET_T , but no comparisons to FLUXCOM because FLUXCOM did not include ET_T . All comparisons are done for time series with a resolution of 16 days and 0.05 degrees for the years 2001-2020. Semi-transparent areas mark pixels in which the correlation of at least one of the data sets is negative.

empirical upscaling.

We have presented qualitative and quantitative comparisons of the X-BASE products with previous FLUXCOM estimates and independent data sets where possible. Statements on the main causes of (dis-)agreements in the magnitude and spatiotemporal variability in the flux estimates remain speculative as detailed analyses would require further investigation in the form of experiments, which is beyond the scope of this manuscript. In the following we discuss the prominent changes in NEE compared 405 to FLUXCOM as a key scientific highlight in X-BASE and outline potential ways forward to tackle persistent challenges in

4.1 Higher consistency of NEE with atmospheric carbon cycle constraints

Although FLUXCOM-X follows the same fundamental approach as FLUXCOM, we find a substantial improvement of the magnitude of the annually integrated NEE of FLUXCOM-X-BASE over previous FLUXCOM products [\(Jung et al., 2020\)](#page-47-3)

- 410 when compared to independent estimates from atmospheric inversions. The mean global X-BASE NEE of -5.75 $PgC \cdot$ yr^{-1} is slightly smaller than the inferred NEE of -3.92 $PgC \cdot yr^{-1}$ (corrected for fire emissions based on GFED 4.1) from CarboScope. The remaining difference could easily be explained by carbon sources such as aquatic evasion and volatile organic [c](#page-47-3)ompounds that are included in the atmospherically based estimate but not in eddy-covariance based FLUXCOM (see [Jung](#page-47-3) [et al.](#page-47-3) [\(2020\)](#page-47-3) and [Zscheischler et al.](#page-55-0) [\(2017\)](#page-55-0) for further discussion).
- 415 The improved global NEE of FLUXCOM-X-BASE originates most likely from enhanced quality of eddy covariance measurements in the training resulting from years of consistent improvements in instrumentation, method development, and quality assurance from the point of measurement to the synthesis datasets. Previous up-scaling-based NEE products of [Jung et al.](#page-47-2) [\(2011,](#page-47-2) [2020\)](#page-47-3); [Bodesheim et al.](#page-43-25) [\(2018\)](#page-43-25) - all based on the La Thuile FLUXNET dataset but varying with respect to machine learning methods, predictor variables, and temporal resolution - consistently estimated a nearly three-fold larger global ter-
- 420 restrial carbon uptake compared to X-BASE. As discussed and speculated in [Jung et al.](#page-47-3) [\(2020\)](#page-47-3), La Thuile likely contained biased NEE measurements, in particular for some tropical sites [\(Fu et al., 2018\)](#page-45-25), and together with the sparsity of data in the tropics, these biases were propagated to unrealistic tropical and global NEE estimates. The fact that we can now reconcile bottom-up global eddy-covariance-based NEE and estimates from top-down atmospheric inversions is a major achievement of the FLUXNET community. For context: $1 P g C \cdot yr^{-1}$ over the global vegetated area $(145 \times 10^6 km^2)$ corresponds to ~7
- 425 $gC \cdot m^2 \cdot yr^{-1}$, which marks a challenge for achieving such accuracy of mean NEE at any one flux tower site. The lesson learned here emphasizes once more that it is crucial to control for and minimize systematic biases of in-situ eddy covariance measurements [\(Moncrieff et al., 1996\)](#page-49-14).

The improved seasonality of X-BASE NEE , in particular for boreal regions, likely also results from enhanced information in the training data due to the hourly resolution. Similar improvements were observed in [Bodesheim et al.](#page-43-25) [\(2018\)](#page-43-25) who extended 430 RS+METEO by training on half-hourly flux observations. The hourly resolution improves the seasonal high-latitude NEE

likely due to better capturing the responses to light when daylength varies strongly.

4.2 New opportunities by X-BASE products

[T](#page-49-15)he improvements of NEE make X-BASE attractive as a data-driven biogenic prior for atmospheric inversions [\(Munassar](#page-49-15) [et al., 2022\)](#page-49-15). Moreover, its hourly resolution facilitates better integration in inversion systems due to the accounting of diurnal

435 flux and atmospheric transport variations, while its high spatial variations can provide patterns of flux variations that cannot be resolved by atmospheric constraints alone.

