Biological nitrogen fixation of natural and agricultural vegetation simulated with LPJmL 5.7.9

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Abstract. Biological nitrogen fixation (BNF) by symbiotic and free living bacteria is an important source of plant-available nitrogen (N) in terrestrial ecosystems supporting carbon (C) sequestration and food production worldwide. Dynamic global vegetation models (DGVMs) are frequently used to assess the N and C cycle under dynamic land use and climate. BNF plays an important role for the components of both these cycles making a robust representation of the processes and variables that

5   BNF depends on important to reduce uncertainty within the C and N cycles and improve the ability of DGVMs to project future ecosystem productivity, vegetation patterns or the land carbon sink. Still, BNF is often modelled as a function of net primary productivity or evapotranspiration neglecting the actual drivers. We implemented plant functional type-specific limitations for BNF dependent on soil temperature and soil water content as well as a cost of BNF in the Lund Potsdam Jena managed Land (LPJmL) DGVM and compare the new (*C-costly*) against the previous (*Original*) approach and data from the scientific

10   literature. For our comparison we simulated a potential natural vegetation scenario and one including anthropogenic land use for the period from 1901 to 2016 for which we evaluate BNF and legume crop yields. Our results show stronger agreement with BNF observations for the *C-costly* than the *Original* approach for natural vegetation and agricultural areas. The *C-costly* approach reduced the overestimation of BNF especially in hot spots of legume crop production. Despite the reduced BNF in the *C-costly* approach, yields of legume crops were similar to the *Original* approach. While the net C and N balances were

15   similar between the two approaches, the reduced BNF in the *C-costly* approach results in a slight underestimation of N losses from leaching, emissions and harvest compared to literature values, supporting further investigation of underlying reasons, such as processes represented in DGVMs and scenario assumptions. While we see potential for further model development, for example to separate symbiotic and free living BNF, the *C-costly* approach is a major improvement over the simple *Original* approach because of the separate representation of important drivers and limiting factors of BNF and improves the ability of

20   LPJmL to project future C and N cycle dynamics.

1 Introduction

Biological nitrogen fixation (BNF) is an important source of plant-available nitrogen (N) in terrestrial ecosystems (Galloway et al., 1995). It can be separated into symbiotic (Granhall, 1981) and free living (Reed et al., 2011) BNF, which account for the total BNF with different shares in different ecosystems (Davies-Barnard and Friedlingstein, 2020a). In natural terrestrial ecosystems, N deposition, N-fixation through lightning, and BNF are the only processes that introduce additional reactive nitrogen into the system (Yu and Zhuang, 2020). In agricultural systems, increased N inputs are - together with the extensive manure recycling - a major source of nitrous oxide (N_2O) and ammonium (NH_4) emissions (Reay et al., 2012; Tian et al., 2020) and nitrate (NO_3^-) pollution (Moss, 2007). These inputs result from increased BNF and deposition of additional anthropogenic N inputs, which originate mainly from synthetic fertiliser application (Lu and Tian, 2017). Promoting N-fixing crops such as forage and grain legumes for usage as green manure has been discussed (Becker et al., 1995; Fageria, 2007; Northup and Rao, 2016) to reduce N losses from nitrification, volatilization, denitrification and leaching on agricultural land. Generally, symbiotic as well as free living BNF can be important for plant growth in N limited ecosystems and supports carbon (C) sequestration and food production across the globe.

Briefly summarised, BNF describes the transformation of atmospheric N_2 to ammonia (NH_4) by a variety of soil microorganisms providing a source of mineral N for plants at the expense of C (Yu and Zhuang, 2020). The underlying mechanisms of BNF as well as its role within the C and N cycles and for ecosystem productivity have been described in detail in multiple studies (e.g., Yu and Zhuang, 2020; Davies-Barnard and Friedlingstein, 2020a; Cleveland et al., 1999). Here, we focus on the representation of BNF in the Lund Potsdam Jena managed Land (LPJmL) DGVM (Schaphoff et al., 2018b; von Bloh et al., 2018; Lutz et al., 2019; Herzfeld et al., 2021; Porwollik et al., 2022; Heinke et al., 2023). We do not distinguish between symbiotic and free living BNF throughout this study but only consider total BNF as the sum of both forms.

DGVMs such as LPJmL can be used to assess the role of BNF for the productivity of natural and agricultural ecosystems and its effects on the N and C cycle under dynamic land use and climate. A solid representation of the processes behind BNF is important to reduce uncertainty and improve model results of DGVMs, which are frequently used in impact assessments and to inform policy makers. A variety of approaches of different complexity to model BNF have been developed. A key difference between approaches is the selection of variables that control BNF and the accounting of the C cost of BNF. For example, Cleveland et al. (1999) use actual evapotranspiration as a single explanatory variable, while Yu and Zhuang (2020) consider soil temperature, soil water content, soil mineral N and soil C content. Both these approaches do not consider the cost of BNF neglecting the reduced C assimilation (Cleveland et al., 1999; Yu and Zhuang, 2020), while others explicitly consider a cost per amount of N fixed and a maximum amount of C that can be invested in BNF (e.g., Ma et al., 2022). Even more complex approaches consider the different pathways of N uptake that are associated with a cost (active N uptake, retranslocation and BNF) and optimise for the minimum cost (e.g., Fisher et al., 2010). Depending on the considered variables, the simulated BNF and how it is affected by climate change may strongly differ, which in turn can have strong effects on the simulated C and N fluxes and pools.

A comparison to data published by Davies-Barnard and Friedlingstein (2020a) suggests that the approach that was implemented in LPJmL von Bloh et al. (2018) based on Cleveland et al. (1999) - in the following defined as the *Original* approach - overestimates global BNF. In addition, we identified several shortcomings of the *Original* approach in LPJmL: In the *Original* approach, BNF is a function of actual evapotranspiration, which leads to an overestimation of BNF in moist but not necessarily N-limited ecosystems and an underestimation in dry but N-limited ecosystems. In this simplified implementation, BNF is not constrained by the availability of reactive forms of N and additional N is fixed even if the reactive soil N is sufficient to fulfil the N demand, which potentially leads to an overestimation of the ammonia pool and N losses. For cultivated grain legumes, the approach assumes no limitation of BNF at all but simply supplies all N requested by the plant that cannot be fulfilled through N uptake from mineral N pools in the soil. This leads to an overestimation of cropland BNF. In order to overcome these deficiencies, we here describe a revision of the *Original* approach in LPJmL with a more complex approach, referred to as *C-costly* approach in the following. The *C-costly* approach is inspired by Ma et al. (2022) and Yu and Zhuang (2020) and introduces plant functional type (PFT)-specific limitations for BNF dependent on soil temperature and soil water content as well as a C cost of BNF. In the following, we present the *C-costly* BNF approach and evaluate its performance against global and site-specific data. We discuss the differences between the *Original* and the *C-costly* BNF approach for the N-cycle and plant productivity.

2 Methods

2.1 Model description

LPJmL is a dynamic global vegetation model (DGVM) with the full terrestrial hydrology and explicit representation of agricultural management systems for cropland and pastures. We have implemented the BNF module in the most recent development branch, which is based on a consolidated version of the carbon-only model (LPJmL4, Schaphoff et al., 2018b, a), the nitrogen cycle (LPJmL5, von Bloh et al., 2018), tillage (Lutz et al., 2019), manure (Herzfeld et al., 2021), cover crop (Porwollik et al., 2022), and grazing management (Heinke et al., 2023) modules. There have been further model improvements that have not been described in publications elsewhere, including improved online coupling options with other models such as IMAGE (Müller et al., 2016) or copan:CORE (Donges et al., 2020). For a better representation of crops that are not explicitly represented (referred to as *others*), these are no longer assumed to be identical to managed grassland (Bondeau et al., 2007), but can be simulated as separate stands with distinct management inputs (e.g. fertiliser amounts).

