1	CEDAR-GPP: spatiotemporally upscaled estimates of gross primary
2	productivity incorporating CO ₂ fertilization
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14 15 16 17 18	This paper is a non-peer-reviewed preprint submitted to EarthArXiv. Subsequent versions of this paper may contain revisions and updates.

Abstract: Gross primary productivity (GPP) is the largest carbon flux in the Earth system, playing a crucial role in removing atmospheric carbon dioxide and providing the sugars and starches needed for ecosystem metabolism. Despite the importance of GPP, however, existing estimates present significant uncertainties and discrepancies. A key issue is the underrepresentation of the CO₂ fertilization effect, a major factor contributing to the increased terrestrial carbon sink over recent decades. This omission could potentially bias our understanding of ecosystem responses to climate change.

26 Here, we introduce CEDAR-GPP, the first global upscaled GPP product that incorporates 27 the direct CO₂ fertilization effect on photosynthesis. Our product is comprised of monthly GPP 28 estimates and their uncertainty at 0.05° resolution from 1982 to 2020, generated using a 29 comprehensive set of eddy covariance measurements, multi-source satellite observations, climate 30 variables, and machine learning models. Importantly, we used both theoretical and data-driven 31 approaches to incorporate the direct CO_2 effects. Our machine learning models effectively predicted monthly GPP ($\mathbb{R}^2 \sim 0.74$), the mean seasonal cycles ($\mathbb{R}^2 \sim 0.79$), and spatial variabilities ($\mathbb{R}^2 \sim 0.67$). 32 33 Incorporation of the direct CO₂ effects substantially improved the models' ability to estimate long-34 term GPP trends across global flux sites. While the global patterns of annual mean GPP, seasonality, 35 and interannual variability generally aligned with existing satellite-based products, CEDAR-GPP 36 demonstrated higher long-term trends globally after incorporating CO₂ fertilization, particularly in 37 the tropics, reflecting a strong temperature control on direct CO₂ effects. CEDAR-GPP offers a 38 comprehensive representation of GPP temporal and spatial dynamics, providing valuable insights 39 into ecosystem-climate interactions.

41 **1. Introduction**

42 Terrestrial ecosystem photosynthesis, known as Gross Primary Productivity (GPP), is the 43 primary source of food and energy for the Earth system and human society. Through 44 photosynthesis, terrestrial ecosystems also mitigate climate change, by removing thirty percent of 45 anthropogenic carbon emissions from the atmosphere each year (Friedlingstein et al., 2023). 46 However, due to the lack of direct measurements at the global scale, our understanding of 47 photosynthesis and its spatiotemporal dynamics is limited, leading to considerable disagreements 48 among various GPP estimates (Anav et al., 2015; O'Sullivan et al., 2020; Smith et al., 2016; Yang et 49 al., 2022). Addressing these uncertainties is crucial for improving the predictability of ecosystem 50 dynamics under climate change (Friedlingstein et al., 2014). 51 Over the past three decades, global networks of eddy covariance flux towers collected *in situ* 52 carbon flux measurements that allow for accurate estimates of GPP, providing valuable insights into 53 photosynthesis dynamics under various environmental conditions (Baldocchi, 2020; Beer et al., 54 2010). To quantify and understand GPP at scales and locations beyond the ~ 1km2 flux tower 55 footprints, machine learning has been employed with gridded satellite and climate datasets to upscale 56 site-based measurements and produce wall-to-wall GPP maps (Yang et al., 2007; Xiao et al., 2008; 57 Jung et al., 2011; Tramontana et al., 2016; Joiner and Yoshida, 2020; Zeng et al., 2020; Dannenberg 58 et al., 2023). This approach provides important observational constraints of global carbon dynamics, 59 complementing process-based and semi-process-based modeling such as Terrestrial biosphere 60 models or the Light Use Efficiency (LUE) models (Beer et al., 2010; Jung et al., 2017; Schwalm et 61 al., 2017; Gampe et al., 2021).

62 Effective machine learning upscaling depends on a complete set of input predictors that fully 63 explain GPP dynamics. Upscaled datasets have primarily relied on satellite-observed greenness 64 indicators, such as vegetation indexes (VIs), Leaf Area Index (LAI), the fraction of absorbed 65 photosynthetically active radiation (fAPAR), which effectively capture canopy-level GPP dynamics 66 related to leaf area changes (Tramontana et al., 2016; Ryu et al., 2019; Joiner and Yoshida, 2020). 67 However, important aspects of leaf-level physiology, such as those controlled by climate factors, are 68 often omitted in major upscaled datasets, preventing accurate characterization of GPP responses to 69 climate change (Stocker et al., 2019; Bloomfield et al., 2023). In particular, none of the previous 70 upscaled datasets have considered the direct effect of atmospheric CO₂ on leaf-level photosynthesis, 71 which is a key factor contributing to at least half of the enhanced land carbon sink observed over the 72 past decades (Keenan et al., 2016; Keenan and Williams, 2018; Walker et al., 2021; Ruehr et al.,

73 2023). This omission can lead to incorrect inference regarding long term trends in various

74 components of the terrestrial carbon cycle (De Kauwe et al., 2016).

75 Multiple independent lines of evidence from atmospheric inversion (Wenzel et al., 2016),

atmospheric ${}^{13}C/{}^{12}C$ measurements (Keeling et al., 2017), ice core records of carbonylsulfide

77 (Campbell et al., 2017), glucose isotopomers (Ehlers et al., 2015), as well as free-air CO₂ enrichment

experiments (FACE) (Walker et al., 2021), suggest a widespread positive effect of elevated

atmospheric CO_2 on GPP from site to global scales. Increasing CO_2 *directly* stimulates the

80 biochemical rate of leaf-level photosynthesis, leading to an increase in net carbon assimilation and

81 leaf area, which enhances canopy-level GPP. Furthermore, high CO₂ concentration is expected to

82 reduce stomatal conductance and increase water use efficiency, indirectly enhancing photosynthesis

83 under water-limited conditions (De Kauwe et al., 2013; Keenan et al., 2013). The direct biochemical

effect has been found to dominate GPP responses to CO₂, from both theoretical and observational
analyses (Haverd et al., 2020; Chen et al., 2022).

86 Satellite-based estimates have shown an increasing global GPP trend in the past few decades 87 largely attributable to CO₂-induced increases in LAI (De Kauwe et al., 2016; Zhu et al., 2016; Chen 88 et al., 2019; Piao et al., 2020). However, previous upscaled GPP datasets, as well as most LUE 89 models such as the MODIS GPP product, have failed to consider the direct CO₂ effects on leaf-90 level biochemical processes (Jung et al., 2020; Zheng et al., 2020). Consequently, these products 91 likely underestimated the long-term trend of global GPP, leading to large discrepancies when 92 compared to process-based models, which typically consider leaf-level CO₂ effects (Anav et al., 93 2015; De Kauwe et al., 2016; O'Sullivan et al., 2020). Notably, recent improvements in LUE models 94 have included the CO₂ response and show improved long-term changes in GPP globally (Zheng et 95 al., 2020), yet, this important mechanism is still missing in GPP products upscaled from *in situ* eddy 96 covariance flux measurements.

97 To improve the quantification of GPP spatial and temporal dynamics and provide a robust 98 representation of long-term dynamics in global photosynthesis, we developed the CEDAR-GPP¹ 99 data product. CEDAR-GPP was upscaled from global eddy covariance carbon flux measurements 100 using machine learning along with a broad range of multi-source satellite observations and climate 101 variables. In addition to incorporating direct CO_2 fertilization effects on photosynthesis, we also

¹ CEDAR stands for upsCaling Ecosystem Dynamics with ARtificial inteligence

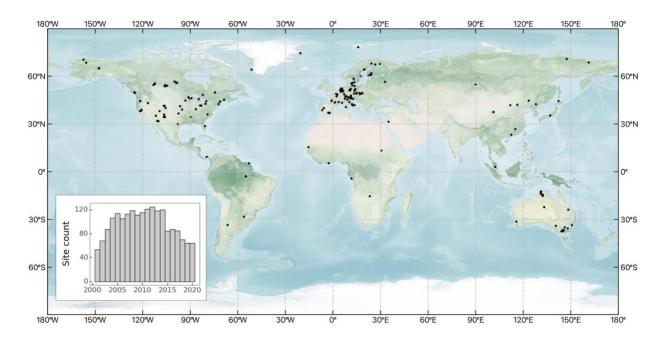
102 account for indirect effects via greenness indicators, and include novel satellite datasets such as 103 solar-induced fluorescence (SIF), Land Surface Temperature (LST) and soil moisture to explain 104 variability under environmental stresses. We provide monthly GPP estimations and associated 105 uncertainties at 0.05° resolution derived from ten model setups. These setups differ by the temporal 106 range depending on satellite data availability, the method for incorporating the direct CO₂ 107 fertilization effects, and the partitioning approach used to derive GPP from eddy covariance 108 measurements. Short-term GPP datasets were from 2001 to 2020, primarily based on data derived 109 from MODIS satellites, and long-term datasets spaned 1982 to 2020 using combined Advanced 110 Very High Resolution Radiometer (AVHRR) and MODIS data. We used two approaches to incorporate the direct CO₂ fertilization effects including direct prescription with eco-evolutionary 111 112 theory and machine learning inference from the eddy-covariance data. Additionally, we provided a 113 baseline configuration that did not incorporate the direct CO₂ effects. Uncertainties in GPP 114 estimation were quantified using bootstrapped model ensembles. We evaluate the machine learning 115 models' skills in predicting monthly GPP, seasonality, interannual variability, and trend against eddy 116 covariance measurements, and compare the CEDAR-GPP spatial and temporal variability to 117 existing satellite-based GPP estimates.