For the first time, X-BASE includes a global data-driven product of ecosystem transpiration. The estimated global ET_T/ET [r](#page-44-30)atio of 57% is consistent with independent top-down assessments from isotope base methods [\(Good et al., 2015;](#page-46-25) [Coenders-](#page-44-30)[Gerrits et al., 2014\)](#page-44-30) and past up-scaling estimates [\(Wei et al., 2017;](#page-54-17) [Schlesinger and Jasechko, 2014\)](#page-52-27). The spatially and tem-

- 440 porally high resolution data-driven X-BASE ET_T product provides a valuable complementary perspective to simulations from [p](#page-42-30)rocess-based land surface models, which show large disagreements and often indicate global ET_T/ET below 50% [\(Berg](#page-42-30) [and Sheffield, 2019;](#page-42-30) [Miralles et al., 2016\)](#page-49-16). This advancement opens new opportunities for large scale studies of carbon- water relations on a diurnal time scale. The generation of the X-BASE ET_T product was facilitated by the development of site-level evapotranspiration partitioning methods [\(Nelson et al., 2018,](#page-49-10) [2020\)](#page-49-17) underlining once more the importance of advances by the 445 FLUXNET community for Earth system science.
	-

5 Tackling persistent challenges

Next to the improvements and opportunities that X-BASE brings through the enhancement in site-level training data quality and quantity as well as the higher spatiotemporal resolution, we find that some key issues previously identified in FLUXCOM [\(Tramontana et al., 2016;](#page-53-4) [Jung et al., 2020;](#page-47-3) [Bodesheim et al., 2018\)](#page-43-25) persist in X-BASE. These include 1) the insufficient

- 450 representation of water-related effects, 2) the limited predictability of the spatial patterns of mean NEE , as well as 3) severe limitations with respect to the variability between years and over decades. In the following, we outline what we consider the most promising ways forward to tackle these (partly interrelated) challenges in future developments beyond X-BASE: novel additional predictor variables, more in-situ observations especially for some key ecosystems as well as innovative approaches of constraining machine learning models.
- 455 The persistent challenge and importance of capturing water effects on land-atmosphere flux variations is illustrated by the overestimation of mean ET in very dry, sparsely vegetated areas (Fig. [C3\)](#page-39-0), as well as by the poorer consistency of NEE sea-sonality with inversions in water limited regions (Fig. [5\)](#page-19-0). For GPP temporal patterns we find that X-BASE shows improved agreement with SIF in water limited regions compared to RS+METEO (Fig. [7\)](#page-22-0), which is likely because X-BASE uses concomitantly changing remote sensing observations opposed to a mean seasonal cycle only in RS+METEO. However, X-BASE
- 460 shows deteriorated agreement with SIF when compared to RS, even though X-BASE was trained on hourly flux observations with improved coverage of dry conditions (Fig. [1\)](#page-16-0). This decrease in performance indicates clearly the importance and uncertainty related to the predictor variable set for capturing water related effects. Uncertainties due to water limitation effects are also seen in the divergence of ET and ET_T estimates is semi-arid regions such as the Sahel and South American Caatinga (Figs. [8](#page-24-0) and [9\)](#page-25-0). Thus, there is considerable potential for advancements by including remote sensing based predictors on soil
- 465 moisture, sub-daily varying land surface temperature from geostationary satellites, SIF, and vegetation optical depth. Here, key challenges reside in achieving a sensible integration of flux observations with footprints that are much smaller than corresponding Earth observation products on the one hand, and an integration of disparate Earth observation products with each other on the other hand. This is one research priority for further FLUXCOM-X developments.
- Missing predictor variables is likely also a main reason for the limited skill of predicting between site variability of mean 470 *NEE* (Fig. [2\)](#page-16-1), which can depend on legacy effects of disturbances and management that are not accounted for. Novel and complementary Earth observation products that characterise ecosystem structure and states related to biomass and canopy heights from SAR and LIDAR should help raise the accuracy of FLUXCOM-X based mean NEE in future efforts. Also high resolution Earth observation products such as from Landsat may help to better resolve spatial details. X-BASE shows a prominent pattern of carbon flux to the atmosphere in sub-tropical and crop dominated regions of India and the Sahel, which 475 emphasizes the need to improve in-situ data coverage for agricultural systems, especially outside the temperate zone, and including important meta-data to better characterize these ecosystems and their site history. Despite the greatly reduced overall

bias of mean NEE, we emphasize that X-BASE products are pre-mature for diagnosing spatial variations of mean NEE.