The original spinup protocol for LPJmL4, described in Schaphoff et al. (2013), was modified to account for the interaction between soils and plants through N supply in LPJmL5. The principal technique to accelerate the spinup by calculating the equilibrium soil C stocks from litter decomposition (i.e., the flux of C into the soil C pools) and soil C turnover rates (or residence time) remains the same as in Schaphoff et al. (2013). However, the original code was refactored to improve the accuracy of estimates of equilibrium stocks and to apply the technique to soil C and N pools simultaneously.

In LPJmL5, an adjustment of N pools can lead to a change in plant productivity through a change in N supply from mineralisation. To account for this feedback, the C- and N-stock adjustments need to be repeated multiple times until the soil and

the vegetation reach equilibria. The revised spinup procedure starts with an initial period of 300 years during which vegetation is allowed to establish. This is followed by a 2400-year period, during which soil C and N pools are updated every 15 years based on litter decomposition and soil pool turnover rates of the preceding ten years. This long period with repeated adjustment

90 (160 times) of C and N pools is required to reach an equilibrium in regions with very low turnover rates (e.g., in the boreal zone). To reduce the effect of inter-annual variability on estimates of equilibrium stocks, a final adjustment is applied after 300 simulation years using litter decomposition and soil pool turnover rates over that period. Finally, the model is allowed to adjust to the new C and N stocks for another 500 simulation years.

To assess the effectiveness of the spinup procedure, we conducted a 1000-year model run under the same conditions as during

95 the spinup period (i.e., stable pre-industrial atmospheric CO_2 concentration, and atmospheric N deposition, and climate) for which present results in appendix B.

Further changes to the code since the last published version (see Porwollik et al., 2022) include various bug fixes concerning fertiliser and manure application, data output, environmental flow requirements (Jägermeyr et al., 2017), soil temperature (Schaphoff et al., 2013), and bioenergy plantations (Beringer et al., 2011). Latest code changes are now also documented in a

100 `CHANGELOG.md` file as part of the code repository (section 5).

2.2 Representation of biological nitrogen fixation

A key feature is the connection of BNF to an associated cost represented as a reduction of net primary production (NPP).

The *C-costly* approach calculates actual BNF (N_{fix}) from the potential BNF ($N_{fix,pot}$) using several reduction factors. First, the nitrogen fixation rate for the environmental conditions $N_{fix,env}$ is calculated from $N_{fix,pot}$ accounting for reductions by

105 dimensionless soil temperature and soil water content (SWC) limitations functions (f_T, f_W) in the interval $[0, 1]$ (Ma et al., 2022):

$$N_{fix,env} = N_{fix,pot} \cdot f_T(T_{soil}) \cdot f_W(SWC) \tag{1}$$

The soil temperature limitation is increasing linearly outside the optimal temperature range ($< T_{opt,low}$ or $> T_{opt,high}$ Eq. 2, Fig. 1 a) and prohibits BNF if outside the tolerable temperature range ($< T_{min}$ or $> T_{max}$), while the soil water limitation is

110 linearly dependent on the relative soil water content SWC (Eq. 3, Fig. 1 b).

$$f_T(T_{soil}) = \begin{cases} 0, & \text{if } T_{soil} < T_{min} \text{ or } T_{soil} > T_{max} \\ \frac{T_{soil} - T_{min}}{T_{opt,low} - T_{min}}, & \text{if } T_{min} \leq T_{soil} < T_{opt,low} \\ 1, & \text{if } T_{opt,low} \leq T_{soil} \leq T_{opt,high} \\ \frac{T_{max} - T_{soil}}{T_{max} - T_{opt,high}}, & \text{if } T_{opt,high} < T_{soil} \leq T_{max} \end{cases} \tag{2}$$

$$f_W(SWC) = \begin{cases} 0, & \text{if } SWC \leq SWC_{low} \\ \varphi_1 + SWC \cdot \varphi_2, & \text{if } SWC_{low} < SWC < SWC_{high} \\ 1, & \text{if } SWC \geq SWC_{high} \end{cases} \tag{3}$$
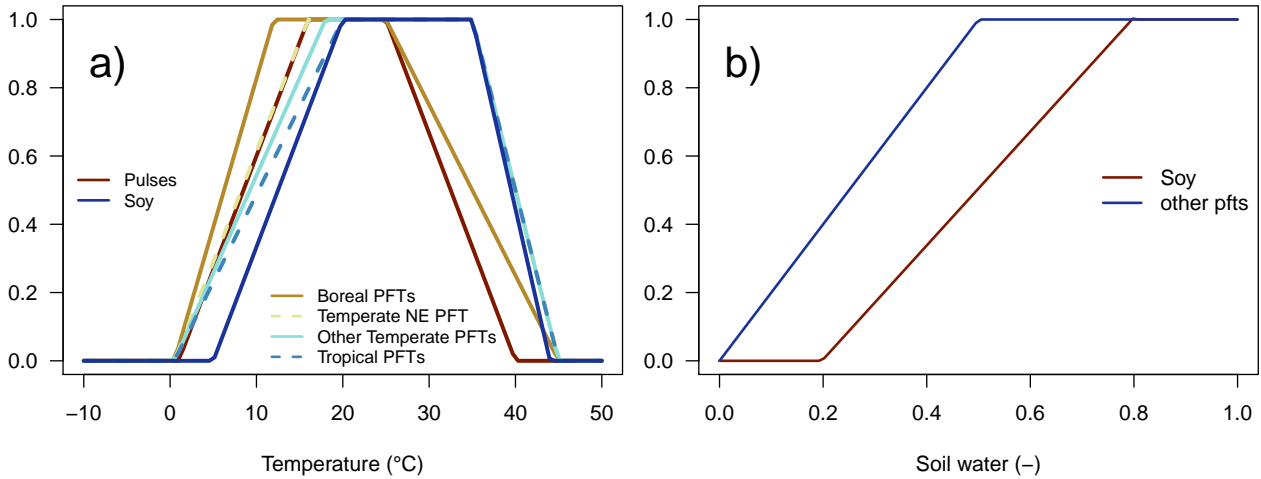
Figure 1. Dimensionless temperature limitation function $f_T(T)$ (a) and soil water limitation function $f_W(SWC)$ (b)

$N_{fix,pot}$, T_{min}, $T_{opt,low}$, $T_{opt,high}$, T_{max}, SWC_{low}, SWC_{high}, φ_1 and φ_2 are PFT-specific parameters (Tab. 1) and their
values are adopted from Yu and Zhuang (2020) for the natural vegetation PFTs and from Ma et al. (2022) for soybean and
pulses.

If $N_{fix,env}$ exceeds the amount of N missing to fulfil the N demand of the current day (the N deficit $N_{deficit}$), the N fixation
is reduced:

$$N_{fix,need} = \min(N_{deficit}, N_{fix,env}) \tag{4}$$

Finally, if the cost of N fixation exceeds the NPP available for BNF, nitrogen fixation is further reduced to match the maximum
amount that can be fixed with the current day's NPP share available for BNF.

$$N_{fix}(NPP) = \begin{cases} N_{fix,need}, & \text{if } cost_{\text{BNF}} \cdot N_{fix,need} < f_{legume} \cdot f_{\text{NPP}} \cdot \text{NPP} \\ f_{legume} \cdot f_{\text{NPP}} \cdot \text{NPP}/cost_{\text{BNF}}, & \text{otherwise}, \end{cases} \tag{5}$$

where f_{NPP} is the maximum share (dimensionless) of NPP available for BNF, which is set to 0.14 (Kull, 2002) for the natural
PFTs and to 0.25 for soybean and pulses. The average legume fraction (f_{legume}) is set to 0.05 for the tropical, to 0.01 for the
temperate, and to 0.03 for the boreal zone (Yu and Zhuang, 2020). PFTs only fix additional nitrogen if the nitrogen uptake from
other sources is insufficient and the net primary productivity (NPP) is larger than zero. The costs of BNF are set at a moderate
constant value of 6 gC gN^{-1} (Boote et al., 2009; Ryle et al., 1979; Patterson and Larue, 1983; Kaschuk et al., 2009).