118 **2. Data and Methods**

119 2.1 Eddy covariance data

- 120 We obtained monthly eddy covariance GPP measurements from 2001 to 2020 from
- 121 FLUXNET2015 (Pastorello et al., 2020), AmeriFlux FLUXNET
- 122 (https://ameriflux.lbl.gov/data/flux-data-products/), and ICOS Warm Winter 2020 (Warm Winter
- 123 2020 Team and ICOS Ecosystem Thematic Centre., 2022) datasets. All data were processed with the
- 124 ONEFLUX pipeline (Pastorello et al., 2020). Following previous upscaling efforts (Tramontana et
- 125 al., 2016), we selected monthly GPP data that had at least 80% of high-quality hourly or half-hourly
- 126 data for temporal aggregation. We further excluded large negative GPP values, setting a cutoff of -1
- 127 gCm⁻²d⁻¹. We utilized GPP estimates from both the night-time (GPP_REF_NT_VUT) and day-time
- 128 (GPP_REF_DT_VUT) partitioning approaches and trained separate machine learning models for
- 129 each. We classified flux tower sites according to the primary C3 and C4 plant categories reported in
- 130 metadata and related publications when available and used a C4 plant percentage map (Still et al.,

131 2003) otherwise. Our analysis encompassed 233 sites, predominately located in North America,



132 Western Europe, and Australia (Figure 1). In total, our dataset included roughly 18000 site-months.



Figure 1. Global distribution of eddy covariance sites used to generate the CEDAR-GPP product. The inset displays the annual count of sites.

136 2.2 Global input datasets

We compiled an extensive set of covariates from gridded climate reanalysis data, multi-source satellite datasets including optical, thermal, and microwave observations, as well as categorical information on land cover, climate zone, and C3/C4 classification. The datasets that we compiled offer comprehensive information about GPP dynamics and its responses to climatic variabilities and

- 141 stresses. Table 1 lists the inputs datasets and associated variables used to generate CEDAR-GPP.
- Table 1. Datasets and input variables used to generate the CEDAR GPP product. For a list ofselected variables used in different model setups, please refer to Table S1.

Category	Dataset	Temporal	Spatial	Temporal	Variables	Reference
		coverage	resolution	resolution		
Climate	ERA5-Land	1950 -	0.1°	Monthly	Air temperature;	(Sabater,
	Monthly	present			vapor pressure	2019)
	Averaged data				deficit, Precipitation,	
					Air and skin	
					temperature, surface	
					downwelling solar	
					radiation,	
					Potential evaporation	

	ESRA Global Monitoring Laboratory Atmospheric Carbon Dioxide	1976 – present	-	Monthly	Atmospheric CO ₂ concentration averaged from Mauna Loa, Hawaii, US and South Pole, Antarctica	(Thoning et al., 2021)
Satellite- based datasets	MODIS Nadir BRDF-adjusted reflectance (MCD43C4)	2000 – present	0.05°	Daily	Surface reflectance b1 – b7, Vegetation indices (NIRv, NDVI, kNDVI, EVI, GCI, NDWI), percent snow	(Schaaf and Wang, 2015)
	MODIS Terra and Aqua LAI/fPAR (MCD15A3H, MOD15A2H)	2000 – present	500m	4-day, 8- day	LAI, fPAR	(Myneni et al., 2015a, b)
	MODIS Terra and Aqua LST (MYD11A1, MOD11A1)	2000 – present	1 km	Daily	Daytime LST Nighttime LST	(Wan et al., 2015b, a)
	BESS_Rad	2000 – 2020	0.05°	Daily	PAR, diffuse PAR, downwelling solar radiation	(Ryu et al., 2018)
	Continuous- SIF (from OCO-2 and MODIS)	2000 – 2020	0.05°	4-day	all-sky daily average SIF	(Zhang, 2021)
	ESA CCI Soil Moisture Combined Passive and Active	1979 – 2021	0.25°	Daily	Surface soil moisture	(Gruber et al., 2019)
	GIMMS LAI4g	1982 – 2021	0.0833°	Half- month	LAI	(Cao et al., 2023)
	GIMMS NDVI4g	1982 – 2021	0.0833 °	Half- month	NDVI	(Li et al., 2023)
Static categorical datasets	MODIS Land Cover (MCD12Q1)	Average status used between 2001 and 2020	500m	-	Plant function types	(Friedl and Sulla- Menashe, 2019)
	Koppen- Geiger Climate Classification	present	1 km	-	Koppen-Geiger climate classes	(Beck et al., 2018)
	C4 percentage map	present	1°	-	Percentage of C4 plants	(Still et al., 2003, 2009)

145 2.2.1 Climate variables

We obtained air temperature, vapor pressure deficit, precipitation, potential
evapotranspiration, and skin temperature from the EAR5-Land reanalysis dataset (Sabater, 2019)
(Table 1; Table S1). We applied a three-month lag to precipitation, to reflect the memory of soil
moisture and represent the root zone water availability. Averaged monthly atmospheric CO₂
concentrations were calculated as an average of records from the Mauna Loa Observatory and South

Pole Observation stations, retrieved from NOAA's Earth System Research Laboratory (Thoning etal., 2021).

153 2.2.2 Satellite datasets

We assembled a broad collection of satellite-based observations of vegetation greenness and structure, LST, solar radiation, solar-induced fluorescence (SIF), and soil moisture (Table 1, Table S1).

157 Three MODIS products were used: surface reflectance, LAI/fAPAR, and LST. Surface 158 reflectance from optical to infrared bands (band 1 to 7) was sourced from the MODIS Nadir 159 BRDF-adjusted reflectance (NBAR) daily dataset (MCD43C4) (Schaaf and Wang, 2015). From this, 160 we derived several vegetation indexes, including NIRv (Badgley et al., 2019), kNDVI (Camps-Valls 161 et al., 2021), NDVI, Enhanced Vegetation Index (EVI), Normalized Difference Water Index 162 (NDWI) (Gao, 1996), and a green chlorophyll index (CIgreen) (Gitelson, 2003). We also used snow 163 percentages from the NBAR dataset. We used the 4-day LAI and fPAR composite derived from 164 Terra and Aqua satellites (MCD15A3H) (Myneni et al., 2015a; Yan et al., 2016a, b) from July 2002 onwards and the MODIS 8-day LAI and fPAR dataset from Terra only (MOD15A2H) prior to July 165 166 2002 (Myneni et al., 2015b). We used day-time and night-time LST from the Aqua satellite (MYD11A1) (Wan et al., 2015b), with the Terra-based LST product (MOD11A1) used after July 167 168 2002 (Wan et al., 2015a). Terra LST was bias-corrected with the differences in the mean seasonal 169 cycles between Aqua and Terra following Walther et al. (2021). 170 We used the PKU GIMMS NDVI4g dataset (Li et al., 2023) and PKU GIMMS LAI4g (Cao et al., 2023) datasets available from 1982 to 2020. PKU GIMMS NDVI4g is a harmonized time 171 172 series that includes AVHRR-based NDVI from 1982 to 2003 (with biases and corrections mitigated 173 through inter-calibration with Landsat surface reflectance images) and MODIS NDVI from 2004 174 onward. PKU GIMMS LAI4g consisted of AVHRR-based LAI from 1982 to 2003 (generated using

- 175 machine learning models trained with Landsat-based LAI data and NDVI4g) and MODIS BNU
- 176 LAI from 2004 onwards (Yuan et al., 2011).

177 We utilized photosynthetically active radiation (PAR), diffusive PAR, and shortwave

downwelling radiation from the BESS_Rad dataset (Ryu et al., 2018). We also obtained the

179 continuous-SIF (CSIF) dataset (Zhang et al., 2018; Zhang, 2021) produced by a machine learning

180 algorithm trained using OCO-2 SIF observations and MODIS surface reflectance. We also obtained

181 surface soil moisture from the ESA CCI soil moisture combined passive and active product (Dorigo

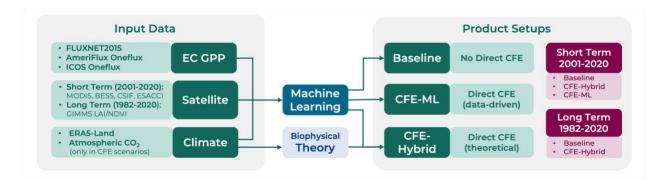
- 182 et al., 2017; Gruber et al., 2019).
- 183 2.2.3 Other categorical datasets

We used plant functional type (PFT) information derived from the MODIS Land Cover 184 185 product (MCD12Q1) (Friedl and Sulla-Menashe, 2019). We followed the International Geosphere-186 Biosphere Program classification scheme but merged several similar categories to maximize the 187 amount of eddy covariance sites/observations available for each category. Closed shrublands and 188 open shrublands are combined into a shrubland category. Woody savannas and savannas are 189 combined into savannas. We generated a static PFT map by taking the mode of the MODIS land 190 cover time series between 2001 - 2020 at each pixel to mitigate uncertainties from misclassification 191 in the MODIS dataset. Nevertheless, changes in vegetation structure induced by land use and land 192 cover change are reflected in the dynamics surface reflectance and LAI/fAPAR datasets we used. 193 We used the Koppen-Geiger main climate groups (tropical, arid, temperate, cold, and polar) (Beck et 194 al., 2018). We also utilized a C4 plant percentage map to account for different photosynthetic 195 pathways when incorporating CO₂ fertilization (Still et al., 2003, 2009).

196 2.2.4 Data preprocessing

197 We implemented a three-step preprocessing strategy for the satellite datasets: 1) quality control, 2) gap-filling, and 3) spatial and temporal aggregation. In the first step, we selected high-198 199 quality data based on the quality control flags of the satellite products when available. For the 200 MODIS NBAR dataset (MCD43C3), we used data with 75% or more high-resolution NBAR pixels 201 retrieved with full inversions for each band. For MODIS LST, we selected the best quality data from 202 the quality control bitmask as well as data where retrieved values had an average emissivity error of 203 no more than 0.02. For MODIS LAI/fAPAR, we used retrievals from the main algorithm with or 204 without saturation. We used all available data in ESA-CCI soil moisture due to the presence of 205 substantial data gaps. In the gap-filling step, missing values in satellite datasets were temporally filled

206 at the native temporal resolution, following a two-step protocol adapted from Walther et al (2021). 207 Short temporal gaps were first filled with medians from a moving window, and the remaining gaps were filled with the mean seasonal cycle. For datasets with a high temporal resolution, including 208 209 MODIS NBAR (daily), LAI/fPAR (4-day), BESS (4-day), CSIF (4-day), ESA-CCI (daily), temporal 210 gaps no longer than 5 days (8 days for 4-day resolution products) were filled with medians of 15-day 211 moving windows in the first step. An exception is MODIS LST (daily), for which we used a shorter 212 moving window of 9 days due to rapid changes in surface temperature. GIMMS LAI4g and 213 NDVI4g data were only filled with mean seasonal cycle due to their low temporal resolution (bi-214 monthly). In the last processing step, all the datasets were aggregated to a monthly time step and



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Figure 2. Schematic overview of the CEDAR-GPP model setups.