The representation of longer term dynamics remains an area with opportunity for improvements in X-BASE. Inter-annual variability is still poorly reproduced in cross validation (Fig. [2\)](#page-16-1), particularly for NEE, which is likely not only due to the 480 complexity of processes shaping inter-annual variations but also due to temporal discontinuities in flux tower time series related to changes in instrumentation and factors like management [\(Jung et al., 2024\)](#page-47-16) that are not accounted for. The complexities of relying on field deployed instrumentation, together with the uncertainties related to linking satellite and flux data, causes poor signal to noise ratios and may impede good cross-validation results for i.a.v.. Globally, comparisons of X-BASE with inversions reveal an underestimated inter-annual variance and a poor correlation for global NEE i.a.v. (Fig. [5](#page-19-0) and Table [C2\)](#page-37-0). Interestingly, 485 X-BASE GPP shows improved correspondence with SIF anomalies compared to RS+METEO, especially in water limited regions (Fig. [7\)](#page-22-0), while no such improvement is evident for global NEE , which is likely due to the compensatory water effects in the global NEE signal [\(Jung et al., 2017\)](#page-47-17). That a comparison of RS+METEO runs with different meteorological forcing data showed the weakest correspondence with inversion i.a.v. when using ERA5 [\(Jung et al., 2020\)](#page-47-3) explains the substantially better correlations of RS+METEO with inversions for NEE i.a.v. in earlier studies [\(Jung et al., 2017,](#page-47-17) [2020\)](#page-47-3), and may also

490 explain the poor correlation of X-BASE. Thus, testing if alternative meteorological forcing data can improve global NEE i.a.v. for X-BASE is an important next step. It remains unclear at this point if accurate inter-annual variations at site-level and globally can be achieved by the FLUXCOM approach in the near future. Additional constraints beyond FLUXNET such as atmospheric CO_2 measurements [\(Upton et al., 2023\)](#page-53-18) or theoretical considerations in the form of hybrid [\(Reichstein et al.,](#page-51-22) [2019\)](#page-51-22) or deep learning models [\(Camps-Valls et al., 2021\)](#page-44-31) are promising and we will foster such endeavours.

495 6 Conclusions

We presented X-BASE, a new set of global high-resolution data-driven products of land-atmosphere fluxes from the FLUX-COM approach. This represents a cornerstone of our developments of the FLUXCOM-X framework designed to explore and mitigate current limitations to up-scaling from site to global scale. Improvements of the eddy covariance data facilitated reconciling estimates of global terrestrial net carbon exchange from X-BASE with top-down atmospheric inversions, and allowed

- 500 for the first time the generation of a global data-driven estimate of ecosystem transpiration. Beyond fostering all activities to enhance quality and coverage of available flux tower observations, most promise for future advancements by FLUXCOM-X relates to the synergistic exploitation of complementary satellite data streams to better capture water-related, site-history, and management effects. This will be challenging as it requires developing strategies and methodologies to better integrate in-situ flux observations and spaceborne Earth observations with very heterogeneous acquisition properties and with spatial resolu-
- 505 tions that are often very coarse compared to flux tower footprints. The recent de-orbiting of the TERRA spacecraft requires employing alternative satellite missions where practical issues of data acquisition and conceptual issues related to temporal consistency and reduced overlap with FLUXNET records pose imminent challenges. With FLUXCOM-X we have prepared the ground for tackling these challenges which can facilitate up-to-date and accurate flux estimates and thereby contribute to increased understanding of the Earth system in the future.

510 Appendix A: Naming conventions

Names of products and modelling environments may create confusion, especially given the legacy of FLUXCOM. We therefore will follow the following naming conventions and require potential users of products and collaborators to also follow this convention.

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Appendix B: Details on processing of Earth Observation Data

515 B1 Dynamic quality control and cutout size

The conditions in the pixels around a given EC station should best represent the conditions of the land surface in the area where the actual fluxes originate from. Given that the actual flux footprints are not generally available or computable for lack of critical information, we assume that the pixel containing the actual EC station (the 'tower pixel') is most representative for the dynamics of the area of influence on a tower. However, data availability and quality in the tower pixel is often in-520 sufficient. An iterative approach therefore selects both the cutout size and the strictness of the BRDF inversion quality from within defined bounds in a way that maximizes data availability and that ensures representativeness of the spatially averaged time series for the given site at the same time. In more detail, we start with a strict criterion for BRDF inversion quality