2.3 Modelling protocol

To compare the two BNF approaches, we simulated two scenarios: First, a potential natural vegetation (PNV) scenario, which
does not include anthropogenic land use or agricultural production systems. Second, a scenario that includes agricultural land

Table 1. BNF related PFT-specific parameter values for the tropical broadleaved evergreen tree (TrBE), tropical broadleaved raingreen tree (TrBR), temperate needleleaved evergreen tree (TeNE), temperate broadleaved evergreen tree (TeBE), temperate broadleaved summergreen tree (TeBS), boreal needleleaved evergreen tree (BoNE), boreal broadleaved summergreen tree (BoBS), boreal needleleaved summergreen tree (BoNS), tropical herbaceous (TrH), temperate herbaceous (TeH), polar herbaceous (PoH), soybean and pulses.

PFT	$N_{fix,pot}$	T_{min}	$T_{opt,low}$	$T_{opt,high}$	T_{max}	SWC_{low}	SWC_{high}	φ_1	φ_2	f_{NPP}	$cost_{BNF}$	f_{legume}
	$gNm^{-2}d^{-1}$	°C	°C	°C	°C	m^3m^{-3}	m^3m^{-3}	-	-	-	$gCg^{-1}N$	-
TrBE	0.01	0.5	20	35	45	0	0.5	0	2.0	0.14	6	0.05
TrBR	0.01	0.5	20	35	45	0	0.5	0	2.0	0.14	6	0.05
TeNE	0.01	0.5	16	35	45	0	0.5	0	2.0	0.14	6	0.01
TeBE	0.01	0.5	18	35	45	0	0.5	0	2.0	0.14	6	0.01
TeBS	0.01	0.5	18	35	45	0	0.5	0	2.0	0.14	6	0.01
BoNE	0.01	0.5	12	25	45	0	0.5	0	2.0	0.14	6	0.03
BoBS	0.01	0.5	12	25	45	0	0.5	0	2.0	0.14	6	0.03
BoNS	0.01	0.5	12	25	45	0	0.5	0	2.0	0.14	6	0.03
TrH	0.01	0.5	20	35	45	0	0.5	0	2.0	0.14	6	0.05
TeH	0.01	0.5	18	35	45	0	0.5	0	2.0	0.14	6	0.01
PoH	0.01	0.5	12	25	45	0	0.5	0	2.0	0.14	6	0.03
Soybean	0.1	5	20	35	44	0.2	0.8	-0.33	1.67	0.25	6	1
Pulses	0.1	1	16	25	40	0	0.5	0	2.0	0.25	6	1

use (LU). The same input datasets were used for all scenarios. We used the climate data from the GSWP3-W5E5 dataset (Kim; Cucchi et al., 2020; Lange et al., 2022), historical atmospheric N deposition (Yang and Tian, 2020), historical atmospheric CO₂ concentrations (Büchner and Reyer, 2022), historical land-use patterns (Ostberg et al., 2023) and grazing management data (Stenzel et al., 2023). For both BNF approaches, we conducted spinup simulations of 3500 years using a random permutation

135 of the climate data from 1901 to 1931. These spinup simulations ensure that the C and N balances are in an equilibrium. Afterwards, land use is introduced and a second spinup period of 390 years is run to capture the effects of historical land-use change on the C and N cycle. Following the two spinup simulations, the model is run from 1901 until 2016 using the transient input data.

2.4 Evaluation data

140 We compared simulated total global BNF against several estimates, which were derived empirically or reported in other modelling studies (Davies-Barnard and Friedlingstein, 2020a). In addition, we compared our results to data obtained at several sites for the natural vegetation (Davies-Barnard and Friedlingstein, 2020a) and legume crops (Ma et al., 2022).

3 Results

3.1 Comparison of the BNF approaches

145 Comparing the simulated BNF of both approaches to data from literature and experiments showed substantial improvement of the global BNF (sect. 3.1.1) as well as the latitudinal and spatial patterns (sect. 3.1.2).

3.1.1 Comparison to data and other models

The two approaches show large differences in the simulated BNF. While the median global BNF between 2001 and 2010 was 191 $TgNyr^{-1}$ for the *Original* approach, for the *C-costly* approach it was substantially lower with a value of 109 $TgNyr^{-1}$

150 (Fig. 2 a). Comparing the global BNF of both approaches to estimates from the scientific literature shows agreement of the *C-costly* values with several other data sources, while the *Original* approach overestimates most of the literature values. Especially the recent estimate by Davies-Barnard and Friedlingstein (2020a) was closely matched by the *C-costly* approach and 60% of the simulated data were within the range of the Davies-Barnard and Friedlingstein (2020a) data (Fig. 2 a). Despite the fact that the *Original* approach was not derived from the empirical relationship of Cleveland et al. (1999) for the legume crops, the data

155 from Cleveland et al. (1999) are well matched by the *Original* approach and only the spread of the Cleveland et al. (1999) data is underestimated. In comparison to the data of Xu-Ri and Prentice (2017), who reported much higher values compared to the other studies, BNF is underestimated by both approaches implemented in LPJmL. However, large differences are to be expected considering that their approach does not calculate the actual BNF but rather the BNF needed to sustain global NPP (Xu-Ri and Prentice, 2017).

160 Comparing the spatial patterns of the two approaches to those of Davies-Barnard and Friedlingstein (2020a) shows that the *Original* approach generally overestimated BNF in large areas of the tropics and temperate zones (Fig. B4 c). The *C-costly* approach still overestimates BNF in the tropics and the production areas of soybean and/or pulses in India and the United States of America (USA) but values are substantially smaller than in the *Original* approach (Fig. B4 f). In both approaches, observed BNF is slightly underestimated in the central to western part of the USA, Canada, China, Kazakhstan, Russia and Mongolia.

165 On croplands, BNF was 21 $TgN\ yr^{-1}$ with the *C-costly* approach, which is within the range of 17 to 31 $TgN\ yr^{-1}$ reported by a recent review (Zhang et al., 2021) and other studies (Bodirsky et al., 2012; Chang et al., 2021). This contrasts the overestimation of cropland BNF in the *Original* approach which was 68 $TgN\ yr^{-1}$. For the two legume crop functional types soybean and pulses, we compared the simulation results to BNF and yield data from experiments (Fig. 2b and c and Fig. B1 a and b). For all except two experiments, the *Original* approach strongly overestimated BNF independent of the crop and the

170 irrigation management. Using the *C-costly* approach, the cropland BNF was strongly reduced by a factor of approximately two leading to substantially lower root mean square errors (RMSE). While simulation results were closer to observations, some deviations remain. Pulses generally showed lower BNF for both approaches compared to soybean, while irrigated simulations generally showed a higher BNF and overestimated BNF compared to observations for all experiments in the *Original* and for the vast majority in the *C-costly* approach. Crop yields barely differed between the two approaches and were comparable to