218 2.3 Machine learning upscaling

0.05-degree spatial resolution.

219 2.3.1 CEDAR-GPP model setups

We trained machine learning model with eddy covariance GPP measurements as targets and climate/satellite variables as input features. We created ten model setups to produce ten different global monthly GPP datasets (Figure 2; Table 2). The model setups were characterized by the temporal range of input datasets used, the configuration of CO2 fertilization effects, and the partitioning approach used to derive the GPP from eddy covariance measurements.

We provided a short-term (ST) configuration producing GPP estimates from 2001 to 2020, and a long-term (LT) configuration spanning 1982 to 2020. Each temporal configuration uses a different set of input variables depending on their temporal availability. Inputs for the short-term configuration included MODIS, CSIF, BESS PAR, ESA-CCI soil moisture, ERA5-Land, as well as PFT and Koppen Climate zone as categorical variables with one-hot encoding. The long-term used GIMMS NDVI4g and LAI4g data, ERA5-land, PFT and Koppen climate. ESA CCI soil moisture 231 datasets were excluded from the long-term model setups due to concerns about the product quality 232 in the early years when the number and quality of microwave satellite data were limited (Dorigo et

233 al., 2015). A detailed list of input features for each setup is provided in Table S1.

234 Regarding the direct CO₂ fertilization effects (CFE), we established a "Baseline" configuration 235 that did not incorporate these effects, a "CFE-Hybrid" configuration that incorporated the effects

236 via eco-evolutionary theory, and a "CFE-ML" configuration that inferred direct effects from eddy

237 covariance data using machine learning. Detailed information about these approaches is provided in

- 238 Section 2.4.2. Furthermore, separate models were trained for GPP target variables from the night-
- 239 time (NT) and daytime (DT) partitioning approaches.

240 Table 2 lists the characteristics of ten model setups. Note due to the limited availability of

241 eddy covariance observations before 2001, we did not apply the CFE-ML approach to the long-term

- 242 setups, as the machine learning inferred CO2 fertilization effects cannot be robustly extrapolate
- 243 GPP back to 1982.

244 Table 2. Specifications of the CEDAR-GPP model setups.

Model Setup Name	Temporal range	Direct CO ₂ Fertilization Effects		GPP Partitioning Method
		Configuration	Method	_
ST_Baseline_NT	Short-term (ST)	Baseline	Not incorporated	Night-time (NT)
ST_Baseline_DT	2001 - 2020			Day-time (DT)
ST_CFE-Hybrid_NT		CFE-Hybrid	Theoretical	NT
ST_CFE-Hybrid_DT				DT
ST_CFE-ML_NT		CFE-ML	Data-driven	NT
ST_CFE-ML_DT				DT
LT_Baseline_NT	Long-term (LT)	Baseline	Not incorporated	NT
LT_Baseline_DT	1982 - 2020			DT
LT_CFE-Hybrid_NT		CFE-Hybrid	Theoretical	NT
LT_CFE-Hybrid_DT				DT

245

246 2.3.2 CO_2 fertilization effect

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We established three configurations considering the direct CO₂ fertilization effects on

248 photosynthesis. In the baseline configuration, we trained machine learning models with eddy

249 covariance GPP measurements, input climate and satellite features, but excluding CO₂

250 concentration. As such, the models only include indirect CO2 effects from the satellite-based proxies

251 of vegetation greenness and structure and do not consider the direct effect of CO_2 on light use

252 efficiency. Our baseline model is therefore directly comparable to other satellite-derived GPP

253 products that only account for indirect CO2 effects (ref FLUXCOM, FLUXSAT, MODIS). 254 In the CFE-ML configuration, we added trained monthly CO_2 concentration into the feature

set in addition to those incorporated in the baseline models. Thus, models inferred the functional

relationship between GPP and CO₂ from the eddy covariance data, encompassing both CO₂

257 fertilization pathways - direct effects on LUE and indirect effects from the satellite-based proxies of

258 vegetation greenness and structure.

259 In the CFE-Hybrid configuration, we applied biophysical theory to estimate the response of 260 LUE to elevated CO₂. First, we estimated a reference GPP, where LUE is not affected by any 261 increase in atmospheric CO₂, by applying the CFE-ML model with a constant atmospheric CO₂ 262 concentration equal to the 2001 level while keeping all other variables temporally dynamic. Then, the 263 impacts of CO_2 on LUE were prescribed onto the reference GPP estimates using a theoretical CO_2 264 sensitivity function of LUE according to eco-evolutionary theories (Supplementary Text S1). The 265 theoretical CO₂ sensitivity function represents a CO₂ sensitivity that is equivalent to that of the 266 electron-transport-limited (light-limited) photosynthetic rate. When light is limited, elevated CO_2 267 suppresses photorespiration leading to increased photosynthesis at a lower rate than when 268 photosynthesis is limited by CO₂ (Lloyd and Farquhar, 1996; Smith and Keenan, 2020). Thus, the 269 CFE-Hybrid scenario provides a conservative estimation of the direct CO₂ effects on LUE. Note 270 that the theoretical sensitivity function describes the fractional change in LUE due to direct CO₂ 271 effects relative to a reference period (i.e. 2001). Therefore, we used the CFE-ML model to establish 272 this reference GPP by fixing the CO_2 effects to the 2001 level, rather than simply using the GPP 273 from the Baseline model in which the direct CO_2 effects were not clearly represented.

274 For both CFE-ML and CFE-Hybrid scenarios, we made another conservative assumption that 275 C4 plants do not benefit from elevated CO_2 , despite potential increases in photosynthesis during 276 water-limited conditions due to enhanced WUE. Data from flux tower sites dominated by C4 plants 277 were removed from our training set, so the machine learning models inferred CO₂ fertilization only 278 from flux tower sites dominated by C3 plants. When applying models globally, we assumed the 279 reference GPP values (with constant atmospheric CO_2 concentration equal to the 2001 level) to 280 represent C4 plants, and GPP estimates from CFE-ML or CFE-Hybrid models wereapplied in 281 proportion to the percentage of C3 plants in a grid cell.

282 2.3.3 Machine learning model training and validation

283 We employed the state-of-the-art XGBoost machine learning model, known for its high 284 accuracy in regression problems across various domains, including environmental and ecological

predictions (Chen and Guestrin, 2016; Kang et al., 2020; Berdugo et al., 2022). XGBoost is a
scalable and parallelized implementation of the gradient boosting technique that iteratively trains an
ensemble of decision trees, with each iteration targeting to minimize the residuals from the last
iteration. A notable merit of XGBoost is its ability to make prediction in the presence of missing
values, a common issue in remote sensing datasets.

We used five-fold cross-validation for model evaluation. Training data was randomly split into five groups (folds), with each fold held out for testing while the rest four folds were used for model training. We imposed two restrictions on fold splitting: each flux site was entirely assigned to a fold to test model performance over unseen locations; the random sampling was stratified based on PFT to ensure coverage of the full range of PFTs in both training and testing. Within each training set, we performed a randomized search using three-fold cross-validation to determine the optimal hyperparameter set, to reduce the risk of overfitting and improve the robustness of the evaluation.

297 We assessed the models' ability to capture the temporal and spatial characteristics of GPP, 298 including monthly variabilities, mean seasonal cycles, monthly anomalies, cross-site variability. 299 Model performance was assessed separately for each model setup (Table 2) and summarized by PFT 300 and Koppen climate zone. Mean seasonal cycles were calculated as the mean monthly GPP over the 301 site observation period, and monthly anomalies were the residuals of monthly GPP after subtracting 302 mean seasonal cycles. Monthly GPP averaged over years for each site was used to assess cross-site 303 variability. Goodness-of-fit metrics include RMSE, bias, and coefficient of determination (R^2, R^2) 304 equivalent to NSE Nash-Sutcliffe model efficiency coefficient).

To evaluate the models' ability to capture long-term GPP trends, we aggregated the monthly GPP to annual values for sites with at least 5 years of observations following Chen et al. (2022). GPP anomalies were computed by subtracting the multi-year mean GPP from the annual GPP for each site. Anomalies were aggregated across site to achieve a single multi-site GPP anomaly per year. We used the Sen slope and Mann-Kendall test to examine the GPP trends from 2002 to 2019, excluding 2001 and 2020 due to the limited number of available sites.

311 2.3.4 Product generation and uncertainty quantification

In the CEDAR-GPP product, we generated a GPP dataset for each of the ten model setups, by applying the model to global gridded datasets within the corresponding temporal range (Table 2). GPP datasets were named after the corresponding model setups. For each model setup, we first generated 30 sample set using bootstrapping, which were then used to train an ensemble of 30 316 XGBoost models. The bootstrapping was performed at the site level, and each bootstrapped sample

- 317 set contained around 140 to 150 unique sites, 17000 to 19000 site months covering all PFTs. The
- 318 relative composition of sites in each PFT was consistent with the full dataset. The 30 models trained
- 319 with bootstrapped samples generated an ensemble of 30 GPP values. We provided the ensemble
- 320 GPP mean and standard deviation from each of the ten model setups.