(BRDF_Albedo_Band_Quality_Bandx_flag in MCD43A2 $\lt=$ 2, meaning only full inversions). Then three options regarding the cutout size are considered:

- 525 A) only the tower pixel,
	- B) those 20% of pixels within 4x4 km² around a tower that are best correlated with the tower pixel are linearly regressed against the tower pixel and subsequently spatially averaged,
	- C) the 25% of pixels within a $4x4 \text{ km}^2$ area that are closest to the tower are averaged with the inverse of the distance to the tower as weight.
- 530 The criteria for selection between options A-C is based on the number of available good quality observations n in the resulting spatial average time series per site as follows:

```
if (n A >= 60 %) & (n B <= 70 %):
       select A
    elif (n A >= 60 %) & (n B >= 70 %):
535 select B
    elif (n A < 60 %) & (n A > 15 %):
        select B
    else:
        select C
```
540 If after the previous steps still less than 40% of good quality observations outside of snow covered times are available in the resulting average time series for a given site and index, the BRDF inversion quality threshold is relaxed to also allow magnitude inversions (MCD43A2 BRDF inversion quality flag \leq = 3), and the procedure to select the pixels contributing to the average described above is repeated. Consequently, the size of the area that a MODIS reflectance time series represents varies between sites, and so does the BRDF inversion quality.

545 For the global gridded MODIS data, the BRDF inversion quality is consistently selected as $\langle =2 \text{ or } \langle =3 \rangle$ based on the number of available good quality observations in a pixel.

B2 Details on the treatment of land cover information

Land cover information was passed through an intermediary classification system to both act as an encoding mechanism and to allow for arbitrary links between classification schemes. Rather than simple true/false classification for each category, different 550 attributes are classified based on whether the classification has (value=1.0), might have (value=0.5), does not have (value=0.0) a specific feature, or is unknown (value=-1.0). In the specific case of the MCD12C1 classification scheme, the conversion is as seen in table [B1.](#page-32-1)

Table B1: Land cover intermediary classification encoding for MCD12C1 classifications where the classification has (value=1.0), might have (value=0.5), or does not have (value=0.0) a specific feature, or is unknown (value=-1.0).

	ENF	EBF	DNF	DBF	MF	CSH	OSH	WSA	SAV	GRA	SNO	CRO	WET
Trees	J.			1	1	0.5	$\boldsymbol{0}$	1	0.5	$\boldsymbol{0}$	-1	$\boldsymbol{0}$	$\boldsymbol{0}$
Shrubs	Ω	$\mathbf{0}$	$\boldsymbol{0}$	θ	θ	1		0.5	0.5	$\mathbf{0}$	-1	$\boldsymbol{0}$	Ω
Grasses	$\mathbf{0}$	$\mathbf{0}$	$\boldsymbol{0}$	θ	$\boldsymbol{0}$	$\boldsymbol{0}$	0.5	0.5	1	1	-1	$\boldsymbol{0}$	Ω
Crops	$\boldsymbol{0}$	$\boldsymbol{0}$	$\boldsymbol{0}$	$\overline{0}$	θ	0	$\boldsymbol{0}$	$\boldsymbol{0}$	$\boldsymbol{0}$	$\mathbf{0}$	-1	1	Ω
Unveg	$\boldsymbol{0}$	$\boldsymbol{0}$	$\boldsymbol{0}$	$\overline{0}$	$\boldsymbol{0}$	$\boldsymbol{0}$	0.5	$\overline{0}$	$\boldsymbol{0}$	$\mathbf{0}$	Ω	$\overline{0}$	Ω
Water	Ω	$\boldsymbol{0}$	$\boldsymbol{0}$	$\overline{0}$	$\boldsymbol{0}$	0	$\boldsymbol{0}$	$\boldsymbol{0}$	$\boldsymbol{0}$	$\overline{0}$	0.5	$\boldsymbol{0}$	
Wetland	Ω	$\mathbf{0}$	$\overline{0}$	θ	θ	$\boldsymbol{0}$	$\boldsymbol{0}$	θ	$\boldsymbol{0}$	$\boldsymbol{0}$		$\overline{0}$	Ω
$C4$ _photo	$\overline{0}$	$\boldsymbol{0}$	$\boldsymbol{0}$	$\overline{0}$	$\boldsymbol{0}$	-1	-1	-1	-1	-1	$\overline{0}$	-1	Ω
Managed -1		-1	-1	-1	-1	-1	-1	-1	-1	-1	Ω		Ω
Needleleaf 1		$\mathbf{0}$	$\mathbf{1}$	θ	-1	-1	-1	-1	-1	$\mathbf{0}$	-1	$\overline{0}$	Ω
Broadleaf 0		1	$\boldsymbol{0}$		-1	-1	-1	-1	-1	$\mathbf{0}$	-1	$\boldsymbol{0}$	Ω
Deciduous 0		$\boldsymbol{0}$	1	1	-1	-1	-1	-1	-1	θ	-1	$\overline{0}$	Ω
Evergreen	-1	1	$\boldsymbol{0}$	θ	-1	-1	-1	-1	-1	$\overline{0}$	-1	$\boldsymbol{0}$	$\overline{0}$