175 observations (Fig. B1 a and b).
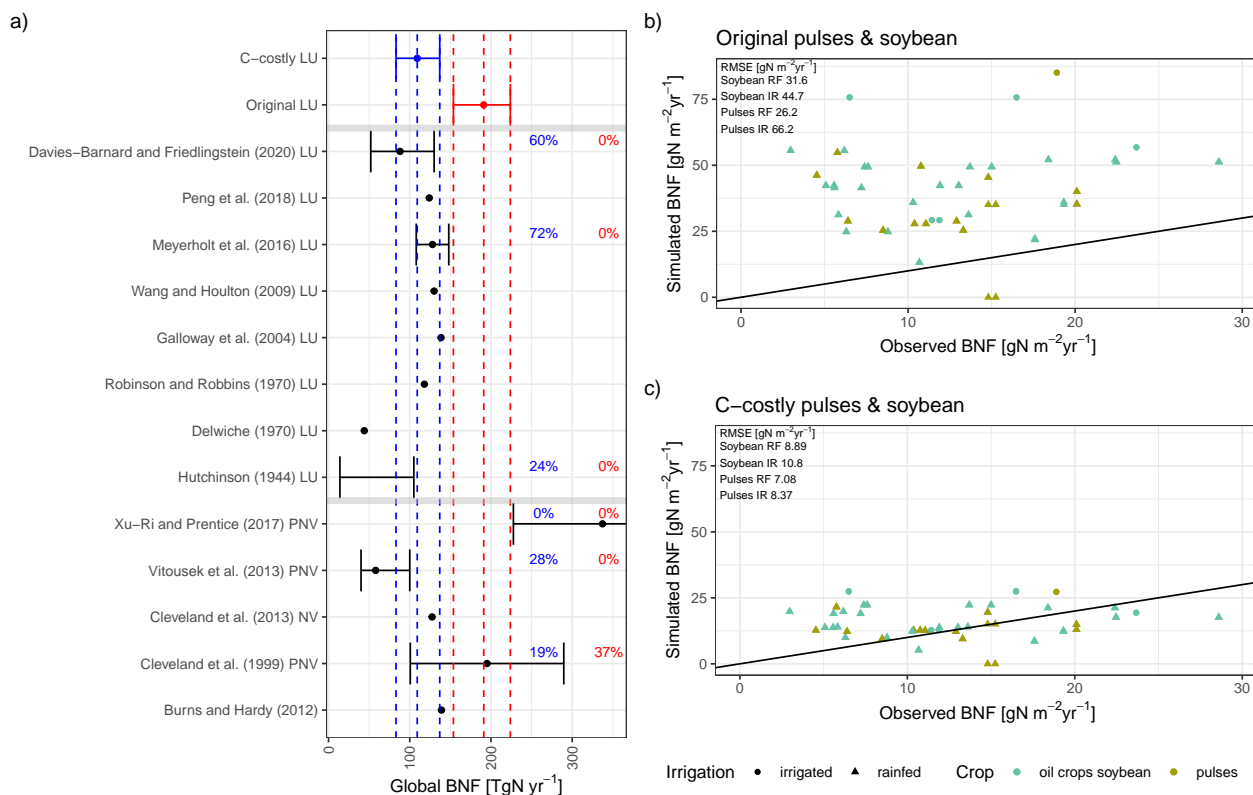
Figure 2. Evaluation against global (a) and site specific data (b, c). Global evaluation plot inspired by Davies-Barnard and Friedlingstein (2020a) showing global BNF in TgN yr^{-1} from different studies (black) compared to the *Original* (red) and *C-costly* (blue) BNF approach implemented in LPJmL. Studies are labelled by author names and whether they consider potential natural vegetation (PNV), actual natural vegetation (NV) or actual land use (LU). We assigned the Davies-Barnard and Friedlingstein (2020a) data to the LU category because they consider cropland area as grasslands and not as potential forest areas. Coloured labels report the overlap between the ranges of the simulation results and the literature estimates. Simulated values are the median between 2001 and 2010 and ranges show minimum and maximum. Site specific evaluation (b, c) comparing data from observations for soybean (red) and pulses (blue) for rainfed (circle) and irrigated (triangle) experiments and simulations results using the *Original* (b) and *C-costly* (c) BNF approach.

3.1.2 Global variation in BNF

Generally, BNF decreases from low to high latitudes with similar gradients but from different levels for the two approaches (Fig. 3). In latitudes with a high share of crop legumes (e.g. 30 to 40°S) the reduction of BNF in the *C-costly* approach is especially large. While both the *Original* as well as the *C-costly* approach underestimate BNF at high latitudes (the *Original*
180 more strongly so) compared to Davies-Barnard and Friedlingstein (2020a), the *C-costly* approach shows good performance in the mid latitudes, but both approaches overestimate BNF compared to observations in the tropics (Fig. 3). In the *Original* approach, especially the high BNF of cropland contributes to the overestimation. For the low latitudes, both approaches exceed the values from Davies-Barnard and Friedlingstein (2020a). However, the higher BNF in the tropics is comparable to the median of the TRENDY-N ensemble (sect. 4 and Kou-Giesbrecht et al., 2023).

185 With the *Original* approach, mineral N was added to the first soil layer and subsequently incorporated by the PFTs via the passive and active N uptake pathway. This did not allow a separate identification of N taken up via BNF from the total N uptake. Using the *C-costly* BNF, the model separates N uptake by BNF from passive and active N uptake against N concentration gradients (Marschner et al., 1991; Fisher et al., 2010)) facilitating the analysis of the share of BNF in total N uptake subsequently referred to as $\mathrm{BNF_{frac}}$. In the PNV simulation, values for $\mathrm{BNF_{frac}}$ were below 15% for most of the grid cells
190 (Fig. B7 and B8 b). For the dynamic land-use simulation, the values for $\mathrm{BNF_{frac}}$ are even smaller with the majority of values below 10% (Fig. B7 and B8 a).

In both approaches, BNF per area is higher for agricultural land than for natural vegetation (Fig. B3 d and f). BNF is especially high in hot spots of legume crop production such as Argentina, Brazil, India and the USA (Fig. 3 a and b). While the spatial pattern is similar between the two approaches, in the *Original* approach, the cropland BNF leads to prominent peaks
195 in the latitudinal distribution (Fig. 3 c). These peaks correspond to hot spots of legume crop production where the *C-costly* approach is up to 15 gN m^{-2} yr^{-1} lower (Fig. B4).

For natural vegetation, the differences are smaller and the BNF in the *Original* approach is only up to 4 gN m^{-2} yr^{-1} higher compared to the *C-costly* approach (Fig. B4). Here, the spatial patterns differ and show a stronger reduction of BNF in dry regions (e.g. central Australia, the Eurasian steppe regions, south east China and parts of Africa).