321 2.4 Product inter-comparison

322 We compared the global spatial and temporal patterns of CEDAR-GPP with other major 323 satellite-based GPP products including three machine learning upscaled and two LUE-based 324 datasets. We obtained two FLUXCOM products (Jung et al., 2020), the latest version of 325 FLUXCOM-RS (FLUXCOM-RSv006) available from 2001 to 2020 based on remote sensing 326 (MODIS collection 6) datasets only, as well as the FLUXCOM-RS+METEO ensemble available 327 between 1979 to 2018 and based on the climatology of remote sensing observations and ERA5 328 forcings (hereafter FLUXCOM-ERA5). We used FluxSat (Joiner and Yoshida, 2020), available from 329 2001 to 2019, which is an upscaled dataset based on MODIS NBAR surface reflectance and PAR 330 from Modern-Era Retrospective analysis for Research and Applications 2 (MERRA-2). Importantly, 331 FluxSat does not incorporate climate forcings. We used the MODIS GPP product (MOD17) 332 available since 2001, which was generated based on MODIS fAPAR and LUE as a function of air 333 temperature and vapor pressure deficit but not atmospheric CO₂ concentration (Running et al., 334 2015). We also used the rEC-LUE products, available from 1982 to 2018 and based on a revised 335 LUE model that incorporated the effect of atmospheric CO₂ concentration and the fraction of 336 diffuse PAR on LUE in addition to air temperature and vapor pressure deficit (Zheng et al., 2020). 337 All datasets were resampled to 0.1 ° spatial resolution, and a common mask for the vegetated land 338 area was applied. We evaluated global mean annual GPP, mean seasonal cycle, interannual 339 variability, and trend among different datasets, comparing them over a common time period 340 determined by their data availability. Global total GPP was computed by scaling the global average 341 GPP flux with the global land area (122.4 million km2) following Jung et al. (2020). Mean seasonal 342 cycle was defined as above (Sec 2.3.3). We used the standard deviation of annual GPP to indicate the 343 magnitude of interannual variability, the Sen slope to indicate GPP annual trend and the Mann-344 Kendall test for the statistical significance of trends.

345 **3. Results**

346 3.1 Evaluation of model performance

347 3.1.1 Overall performance

The short-term and long-term models explained approximately 74% and 68%, respectively, of 348 349 the variation in eddy covariance estimated monthly GPP across global sites (Figure 3a). The long-350 term models consistently yielded lower performance than the short-term models, likely due to 351 differences in the satellite remote sensing datasets used, as the short-term models benefited from a 352 richer information including surface reflectance from individual bands, LST, CSIF, as well as soil 353 moisture, while the long-term model only exploited NDVI and LAI. The models with different CFE 354 scenarios and target GPP variables had similar performance on predicting monthly GPP (Figure 3b, 355 Table 3, Table S2). All models exhibited minimal bias less than 0.15. 356 Model performance in terms of the different temporal and spatial characteristics of monthly 357 GPP was variable (Figure 3c-h). The models were most successful at predicting mean seasonal

cycles, with the short-term and long-term models explaining around 79% and 72% of the variability,

respectively (Figure 3c-d). The short-term and long-term models captured 66% and 54%,

360 respectively of the spatial variabilities of multi-year mean GPP across global sites (i.e., cross-site

361 variability) (Figure 3g-h). However, all models predicted monthly anomalies across the sites, with R^2

362 values below 0.11 (Figure 3e-f). The CFE-ML and CFE-Hybrid models showed slightly higher

363 accuracy than the Baseline model across all temporal and spatial characteristics.

Model Setup Name	Monthly		Mean seasonal cycles		Monthly anomalies			Cross-site				
	RMSE	Bias	R ²	RMSE	Bias	R ²	RMSE	Bias	R ²	RMSE	Bias	R ²
ST_Baseline_NT	1.96	-0.05	0.74	1.57	0.02	0.79	1.22	0.00	0.11	1.11	0.03	0.66
ST_CFE-ML_NT	1.95	-0.05	0.74	1.56	0.02	0.80	1.22	0.00	0.12	1.10	0.03	0.67
ST_CFE-	1.96	-0.05	0.74	1.57	0.03	0.79	1.23	0.00	0.12	1.10	0.04	0.67
Hybrid_NT												
LT_Baseline_NT	2.18	-0.10	0.68	1.82	0.01	0.72	1.26	0.00	0.06	1.29	0.03	0.54
LT_CFE-	2.16	-0.11	0.69	1.79	0.01	0.73	1.25	0.00	0.07	1.27	0.03	0.56
Hybrid_NT												

Table 3. Machine learning model performance for five CEDAR-GPP setups based on NT GPP (Table 2). Results of DT setups can be found in Table S2.

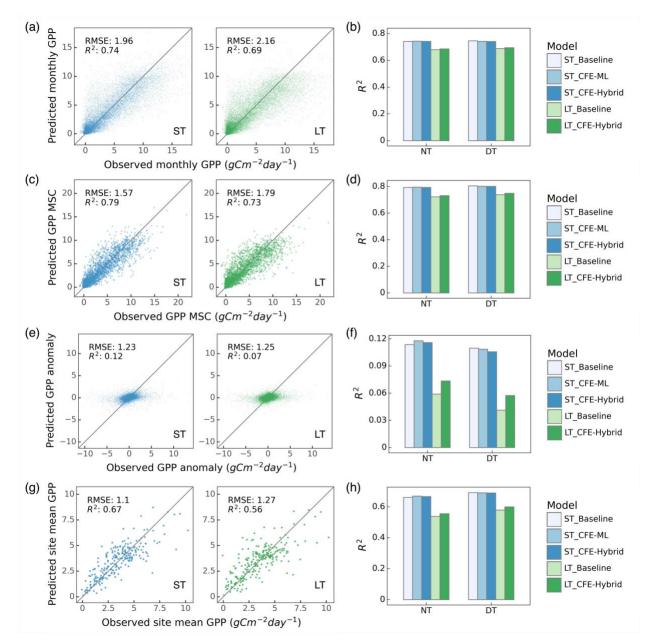


Figure 3. Machine learning model performance in predicting monthly GPP and its spatial and temporal variability. Scatter plots illustrated relationships between model predictions and observations for monthly GPP (a), mean seasonal cycles (MSC (c), monthly anomaly (e), and cross-site variability (g) for ST_CFE-Hybrid_NT (left, blue) and LT_CFE-Hybrid_NT (right, green) models. Corresponding bar plots show the R² values for all ten model setups in predicting monthly GPP (b), MSC (d), monthly anomaly (f), and cross-site variability (h).

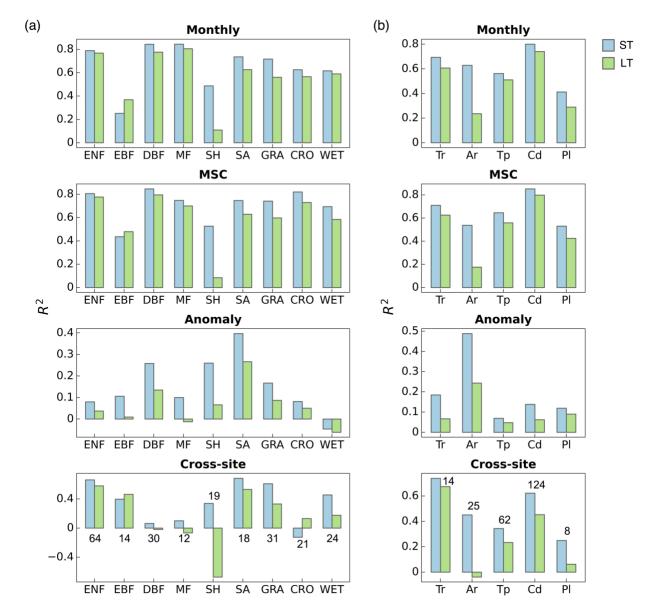
375 3.1.2 Performance by biome and climate zone

The predictive ability of our models varied across different PFTs and Koppen climate zones (Figure 4). Here we present results from the CFE-Hybrid models and note that patterns for the other CFE configurations were similar.

379 Model performance in terms of monthly GPP was highest for forests with distinct seasonality, 380 including deciduous broadleaf forests, mixed forests, and evergreen needleleaf forests, with R² values 381 above 0.78. Model accuracies were also high for savannas, and grasslands, followed by croplands and wetlands, with R² values between 0.57 and 0.74. Model accuracies were lowest in evergreen 382 383 broadleaf forests and shrublands, with R² values as low as 0.14. Across climate zones, models 384 achieved the highest accuracy in predicting monthly GPP in cold and tropical climate zones with R^2 385 values between 0.64 and 0.80. The short-term models had lowest performance in polar regions with 386 an R² value around 0.42 and the long-term model had the lowest performance in arid regions with an R^2 value of 0.25. 387

388 Model performance in terms of mean seasonal cycles across PFTs and climate zones followed 389 patterns for monthly GPP, while disparities emerged for performance in terms of GPP anomaly and 390 cross-site variability (Figure 4). The short-term model showed the highest predictive power in explaining monthly anomalies in arid regions with an R^2 value of 0.49, where savanna and 391 shrublands sites are primarily located. Model performance in all other climate zones was significantly 392 lower with R² values below 0.2, and as low as 0.07 in temperate regions. Besides, the short-term 393 394 model demonstrated good performance in capturing anomalies in deciduous broadleaf forests. The 395 long-term model's relative performance between PFTs and climate zones was mostly consistent with 396 that of the short-term model, with lower accuracy in shrublands when compared to the short-term 397 model.

398 Model performance in terms of cross-site variability demonstrated highest accuracy in 399 savannas, grasslands, evergreen needleleaf forests, and evergreen broadleaf forests ($R^2 > 0.36$) and lowest accuracy in deciduous broadleaf forests, mixed forests, and croplands ($R^2 < 0.20$). The short-400 term model additionally showed good performance in shrublands and wetlands ($R^2 > 0.36$), whereas 401 402 the long-term model failed to capture any variability for shrublands. In terms of climate zones, 403 models were most successful at explaining the variabilities across tropical and cold climate zones 404 $(R^2 > 0.46)$, the short-term model was least successful across polar regions, with a R^2 value of 0.29, 405 and the long-term model had low performance for both polar and arid regions with R² values below 406 0.15.