555 C1 Additional cross-validation results

Figure C1. Cross-validation sampling in meteorological space: Number of unique sites contributing to sampling for NEE for FLUXCOM RS+METEO (left) compared to the sampling in the X-BASE set-up (right). Color corresponds to number of unique sites per bin in log scale.

C2 Large carbon release in tropical croplands

Figure C2. Large carbon release in tropical croplands

C3 Global magnitude of all fluxes

Table C1: Global magnitude of all fluxes. Column *Global Total* is the globally integrated flux for all areas including sparsely vegetated dry areas from 2001-2020. The column *Veg. Areas* includes a common mask which removes sparsely vegetated areas which are not computed for the RS and RS+METEO products. Values reported after the \pm correspond to the standard deviation across years.

C4 Linear trends and inter-annual variability for all fluxes

Table C2: Long-term variability of fluxes. Column *linear trend* is the linear slope of annually integrated fluxes over the years 2001-2020. The column *inter-annual variability* is computed as the standard deviation of annually integrated fluxes after the trend is removed.

C5 Potential overestimation of ET in dryland areas

560 Maps in Fig. [C3](#page-39-0) show the extend where ET and ET_T exceed precipitation as the ratio between the total of each flux to total precipitation (from GPCC [Schneider et al.](#page-52-26) [\(2022\)](#page-52-26)). Overall, X-BASE ET largely exceeds precipitation in most dry, sparsely vegetated areas, indicating overestimation. In contrast, ET_T does not show such extensive overestimation, limited instead to only smaller regions of the Sahara.

The amount of overestimation of X-BASE ET can be roughly estimated by replacing areas where annual ET exceeds pre-565 cipitation inputs with the corresponding annual precipitation inputs for each grid cell, i.e. replacing areas where the $ET/precip$ ratio is more than a threshold with the precipitation rather than the estimated ET . Using thresholds from 1.25 to 2.5 gives an excess of ET (i.e. original ET minus precipitation corrected) from $3.9x10^3$ to $6.1x10^3$ $km^3 \cdot yr^{-1}$.

Figure C3. Potential ET overestimation based on the ratio of estimated ET to precipitation from the Global Precipitation Climatology Centre (GPCC [Schneider et al.](#page-52-26) [\(2022\)](#page-52-26)).

Data availability. All data FLUXCOM-X-BASE data covering the years 2001-2021 (this manuscript only shows 2001-2020) is available as aggregated NetCDF file formats, to ease data handling for common use cases, from the ICOS Carbon Portal (https://doi.org/10.18160/5NZG-

570 JMJE). Furthermore, the full resolution data is accessible in the zarr format and in a publicly available object store provided by German Climate Computing Center (Deutsches Klimarechenzentrum, DKRZ). Instructions on how to all data, as well as the full dataset, can be found at the associated repository (https://gitlab.gwdg.de/fluxcom/fluxcomxdata).

Author contributions. JN, SW and MJ wrote the manuscript, and all authors contributed to the editing and structuring of it. JN, SW, FG, BK, ZH wrote the code which constitutes the modelling environment FLUXCOM-X, structuring it according to discussions including MJ, UW, 575 GD, and MM. Editorial input was provided by AI, AK, AK, AS, BB, BK, DB, DP, FT, GCV, GD, GN, GW, JA, JC, KI, KMK, KN, LH, LS, MK, MM, MR, NB, RLS, SS, TT, and WZ. All other authors contributed through their work at one or more eddy-covariance stations through the acquisition of funding, set-up and maintenance, pre-processing and quality control, administration, and their insertion into regional or global networks.

Competing interests. We declare that one or more of the coauthors of this manuscript is a member of the editorial board of Biogeosciences.

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