200 The various natural PFTs contribute differently to the lower overall BNF in the *C-costly* approach (Fig. B5 and B6). To some extent this reflects changes in the PFT distribution (Fig. S1 and 2). For the tropical PFTs, BNF is lower for the broadleaved raingreen tree ($\Delta 5.25$ TgN yr^{-1} Fig. B5 b) and the herbaceous PFT ($\Delta 14.1$ TgN yr^{-1} Fig. B5 i) and higher for the broadleaved evergreen tree ($\Delta 7.3$ TgN yr^{-1} Fig. B5 a). While the temperate needleleaved evergreen tree PFT contributed to biological N fixation in low latitudes outside its expected habitat (e.g. in India and Brasil) in the *Original* approach, this issue was resolved
205 with the *C-costly* approach (Fig. B5 c). The temperate PFTs all fix less N in the *C-costly* approach than in the *Original* approach. The reductions are smaller for the broadleaved evergreen ($\Delta 3.6$ TgNyr^{-1} Fig. B5 d) and summergreen ($\Delta 3.8$ TgNyr^{-1} Fig. B5 e) tree and the herbaceous PFT ($\Delta 4.7$ TgNyr^{-1} Fig. B5 j) compared to the needleleaved evergreen tree ($\Delta 9.1$ TgNyr^{-1} Fig. B5 c). The boreal PFTs' BNF is similar (Δ around 0.5TgNyr^{-1} Fig. B5 f,g,k) for all PFTs except the needleleaved summergreen tree ($\Delta 1.2$ TgNyr^{-1} Fig. B5 h), which fixes less N in the *C-costly* approach. In the *Original* approach, the temperate
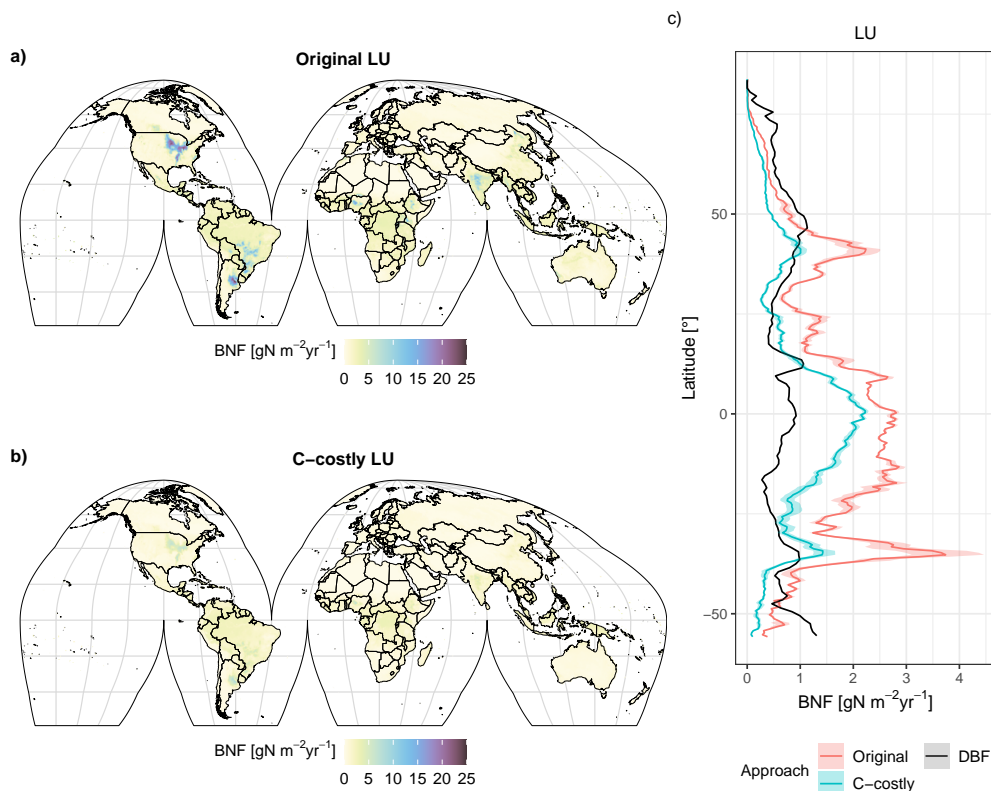
Figure 3. Simulated average annual BNF in $\mathrm{gNm^{-2}yr^{-1}}$ for years 2001 to 2010 using the *Original* (a) and *C-costly* (b) approach. Average (line) and 5th to 95th percentile (shading) of simulated BNF per latitude in $\mathrm{gNm^{-2}yr^{-1}}$ using the *Original* (red) and *C-costly* (blue) approach (c).

210 herbaceous contributed twice as much as in the *C-costly* to the biological N fixation of the polar vegetation (Fig. B5 j). For the pulses, the BNF was 14.6 $\mathrm{TgNyr^{-1}}$ and for soybean 6.4 $\mathrm{TgNyr^{-1}}$ lower with the *C-costly* approach.

3.2 Effects on the nitrogen cycle and productivity

In LPJmL the carbon and nitrogen cycles are coupled via, for example, the N limitation of gross primary productivity (GPP), which controls the amount of assimilated C, the role of plant organ carbon-to-nitrogen (C:N) ratios for maintenance respiration
215 and the availability of the resulting NPP for BNF. Additionally, the N content of the different plant organs (leaves, roots, sapwood, heartwood and storage organs) is derived dependent on the respective carbon content ensuring that their C:N ratios remain within a prescribed range. As a result, the N balance components presented in the following section are strongly shaped by their C cycle counterparts as the overall C and N balances represented by LPJmL are intimately linked.

We describe the N balance as the sum over in- and outfluxes of the vegetation and the soil. Therefore, the overall balance
220 contains a change in vegetation and soil N stocks including organic and mineral forms of N.
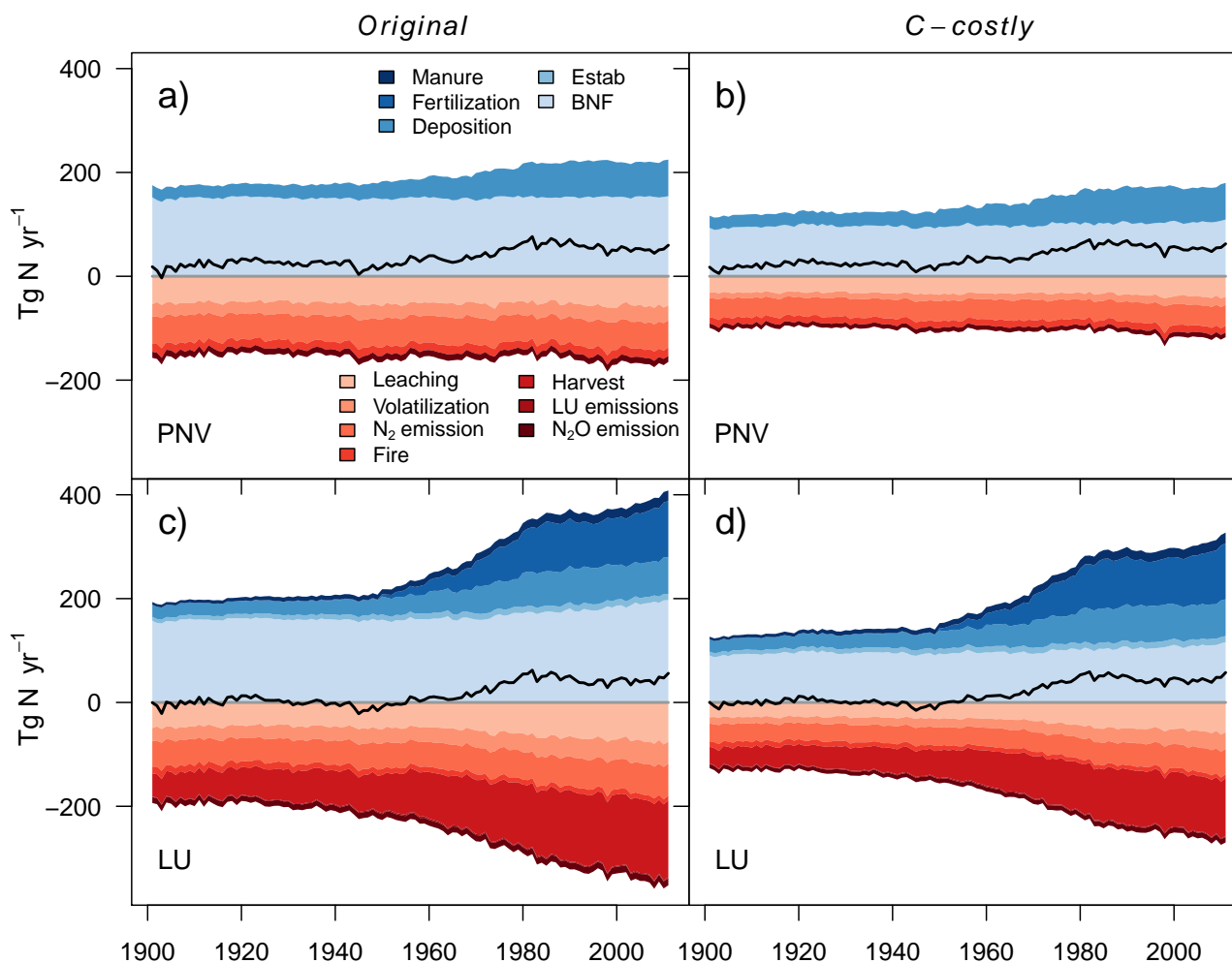
Figure 4. Global terrestrial N balance. Scenarios include the *Original* approach, the *C-costly* approach for natural vegetation and actual land use. Net balance is denoted by the black line. N losses include leaching, volatilization, N_2 emissions, fire N, harvested N, land-use change emissions (= deforestation, product turnover and timber harvest) and N_2O emissions from nitrification and denitrification.