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412 413

Figure 4. Performance of the ST_Baseline_NT (blue) and LT_Baseline_NT (green) models on GPP spatiotemporal estimation by plant functional types (a) and climate zones (b). The cross-site panels included the number of sites within each category. ENF: evergreen needleleaf forest, EBF: evergreen broadleaf forest, DBF: deciduous broadleaf forest, MF: mixed forest, SH: shrubland, SA: savanna, GRA: grassland, CRO: cropland, WET: wetland. Tr: tropical, Ar: arid, Tp: temperate, Cd: cold, Pl: polar.

414 3.1.3 Prediction of long-term trends

Eddy covariance measured GPP presented a substantial increasing trend in GPP across flux

sites between 2002 and 2019 (Figure 5a). The observed GPP from the night-time partitioning

417 approach indicated an overall trend of 7.7 gCm⁻²year⁻². In contrast, the ST_Baseline_NT model

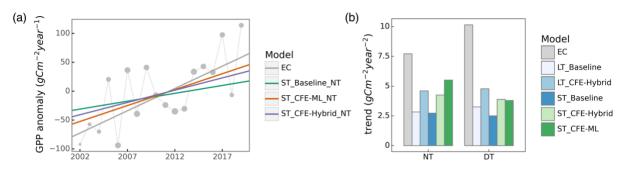
418 predicted a more modest trend of 2.7 gCm⁻²year⁻², primarily reflecting the indirect CO_2 effect

419 manifested through the growth of LAI. Both the ST_CFE-ML_NT and ST_CFE-hybrid_NT

420 models predicted much higher trends of 5.5 and 4.3 gCm⁻²year⁻², respectively, aligning more closely

421 to eddy covariance observations.

Across all model setups, the CFE-ML and CFE-hybrid models consistently outperformed the Baseline models in predicting GPP trends in global eddy covariance towers (Figure 6b) and all trends were statistically significant (p < 0.05). Notably, we found a considerably higher trend in eddy covariance GPP measurements derived from the day-time versus night-time partitioning approach. The predicted trends of different model setups between the partitioning approaches were similar despite a smaller trend predicted by the ST_CFE-ML_DT model compared to the corresponding NT model (Figure 6b).



429

Figure 5. Comparison of observed and predicted GPP trends across eddy covariance flux towers. (a) Aggregated annual GPP anomaly from 2002 to 2019 and trend lines from eddy covariance (EC) measurements, and three CFE model setups (short-term, night-time partitioning). Size of the grey circle markers is proportional to the number of sites. (b) Annual trends from eddy covariance measurements and ten CEDAR-GPP model setups.

436 3.2 Evaluation of GPP spatial and temporal dynamics

437 In this section, we present comparisons between CEDAR-GPP datasets and other upscaled or

438 LUE-based datasets regarding the mean annual GPP (Section 3.2.1), GPP seasonality (Section 3.2.2),

439 interannual variability (Section 3.2.3), and annual trends (Section 3.2.4). CEDAR-GPP model setups

440 generally showed similar patterns in mean annual GPP, seasonality, and interannual variability,

therefore, in corresponding sections, we present the CFE-Hybrid model setups as representative

442 examples for comparisons with other independent datasets, unless otherwise stated. Supplementary

443 figures include comparisons involving all CEDAR-GPP.

444 3.2.1 Mean annual GPP

445 Global patterns of mean annual GPP were generally consistent among CEDAR-GPP model 446 setups, FLUXCOM, FLUXSAT, MODIS, and rEC-LUE, with few noticeable regional differences 447 (Figure 6, Figure S1). Differences among CEDAR-GPP model setups were minimal and only 448 evident between the NT and DT setups in the tropics (Figure 6b-c, Figure S1). CEDAR-GPP short-449 term datasets showed highest consistency with FLUXSAT in terms of mean annual GPP 450 magnitudes (2001 – 2018) and latitudinal variations, although FLUXSAT presented slightly higher GPP values in the tropics compared to CEDAR-GPP (Figure 6b). Mean annual GPP magnitude for 451 452 FLUXCOM-RS006 and MODIS tended to be lower globally than CEDAR-GPP and FLUXSAT, 453 with the most pronounced differences observed in the tropical areas. Among the long-term datasets 454 (CEDAR-GPP LT, FLUXCOM-ERA5, and rEC-LUE), mean annual GPP (1982 - 2018) exhibited 455 greater disparities in the northern mid-latitudes than in the tropics and southern hemisphere (Figure 456 6c). CEDAR-GPP aligned more closely with FLUXCOM-ERA5 than with rEC-LUE, with the latter

457 showing lower annual mean GPP globally, particularly between 20°N to 50° N.

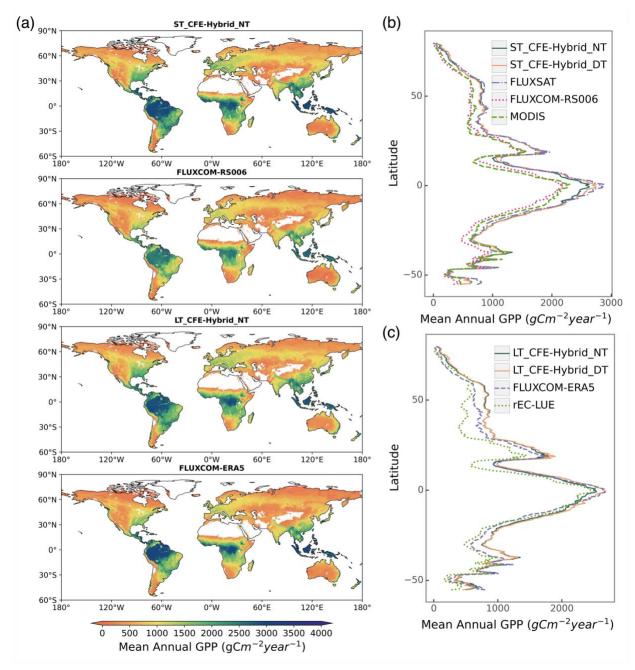
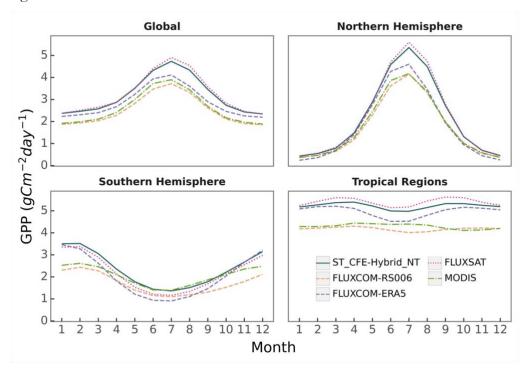


Figure 6. Global distributions of mean annual GPP from CEDAR-GPP and other machine learning upscaled and LUE-based reference datasets. (a) Global patterns of mean annual GPP from ST_CFE-Hybrid_NT, FLUXCOM-RS006, LT_CFE-Hybrid_NT, and FLUXCOM-ERA5. (b) Latitudinal distributions of mean annual GPP (2001 – 2018) from short-term datasets (ST_CFE-Hybrid_NT, ST_CFE-Hybrid_DT, FLUXSAT, FLUXCOM-RS006, and MODIS. (c) Latitudinal distributions of mean annual GPP (1982 – 2018) from long-term datasets (LT_CFE-Hybrid_NT, LT_CFE-Hybrid_DT, FLUXCOM-ERA5, and rEC-LUE.

467 3.2.2 Seasonal variability

CEDAR-GPP and other machine learning upscaled and LUE-based GPP datasets agreed on 468 469 seasonal variabilities (average between 2001 and 2018) at the global scale, characterized by a peak in 470 GPP in July and a nadir between December and January (Figure 7). At the global scale, CEDAR-471 GPP was most closely aligned with FLUXSAT in GPP seasonal magnitude and amplitude, while 472 both FLUXCOM and MODIS displayed a relatively less pronounced magnitude. 473 In the northern hemisphere (20°N - 90°N), all GPP datasets agreed in seasonal GPP variation, despite variances in the magnitude of peak GPP. In the southern hemisphere (20°S - 60°S), all 474 475 datasets exhibited their lowest GPP during June and July, and highest GPP from December to January. However, the seasonal amplitude of GPP was greatest for FLUXCOM-ERA5, followed by 476 CEDAR-GPP and FLUXSAT, and substantially smaller for FLUXCOM-RS006 and MODIS GPP. 477 478 In the tropics (20°N - 20°S), differences between datasets were the strongest, where seasonal 479 variation is not as prominent compared to other regions. CEDAR-GPP, FLUXSAT, and FLUXCOM-ERA5 each showed two GPP peaks, occurring in March-April and September-480 481 October. Although FLUXCOM-RS006 had a similar seasonal pattern, its GPP magnitude was 482 markedly smaller. Interestingly, MODIS showed an inverse season pattern with a small peak from 483 June to August.



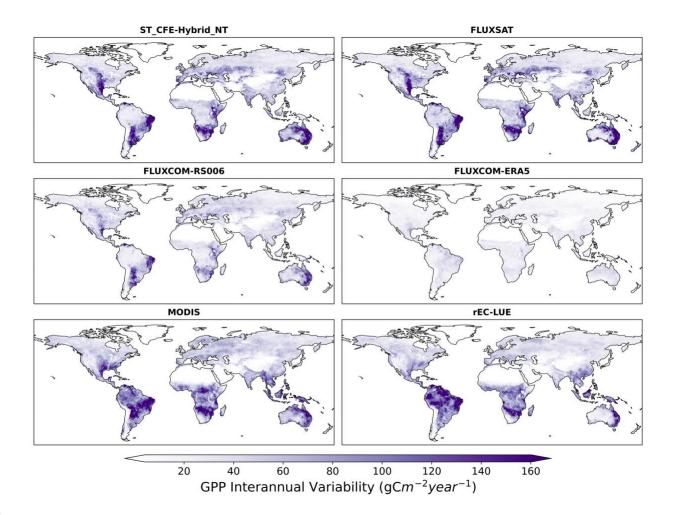
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Figure 7. Comparison of GPP mean seasonal cycle between different datasets on a global scale, and specifically within the Northern Hemisphere (20°N - 90°N), Southern

487 Hemisphere (20°S - 60°S), and Tropical regions (20°N - 20°S). Monthly means were
488 averaged from 2001 to 2018 for all datasets.

489 3.2.3 Interannual variability

490 We found distinct spatial patterns in GPP interannual variability between upscaled and LUE-491 based datasets and a high level of agreement within each category, with the exception of 492 FLUXCOM-ERA5, which showed minimal interannual variability globally (Figure 8). All datasets 493 agreed on the presence of GPP interannual variability hotspots in eastern and southern South 494 America, central North America, southern Africa, and western Australia. These hotspots primarily 495 corresponded to arid and semi-arid areas characterized by grasslands, shrubs, and croplands (Figure 496 9). CEDAR-GPP was highly consistent with FLUXSAT, and both datasets also displayed relatively 497 high interannual variability in the dry subhumid areas of Europe, predominately covered by 498 croplands. FLUXCOM-RS006 mirrored the relative spatial patterns of CEDAR-GPP and 499 FLUXSAT, albeit at lower magnitudes. The LUE-based datasets (MODIS and rEC-LUE) predicted 500 a much higher interannual variability than the upscaled datasets in the tropical areas, particularly in 501 evergreen broadleaf forests and woody savannas (Figure 8, Figure 9). These datasets also depicted 502 slightly higher interannual variability for other types of forests, including evergreen needleleaf forests 503 and deciduous broadleaf forests, compared to the upscaled datasets.



505Figure 8. Spatial patterns of GPP interannual variability extracted over 2001 to 2018506for CEDAR-GPP (ST_CFE-Hybrid_NT), FLUXSAT, FLUXCOM-RS006, MODIS,

507 FLUXCOM-ERA5, and rEC-LUE.

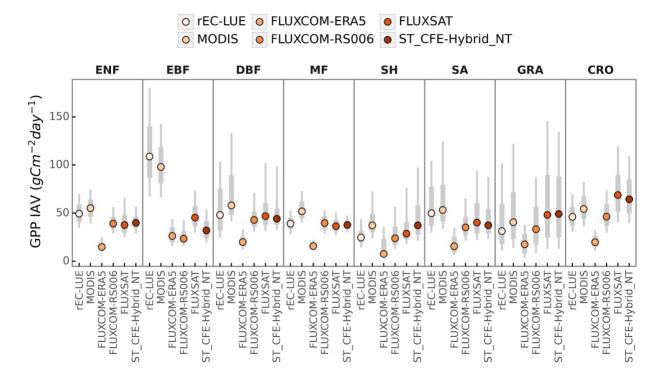


Figure 9. Comparison of GPP interannual variability (IAV across global datasets by
PFT. Colored dots represent the median IAV, thicker grey bars indicate the 25% to
75% percentiles of IAV distributions, and thinner grey bards show the 10% to 90%
percentiles.

513 3.2.4 Trends

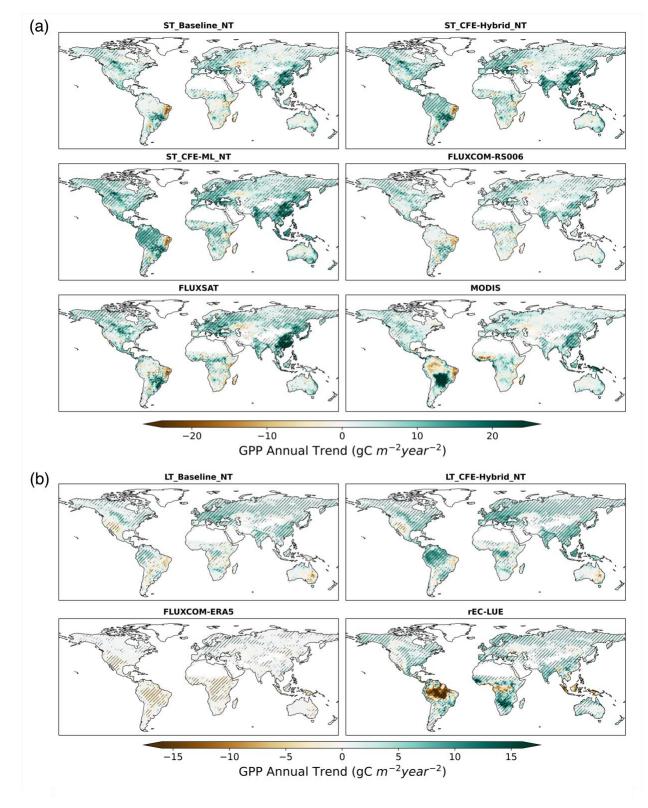
514 Differences in annual GPP trends among CEDAR-GPP model setups and other upscaled and 515 LUE-based datasets mainly reflected the variability in the representation of CO₂ fertilization effects 516 (Figure 10, Figure S4). From 2001 to 2018, the CEDAR-GPP Baseline model setups showed spatial 517 variations in GPP trends consistent with the other upscaled datasets without direct CO₂ fertilization 518 effects, including FLUXSAT and FLUXCOM-RS. In these datasets, substantial increases were seen 519 in southeastern China and India, western Europe, and part of North and South America. These 520 increases were largely associated with rising LAI due to land use changes and indirect CO₂ 521 fertilization effects, as identified by previous studies (Zhu et al., 2016; Chen et al., 2019). Although 522 MODIS, which also does not include a direct CO_2 fertilization effect, generally agreed with these 523 increasing trends, it also showed a declining GPP in the tropical Amazon and a stronger positive 524 trend in central South America. After incorporating the direct CO₂ fertilization effects, both the 525 CFE-Hybrid and CFE-ML setups predicted positive trends in tropical forests, an observation absent

526 in all other datasets. Furthermore, the CFE-Hybrid and CFE-ML models also revealed increasing

527 GPP in temperate and boreal forests of North America and Eurasia. Notably, all datasets agreed on528 a pronounced GPP decrease in eastern Brazil.

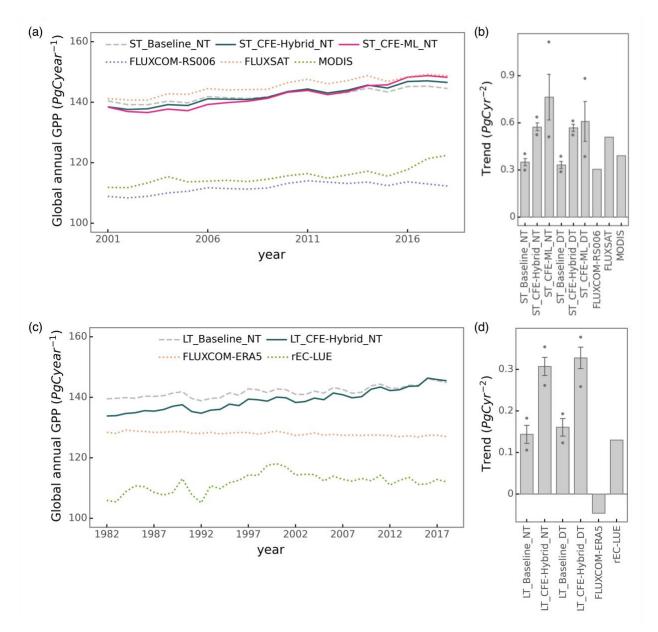
529 From 2001 to 2018, a positive trend in global annual GPP was uniformly detected by all, albeit 530 with varying magnitudes (Figure 11a-b). The ST_Baseline_NT model predicted a GPP growth rate 531 of 0.35 Pg C per year, aligning with FLUXCOM-RS, but lower than FLUXSAT (0.51 Pg C yr⁻¹) and MODIS (0.39Pg C yr⁻¹) (Figure 11b). The CFE-hybrid models estimated a notably faster GPP 532 growth at 0.58 Pg C per year. The CFE-ML models predicted the highest trends, up to 0.76 from 533 534 the ST_CFE-ML_NT model and 0.59 from the ST_CFE-ML_DT model. Also, a higher variance 535 was observed among ensemble members in the ST_CFE-ML setups compared to the ST_Baseline 536 and ST_CFE-Hybrid models. 537 From 1982 to 2018, the LT Baseline models identified increasing GPP trends in large areas of 538 Europe, East and South Asia, as well as Northern Amazon (Figure 10b). The patterns from LT_CFE-Hybrid models aligned closely with the LT_Baseline models but exhibited a stronger 539 540 positive trend in global tropical areas as well as Eurasian boreal forests. In contrast, FLUXCOM-541 ERA5 showed overall negative trends in the tropics, despite a small magnitude. Lastly, rEC-LUE 542 agreed with positive GPP trends identified in CEDAR-GPP in the extratropical areas, but predicted 543 a pronounced negative trend in the tropics. At the global scale, all the CEDAR-GPP long-term 544 models predicted an increasing global GPP trend (Figure 11d). The LT_Baseline models showed a trend of 0.13 to 0.15 Pg C year⁻², while the LT_CFE-Hybrid setups doubled that rate. rEC-LUE 545 showed a two-phased pattern with a strong increase in GPP from 1982 to 2000 (0.54 Pg C year⁻²), 546 547 followed by a decreasing trend after 2001 (-0.20 Pg C year⁻²) (Figure S5). This resulted in an overall 548 positive change at a rate comparable to that of the Baseline model. FLUXCOM-ERA5 exhibited a

549 small negative trend.



551Figure 10. Annual GPP trend over 2001 – 2018 for short-term CEDAR-GPP,552FLUXCOM-RS006, FLUXSAT, and MODIS datasets (a) and over 1982 – 2018 for553long-term CEDAR-GPP, FLUXCOM-ERA5 and rEC-LUE datasets (b). Hatched

areas indicate the GPP trend that is statistically significant at p < 0.05 level under the Mann-Kendal test.