3.2.1 Potential natural vegetation

Simulating only natural vegetation resulted in a positive terrestrial N balance with an average sink of 52 TgN yr^{-1} for the *Original* and 54 TgN yr^{-1} for the *C-costly* approach between 2001 and 2010 (Fig. 4 a, b and Tab. B1). In 1901, N in- and outputs were almost balanced and the sink remained small until the 1950s when N inputs from deposition increased resulting in an increased sink. While the overall N balance was similar for both BNF approaches, the size of several components was different. The total BNF simulated with the *Original* approach was approximately double that of the *C-costly* BNF leading to higher soil mineral N and organic C and N stocks. However, mineral N stocks were not utilised by the vegetation but instead

225

lost to the atmosphere and water bodies leading to higher N emissions and leaching using the *Original* approach. Here, 112 TgN yr^{-1} were emitted and 56 TgN yr^{-1} were leached on average between 2001 and 2010, while for the *C-costly* approach

230 only 79 TgN yr^{-1} were emitted and 39 TgN yr^{-1} were leached. Synchronised with the increase of deposition over time, emissions and leaching also increase in both approaches with stronger increases in the *C-costly* approach. Overall, N inputs increased by 35 TgN in total from 1950 to 2000 in the *Original* approach and by 42 TgN in the *C-costly* approach, while N losses from emissions and leaching increased by 1 TgN and 4 TgN respectively.

3.2.2 Dynamic land use

235 The simulations with dynamic land use include agricultural production and related additional N in- and outputs. Additional inputs are N from application of manure and synthetic fertilisers and additional outputs are N removed through crop harvesting, grazing and emissions from land-use change. The differences of the total BNF, soil mineral N and organic C and N stocks are similar to the PNV simulations. Between 2001 and 2010, LPJmL simulated an average N sink of 44 TgN yr^{-1} for the *Original* and 45 TgN yr^{-1} for the *C-costly* approach (Fig. 4 c, d, and Tab. B1). Already in 1901, the N balances of the PNV and dynamic

240 land-use simulations diverge. Since there are no synthetic fertiliser inputs in 1901, only the relatively small additional inputs from establishment and manure were counteracted by N removal through crop harvesting and land use change emissions, which shifts the total N balance towards a smaller source. This persists even after inputs from manure and fertiliser were increased starting in the 1950s, which not only resulted in higher crop yields and therefore N removed through harvesting but also increased N losses from emissions and leaching. As for the PNV simulations, the overall N balance is similar for

245 both approaches but with different in- and output terms driven by the higher BNF in the *Original* approach. N emissions and leaching for the *Original* approach (128 TgN yr^{-1} and 74 TgN yr^{-1}, resp.) were higher than for the *C-costly* approach (99 TgN yr^{-1} and 55 TgN yr^{-1}, resp.). N removal from harvesting was 142 TgN yr^{-1} on average between 2001 and 2010 for the *Original* and 108 TgN yr^{-1} for the *C-costly* approach. This indicates a stronger N limitation of agricultural areas in the *C-costly* approach. The majority of this reduction can be attributed to managed grassland and not croplands (Fig. S3 and 4).

250 ## 4 Discussion

The *C-costly* approach is not only conceptually superior to the simplistic *Original* approach in LPJmL, it also performs better in comparison to external data. Still, some mismatches with reference data remain, such as an overestimation of BNF in the tropics (Fig 3 c). However, the ensemble mean of a recent study evaluating the N cycle of eleven DGVMs shows a similar overestimation in the tropics and a large bias indicating little agreement between models (Kou-Giesbrecht et al., 2023). They

255 attributed this to the fact that BNF is typically modelled as a function of vegetation activity expressed either through NPP or evapotranspiration. Our results show that the overestimation of tropical BNF is reduced if temperature and water availability are considered as separate limitations, which supports their interpretation. Furthermore, the NPP that can be used for BNF depends on the overall productivity which certainly is higher in the tropics. It is likely that additional variables not considered in our approach constrain BNF there, such as phosphorus limitation (Vitousek, 1984; Lee et al., 2019). However, it has also been

260   suggested that as a result of higher N losses, tropical BNF should be higher than observations imply (Hedin et al., 2009). This could be a result of uncertainties inherent to BNF measurements (Soper et al., 2021) or the limited amount of data available from tropical ecosystems.

     Furthermore, simulated BNF was at the higher end of the range reported by Davies-Barnard and Friedlingstein (2020b) for the *C-costly* approach. One explanation is that Davies-Barnard and Friedlingstein (2020b) aggregate crop- and grassland areas
265   assuming their BNF rates are identical. However, a recent study provides evidence that BNF of crop legumes might actually be substantially higher than that of forage legumes (Herridge et al., 2022; Peoples et al., 2021) and therefore BNF of croplands and grassland cannot be assumed to be similar. Consistent with this, we also had to select much higher potential N fixation rates for the crop PFTs compared to the other PFTs to achieve sufficient cropland BNF (Tab. 1).

     We expected that limiting BNF of legume crops would result in stronger N stress and reduced yields. However, yields for
270   the legume crops were similar between the two approaches. One explanation is the direct link of maintenance respiration of a plant organ to its N content. Reducing the N that is taken up via BNF results in a lower organ N content and maintenance respiration and thus similar NPP. Indeed, C:N ratios are higher for the *C-costly approach* compared to the *Original* approach indicating a lower plant N content (Fig. B2).

     The average contribution of BNF to total N uptake was between 0 and approximately 25%, except in the main cropping
275   areas of legume crops, where the share of BNF was higher. The high share of low values (Fig. B7) indicates that available soil mineral N is still sufficient to fulfil plant N demand in many areas despite being half of that of the *Original* approach. We found a higher fraction of BNF for both the natural vegetation and the cropland in warm and dry areas (Fig. B8) where mineralisation of organic N is limited (Dessureault-Rompré et al., 2010).

     We expected that the differences in the BNF between the two approaches would be reflected by differences in the C stocks
280   and fluxes due to the close link of the C and N cycles in LPJmL. Both the C inflow into terrestrial C stocks from NPP and outflows from harvest and fire were lower in the *C-costly* approach, leading to a similar net C balance for the two approaches (Fig. S5). Because of the close link of the C and N cycles, the net N balance is also similar for the two approaches. The lower BNF in the *C-costly* approach results in lower N outfluxes, i.e. leaching, emissions, and harvests. The *Original* approach added mineral N to the soils of the natural vegetation even if the vegetation was not nitrogen limited. Legume crops that received all
285   N they demanded as in the *Original* approach returned high N content residues to the soil, increasing N inputs and mineral N stocks. As a result, the mineral N content of soils was higher in the *Original* approach, explaining the differences in yields and leaching. Similarly, soil mineral N content influences N emissions except fire emissions, which are controlled by the N content of the burned vegetation and litter. Since this also decreased, fire emissions were lower with the *C-costly* approach. In contrast to the lower BNF, which is in line with observations, N losses from leaching and emissions (from volatilization, denitrification,
290   nitrification, fire and land-use change) are underestimated by LPJmL simulations compared to observational data (see Tab. B1) in both approaches. While one source of differences is the missing representation of NO_x emissions in LPJmL, this is not sufficient to fully explain the difference. However, the models of the TRENDY-N ensemble also underestimated N losses from emissions of NH_3, N_2O, NO_x, and N_2, as well as leaching (Kou-Giesbrecht et al., 2023), suggesting that processes within DGVMs and scenario assumptions need to be revised. For LPJmL, we identified several potential causes: First, the manure

295 input accounts only for manure applied to cropland and the total amount is in line with other sources reporting cropland manure (Zhang et al., 2021) but does not account for manure added to grasslands other than the internal recycling by grazing animals (Heinke et al., 2023). Second, N losses and emissions strongly vary between different agricultural production systems whose representation would require not only the implementation of more detailed management options but also data sets on the spatial patterns of the application of different management specifics of these systems. Third, we conducted our simulations assuming

300 cover cropping outside the growing season on all croplands, which overestimates the extent of cover cropping and reduces N losses. However, data on cover cropping systems are not available (e.g., Porwollik et al., 2022).