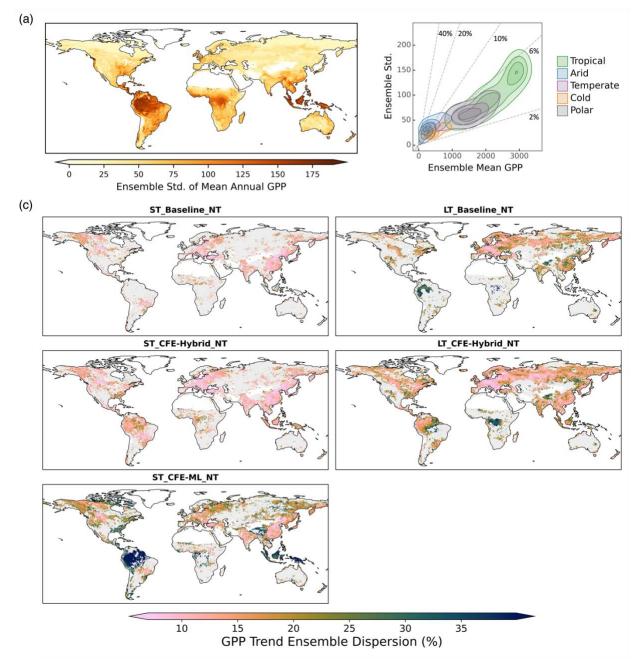
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557 Figure 11. Global annual GPP variations (a) and trends (b) over 2001 to 2018 for 558 short-term CEDAR-GPP, FLUXCOM-RS006, FLUXSAT, and MODIS datasets 559 Global annual GPP variations (c) and trends (d) over 1982 to 2018 for long-term for 560 long-term CEDAR-GPP, FLUXCOM-ERA5, and rEC-LUE datasets. Error bars in 561 (b) and (d) represent the 25% to 75% percentile from the model ensembles of 562 CEDAR-GPP. Dots in (b) and (d) indicate the minimum and maximum from the 563 model ensembles of CEDAR-GPP.

565 3.3 GPP estimation uncertainties

566 We analyzed the spread between the 30 model ensemble members in CEDAR-GPP as an 567 indicator of uncertainties in GPP estimations. The spatial pattern of uncertainty in estimating annual 568 mean GPP largely resembled that of the mean map (Figure 12, Figure 6a). The largest model spread 569 was found in highly productive tropical forests, and this uncertainty decreased in temperate and cold 570 areas (Figure 12a). Tropical ecosystems, with a mean annual GPP between 1000 to 3500 PgCyr⁻¹, 571 only exhibited a 2% and 6% variation within the model ensemble (Figure 12b). Ecosystems in the 572 temperate and cold climates had a smaller annual GPP and proportionally small uncertainties up to 573 6%. However, ecosystems in Arid and Polar climates, despite their similarly low GPP, showed 574 higher model uncertainty, reaching 10% to 40% of the ensemble mean. The estimation uncertainty 575 of GPP trends was generally below 15% to 20% in the CEDAR-GPP datasets under the 576 ST_Baseline and ST_CFE-Hybrid setups (Figure 12c). However, in the ST_CFE-ML setup, the 577 estimation increased substantially, with model spread reaching up to 40% in tropical areas. Notably,

578 the long-term models showed a higher uncertainty compared to the short-term models.



580 Figure 12. CEDAR-GPP estimation uncertainty derived from ensemble spread 581 (standard deviation of 30 model predictions). (a) Spatial patterns of the absolute 582 standard deviation from ensemble members in estimating the mean annual GPP from 2001 to 2018, using data from the ST_CFE-Hybrid_NT setup. (b) Relationships 583 between ensemble standard deviation and ensemble mean in mean annual GPP. 584 Colored contours denote clusters of Koppen climate zones. Dashed lines indicate the 585 ratio between the ensemble standard deviation and the ensemble mean with values 586 587 shown in percentage. (c) Spatial patterns of model uncertainty in GPP long-term trend 588 estimation. Only areas where 90% of the ensemble members showed a statistically 589 significant trend (p < 0.05) are shown in the maps. The trend for the short-term datasets

(left column) was computed between 2001 to 2018. The trend for the long-term datasets (right column) was computed between 1982 to 2018.

592 **4. Discussion**

593 4.1 Uncertainties in GPP upscaling

594 Uncertainties in CEDAR-GPP estimations primarily stem from three components of the 595 machine learning upscaling framework: eddy covariance GPP measurements, input satellite and 596 climate datasets, and the machine learning model itself. Here we examine the three sources of 597 uncertainties, discuss our strategies to reduce their impact, and assess the ability of our model 598 ensemble spread indicator to indicate these uncertainties.

599 4.1.1 Eddy covariance data

600 Measurement and modeling errors inherent in eddy covariance GPP can propagate through 601 the upscaling process. While random measurement errors in monthly GPP are typically very small 602 due to error cancellation through temporal aggregation from the half-hourly data, systematic biases 603 may be introduced by the partitioning approach used to derive GPP from the Net Ecosystem Exchange (NEE) measurements, which could be specific to certain environmental conditions 604 605 (Keenan et al., 2019; Pastorello et al., 2020). This uncertainty was evidenced by a discrepancy 606 between the CEDAR-GPP NT and DT setups. The mean annual GPP from the DT setup was 607 slightly higher than that from the NT setup (Figure 6), and the DT setup also predicted a higher 608 GPP trend in the long-term dataset (Figure 11). Notably, these discrepancies were relatively small 609 compared to the predominant spatiotemporal patterns. Nevertheless, separate DT and NT setups in 610 CEDAR-GPP offered an interesting quantification of the associated uncertainties over space and 611 time, providing insights for future improvements of GPP partitioning approaches. 612 The heavily skewed representativeness of the eddy covariance data remains a key challenge 613 in upscaling, a limitation well-documented in previous studies (Jung et al., 2020). Effective 614 generalization in machine learning models requires a substantial volume of training data that

adequately represents and balances unseen conditions. However, the geographical and temporal

616 limitations of eddy covariance data introduce both systematic and random uncertainties in upscaled

617 GPP estimations. Flux sites are primarily clustered in North America and Western Europe, with

618 sparse availability in critical carbon exchange hotspots such as tropical, subtropical, and boreal

619 regions (Figure 1). Consequently, estimated GPP from upscaling was commonly believed to carry 620 high uncertainties in these areas. However, previous studies have found that humid tropical regions 621 were associated with low extrapolation uncertainty despite the limited amount of flux sites (Jung et 622 al., 2020). A pioneering study employing synthetic datasets from a deterministic terrestrial biosphere 623 model assessed the generalizability of the upscaling approach (Jung et al., 2009). Results indicated 624 that a machine learning model trained with data from the FLUXNET sites' location and times could 625 account for 92% variation of GPP globally. Therefore, to fully understand the upscaling uncertainty, 626 it is essential to carefully evaluate the generalization or extrapolation errors within the predictor 627 space, which indicates the actual environmental controls and mechanisms of the ecosystem carbon 628 fluxes (van der Horst et al., 2019; Villarreal and Vargas, 2021).

629 We compiled a large (~18000 site-months) set of high-quality eddy covariance data in 630 generating CEDAR-GPP to potentially mitigate uncertainties associated with eddy covariance 631 measurements. The FLUXNET2015 dataset was complemented by two regional networks 632 processed under the same ONEFLUX protocol with additional sites and longer records. Data were 633 screened with stringent quality control criteria to reduce measurement uncertainties. Nevertheless, 634 uncertainties in GPP upscaling due to limited eddy covariance data representation remain 635 substantial. Additionally, our analysis suggested that the estimated global GPP magnitudes were 636 related to the eddy covariance GPP data used in the model. Global GPP magnitudes derived from 637 CEDAR-GPP and FLUXSAT aligned closely with that from Terrestrial Biosphere Models (Anav et al., 2015), while FLUXCOM's estimation was much lower (Figure 6, Figure 11). FLUXSAT used 638 639 FLUXNET2015 as the training set, which largely overlapped with that included in CEDAR-GPP 640 (Joiner and Yoshida, 2020). FLUXCOM utilized the FLUXNET La Thuile set combined with 641 CarboAfrica network, which consisted of a very different set of sites, with flux data processed with a 642 different pipeline (Tramontana et al., 2016). The influence from the predictor datasets was minimal 643 since all three datasets relied on MODIS-derived products. For a comprehensive evaluation of the 644 impacts of flux site representativeness on upscaling, future research directions could include 645 conducting synthetic experiments with simulations of ensembles of terrestrial biosphere models. 646 4.1.2 Input predictors and controlling factors

Input predictors, including satellite and climate datasets, bring additional uncertainties to
 upscaled GPP. First, satellite remote sensing data contains noises resulting from atmospheric
 conditions, sun-earth geometry, soil background, and geolocation inaccuracies. The models or

650 algorithms used for variable estimation, such as those for retrieving LAI, fAPAR, LST, and soil 651 moisture, also contain random errors and systematic biases specific to certain regions, biome types, 652 or climatic conditions (Yan et al., 2016b; Fang et al., 2019; Ma et al., 2019). Additionally, satellite 653 observations frequently contain missing values due to clouds, aerosols, snow, and satellite revisit 654 cycles, leading to both systematic and random uncertainties. In producing CEDAR-GPP, we aimed 655 to mitigate these uncertainties through comprehensive preprocessing procedures. Our temporal gap-656 filling strategy improved upon previous upscaling efforts by exploiting both the temporal 657 dependency of vegetation status and long-term climatology, to reduce biases from missing values. 658 Temporal and spatial aggregation further diminished the remaining data gaps and random noises. 659 Nevertheless, it was still likely that considerable uncertainties remained in satellite datasets and 660 propagated into the upscaled estimations.