While the *C-costly* approach improved simulation results for BNF as well as other components of the N balance and model results are in line with other DGVMs that represent the N cycle, we see potential for further improvement. The *C-costly* approach depends on multiple parameters some of which are not well constrained. Values for the potential N fixation rate vary

305 between species and across sites (Ma et al., 2022) and selecting one value to be representative for one PFT or even all PFTs of an entire climate zone is a strong simplification.

In addition, we assume a constant fraction of N fixers present in a community. However, the amount of N fixers changes over time dependent on N stress (Herben et al., 2017; Taylor et al., 2019). N fixation, the share of fixers and/or nodule abundance is low in undisturbed N-rich environments and nodules need to be produced to increase N fixation if N availability decreases

310 (Fisher et al., 2010; Crews, 1999). Similarly, N fixation does not cease instantaneously when N becomes more abundant but is only reduced after the share of fixers and/or nodule abundance has decreased (Thornley et al., 1995; Herben et al., 2017). In contrast, fixers are always present in LPJmL and can instantly fix N if necessary. Therefore, LPJmL likely simulates too quick adaptation to changing N availability and overestimates the short term capability of the community to buffer changes in N availability.

315 While our approach simulates the total amount of BNF well, it does not distinguish symbiotic from free living or heterotrophic N fixation. However, these are two different sources of N and their share of total BNF shows large spatial heterogeneity (Davies-Barnard and Friedlingstein, 2020a). In contrast to symbiotic BNF, free living BNF does not require NPP expenditures and separating the two may further improve simulation results for NPP and dependent variables.

5 Conclusions

320 Compared to the simplistic *Original* BNF implementation in LPJmL, the more complex *C-costly* approach as described here presents a substantial improvement of the representation of BNF in LPJmL. While the original approach led to an overestimation of BNF and was insensitive to soil temperature and soil water conditions, the *C-costly* approach overcomes these issues and can help to better project future BNF and its effects on N limitation of the terrestrial biosphere as well as losses of reactive N to the environment, including the greenhouse gas nitrous oxide (N_2O). Further research is needed, especially with respect to

325 balancing different in- and outfluxes and internal recycling rates. The current improvement of BNF simulations with LPJmL and the associated underestimation of loss terms exemplifies the scope of this problem. Our study highlights the importance of a detailed implementation of the processes controlling BNF for N cycling in DGVMs. While the *C-costly* approach already

improved simulations results, we think that additional benefits would be gained by explicitly separating BNF by symbiotic and free living bacteria and from accounting for the costs of other N uptake sources except passive N uptake.

330 *Code availability.* The source code of LPJmL in the exact form as described here is available at zenodo.org (Wirth et al., 2023) and on https://github.com/PIK-LPJmL/LPJmL.

Data availability. The historical climate data from the GSWP-W5E5 dataset are available from https://doi.org/10.48364/ISIMIP.982724 (Lange et al., 2022). The historical data of atmospheric N deposition and atmospheric CO2 concentrations can be obtained from https://doi.org/10.48364/ISIMIP.600567 (Yang and Tian, 2020) and https://doi.org/10.48364/ISIMIP.664235.2 (Büchner and Reyer, 2022), respectively.

335 All input data, model code, model outputs, and scripts that have been used to produce the results presented in this paper are archived at the Potsdam Institute for Climate Impact Research and are available upon request.

Appendix A: Spinup simulation carbon stocks
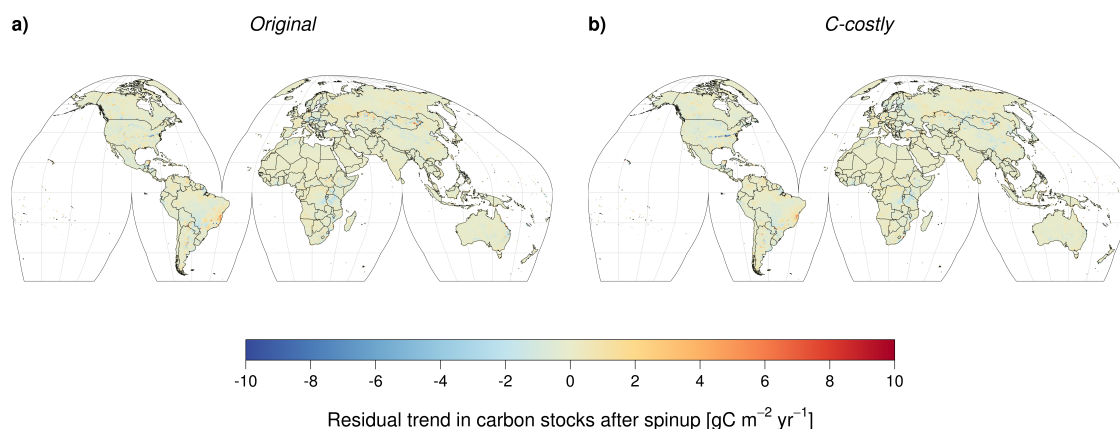
Figure A1. Residual trends in C stocks after the spinup simulation averaged over 1000 years for the Original (a) and the C-costly (b) approach.

With constant forcing (i.e., stable pre-industrial atmospheric CO_2 concentration, and atmospheric N deposition, and climate), the global carbon stocks showed a residual trend of -0.0106 $\mathrm{PgC\ yr^{-1}}$ for the *Original* approach and -0.0121 $\mathrm{PgC\ yr^{-1}}$

340 for the *C-costly* approach. This is 8-10 times lower than the steady-state criterion of 0.1 $\mathrm{PgC\ yr^{-1}}$ residual trend after spinup, which is used by the Global Carbon Project to validate DGVMs for inclusion in their global carbon budget analysis (Friedlingstein et al., 2022). At the grid cell level, the vast majority of cells (94 % for the *Original* approach and 95 % for the *C-costly*

approach) exhibited residual trends in total carbon stocks of less than $\pm 1 \text{ gC m}^2 \text{ yr}^{-1}$. The corresponding maps are shown in Fig. A1.

345 **Appendix B: Additional figures and tables**
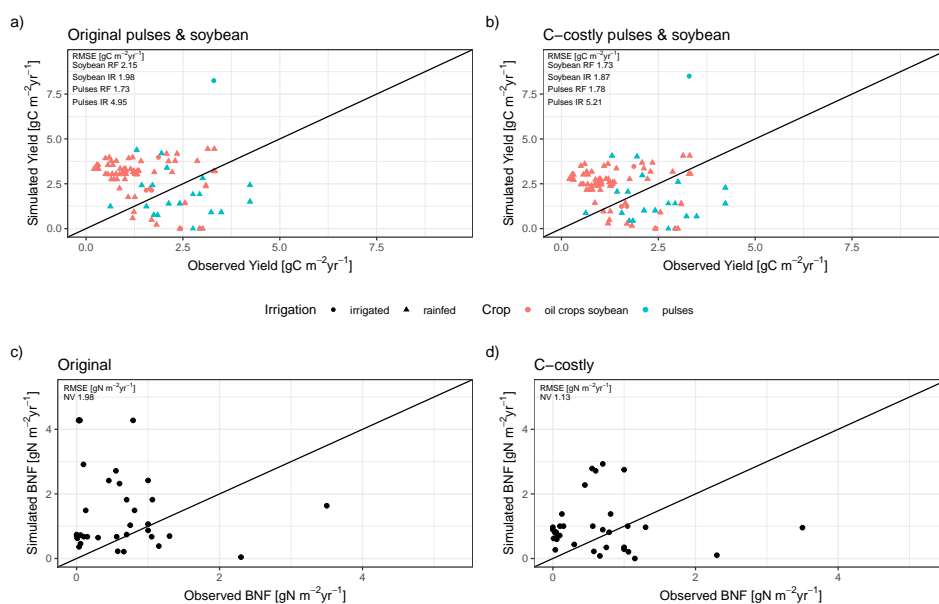
Figure B1. Simulated and observed crop yields (a,b) for soybean (red) and pulses (blue) and BNF in natural vegetation (c,d).