661 The mismatch between the footprint of the eddy covariance measurements and the coarse 662 resolution of satellite observations presents another significant, and potentially more impactful, 663 source of uncertainties. Flux towers typically have a footprint of around $\sim 1 \text{ km}^2$ (Chu et al., 2021), 664 whereas satellite observations employed in CEDAR-GPP and most other upscaled datasets were at 665 5 km or lower resolution. Systematic and random errors could be introduced due to this mismatch, 666 particularly in heterogenous biomes and areas with a mixture of vegetation and non-vegetated land 667 covers. Gaber et al. (in prep) discovered that machine learning models trained with MODIS datasets 668 at their native 500m resolution substantially outperformed those trained with aggregated datasets at 669 0.05-degree resolution, especially in capturing interannual variabilities. One approach to mitigate this 670 issue is by generating upscaled datasets at a higher spatial resolution (e.g. 500m). Alternatively, 671 models could be trained at a high resolution and applied to the coarse resolution to reduce 672 computation and storage requirements (Dannenberg et al., 2023). However, this approach does not 673 address inherent scaling errors in coarse-resolution satellite images (Yan et al., 2016a; Dong et al., 674 2023).

Besides the quality of predictors, successful machine learning upscaling also depends on a
comprehensive set of features representing all controlling factors. Satellite-derived vegetation
structural indicators have been found to be the most influential features in GPP upscaling
(Tramontana et al., 2015); consequently, trends and interannual variabilities in upscaled GPP
reflected that from the underlying vegetation structural datasets. For example, the FLUXCOMRSv006 dataset was generated based on the MODIS collection 6 dataset, showing similar temporal
dynamics globally as CEDAR-GPP and FLUXSAT. However, the previous version that utilized

MODIS collection 5 products exhibited minimal interannual variability and insignificant trend (Ryuet al., 2019).

684 Furthermore, information about resource limitations and stress factors can be crucial for 685 certain biomes and/or under specific conditions (Stocker et al., 2018). For example, Dannenberg et 686 al. (2023) found that incorporating LST from MODIS and soil moisture from the SMAP satellite 687 datasets improved the machine learning estimation accuracy of GPP in drylands from $R^2 \sim 0.4$ to 0.7 for dryland sites in North America. CEDAR-GPP integrated multi-source satellite observations 688 689 (optical, thermal, microwave) as well as climate variables to obtain comprehensive information about 690 GPP dynamics. Nevertheless, as was commonly observed in machine learning upscaling, the models 691 failed to capture interannual anomalies. This could imply that vital information for GPP estimation 692 remained missing or inadequately represented in existing datasets. Examples include factors related 693 to agricultural management practices (crop type, cultivar, irrigation, fertilization), plant hydraulic and 694 physiological properties, as well as root and soil characteristics.

695 4.1.3 Machine learning models and uncertainty quantification

696 The choice of machine learning models and their parameterization has been found to have a relatively minor impact on the upscaling of GPP (Tramontana et al., 2015). CEDAR used the state-697 of-the-art boosting algorithm, XGBoost, which provided near-optimal performance considering the 698 699 current data availability. Further reduction of model uncertainty will likely rely on additional 700 information, such as increasing the number of training samples or incorporating more high-quality 701 predictors. Additionally, temporal dependency of carbon fluxes responses to atmospheric controls 702 may also be exploited with specialized deep neural networks such as recurrent neural networks or 703 transformers (Besnard et al., 2019; Ma and Liang, 2022).

704 A key challenge, however, is the quantification of uncertainties in machine learning upscaling (Reichstein et al., 2019). The limited availability of eddy covariance data hinders a comprehensive 705 706 assessment of the extrapolation errors; consequently, metrics of predictive performance from cross-707 validation are inherently biased. CEDAR derived estimation uncertainty for each GPP prediction 708 using bootstrapping model ensemble, which naturally mimics the biased sampling of flux tower 709 locations. Notably, the choice of input climate reanalysis datasets could also induce systematic 710 differences in GPP spatial and temporal patterns (Tramontana et al., 2015). The FLUXCOM 711 product used model ensembles based on different reanalysis datasets to capture these uncertainties.

712 Additionally, different satellite datasets of vegetation structural proxies, such as LAI, also exhibited

significant discrepancies (Jiang et al., 2017). Thus, an ensemble approach combining site-level

- 514 bootstrapping with multiple sources of input predictors could potentially provide a more
- 715 comprehensive quantification of uncertainties. Future work may also explore Bayesian neural
- 716 networks, which provide uncertainty along with predictions and, at the same time, present high
- 717 predictive power comparable to ensemble tree-based algorithms (Ma et al., 2021).

718 4.2 Long-term GPP changes and CO₂ fertilization effect

719 CEDAR-GPP was constructed using a comprehensive set of climate variables and multi-720 source satellite observations, thus, encapsulating long-term GPP dynamics from both direct and 721 indirect effects of climate controls. Particularly, CEDAR-GPP included the direct CO₂ fertilization 722 effect, which has been shown to dominate the increasing trend of global GPP (Chen et al., 2022). 723 Incorporating these effects substantially improved long-term trends of GPP from site to global 724 scales (Figure 5, 10, 11). CEDAR's CFE-Hybrid setup offered a conservative estimation of the 725 direct CO₂ effects by simulating the light-limited sensitivity on LUE for C3 plants (Walker et al., 726 2021). Nevertheless, the model did not account for the impacts of nutrient availability, which could 727 potentially constrain CO₂ fertilization (Reich et al., 2014; Peñuelas et al., 2017; Terrer et al., 2019). 728 Furthermore, the sensitivity of light-limited photosynthesis is a function of temperature, resulting in 729 the most pronounced increasing trend in the tropics (Figure 10). Yet the model assumed a fixed 730 ratio of leaf-internal to ambient CO₂, and thus did not include any responses to vapor pressure 731 deficit.

732 The CFE-ML model adopted a data-driven approach to infer CO₂ effects directly from eddy 733 covariance data. This strategy allowed the model to capture any physiological pathways of the CO_2 734 impact evidenced in the eddy covariance measurements, including the increases of the biochemical 735 rates as well as enhancements in water use efficiency (Keenan et al., 2013). The model successfully 736 detected a strong positive effect of CO_2 on eddy covariance measured GPP, consistent with 737 previous studies based on process-based and statistical models (Fernández-Martínez et al., 2017; 738 Ueyama et al., 2020; Chen et al., 2022). Notably, the CFE-ML model could have included the 739 impacts of other factors that exhibit a strong temporal correlation with CO₂. For example, 740 industrialization-induced increases in nitrogen deposition could synergistically boost GPP alongside 741 CO₂ (O'Sullivan et al., 2019). Technological and management improvements in agriculture that 742 contribute to a global boost of crop photosynthesis (Zeng et al., 2014), might also be indirectly 743 reflected in the model estimates. As a result, the CFE-ML predicted a GPP trend that more closely

744 aligned with eddy covariance observations, and the upscaled dataset also showed a globally higher 745 trend than CFE-Hybrid (Figure 5; Figure 10). Nevertheless, spatial patterns of GPP trends from the CFE-ML aligned with that from CFE-Hybrid, reflecting a strong temperature dependency, implying 746 747 that the effects of CO₂ likely remained the most significant factor. Additionally, the considerable ensemble spread in the CO₂ trends from the CFE-ML model (Figure 11, Figure 13) underscored a 748 749 high level of uncertainty in the machine learning quantified CO₂ effects. Future work may exploit 750 explainable machine learning and causal inference to investigate the underlying mechanisms of CO₂ 751 effects.

752 **5. Data availability**

The CEDAR-GPP product, comprising ten GPP datasets, is available at zenodo
(https://doi.org/10.5281/zenodo.8212707). These datasets were generated at a spatial resolution of
0.05° and monthly time steps. Each dataset includes an ensemble mean GPP and an ensemble
standard deviation.

757 6. Summary and conclusions

758 We present the CEDAR-GPP product generated by upscaling global eddy covariance 759 measurements with machine learning and a broad range of satellite and climate variables. CEDAR-760 GPP comprises four long-term datasets from 1982 to 2020 and six short-term datasets from 2001 to 761 2020. These datasets encompass three different configurations of the incorporation of direct CO_2 762 fertilization effects and two partitioning approaches to derive GPP from eddy covariance data. The 763 machine learning models of CEDAR-GPP achieved high capability in predicting monthly GPP, its 764 seasonal cycles, and spatial variability within the globally distributed eddy covariance sites, with 765 cross-validated R² between 0.56 to 0.79. Short-term model setups consistently outperformed long-766 term models due to considerably more and higher-quality information from multi-source satellite 767 observations.

CEDAR-GPP advances satellite-based GPP estimations, as the first upscaled dataset that considered the direct biochemical effects of elevated atmospheric CO_2 on photosynthesis, which is responsible for an increasing land carbon sink over the past decades. We showed that incorporating this effect in our CFE-ML and CFE-Hybrid models substantially improved the estimation of GPP trends at eddy covariance sites. Global patterns of long-term GPP trends in the CFE-ML setups
showed a strong temperature dependency consistent with biophysical theories. Aside from the trend,
global spatial and temporal GPP patterns from CEDAR generally aligned with other satellite-based

GPP datasets.

776 In conclusion, CEDAR-GPP, informed by global eddy covariance measurements (~18000 777 site-months) and a broad range of multi-source remote sensing observations and climatic variables, 778 offered a comprehensive representation of global GPP spatial and temporal dynamics over the past 779 four decades. The different CO₂ fertilization configures integrated in CEDAR-GPP offer new 780 opportunities for understanding global ecosystem photosynthesis's response to increases in 781 atmospheric CO₂ along different pathways over space and time. CEDAR-GPP is expected to serve 782 as a valuable tool for benchmarking process-based modeling and constraining the global carbon 783 cycle.

784 Supplement

785 The supplement related to this article is available online.

786 Author contributions

T. K. and Y. K. conceptualized the study. Y. K. performed the formal analysis and generated
the final product. Y. K., T. K., M. B., and M. G. contributed to the development and investigation
of the research. Y. K., M. G., and X. L. contributed to data curation and processing. Y. K. prepared
the manuscript with contributions from all co-authors. T. K. supervised the project.

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