	Original	*C-costly*	Literature	*Original* PNV	*C-costly* PNV	Literature
N losses (TgNyr^{-1})	344	263		168	118	
Leaching	74	55	93[1], 68[2]	56	39	28.6[3]
Volatilization	43	32	-	31	17	-
N$_2$ emissions	60	47	68[1],64.2[2]	52	40	-
N$_2$O emissions	13	10	10.9[4],13[5],10[6],7.4-12.3[7]	12	9	-
Fire	10	8	-	17	13	-
Harvest	142	108	-	0	0	-
LUC	2	2	-	0	0	-
N gains (TgNyr^{-1})	388	307	-	220	172	-
BNF	191	110	see Fig. 2	153	104	19.8-107.9[8]
Establishment fluxes	12	12	-	0	0	-
Deposition	67	67	-	67	67	-
Fertilization	99	99	-	0	0	-
Manure	19	19	-	0	0	-
net balance (TgNyr^{-1})	44	45		52	54	

[1]Bouwman et al. (2013),[2]Zaehle et al. (2010),[3]Braakhekke et al. (2017), [4]Galloway et al. (2004),[5]Sutton et al. (2013),[6]Tian et al. (2019),[7]Tian et al. (2020),[8]Yu and Zhuang (2020)

Table B1. N balance values for 2001 to 2010 shown in figures. LUC includes deforestation emissions, product turnover and negative N fluxes
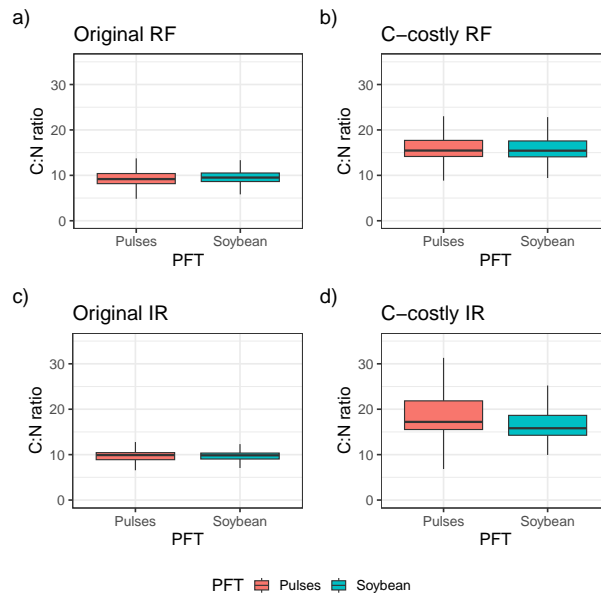
Figure B2. Vegetation C:N ratio for years 2001 to 2010 for rainfed (RF) and irrigated (IR) soybean (red) and pulses (blue) for the *Original* and *C-costly* approach.
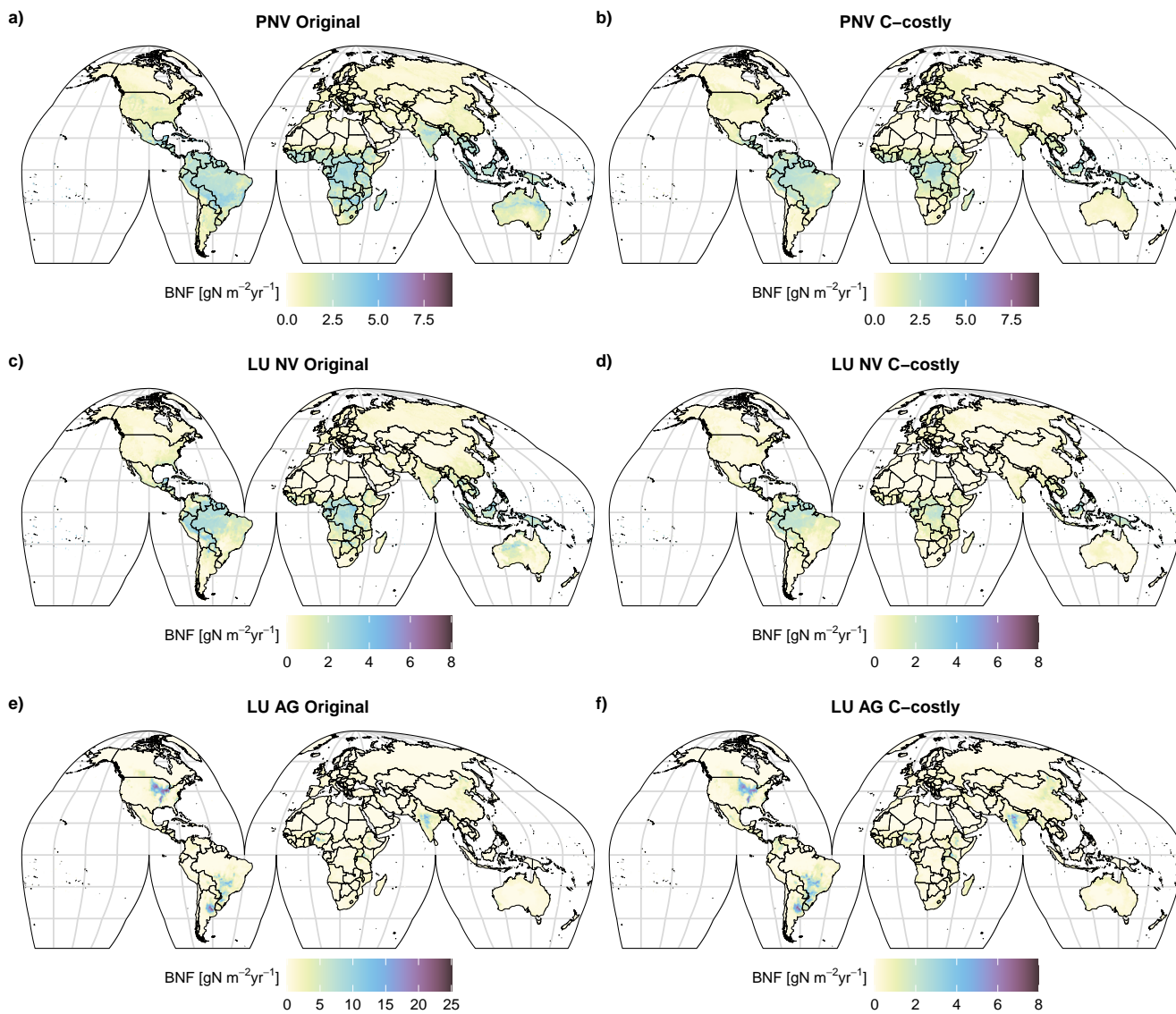
Figure B3. 2001 to 2010 average BNF in $gNm^{-2}yr^{-1}$ of the potential natural vegetation simulations (PNV) (a,b) and of the natural vegetation (NV) (c,d) and managed land (AG) (e,f) area fractions of the dynamic land-use (LU) simulations.
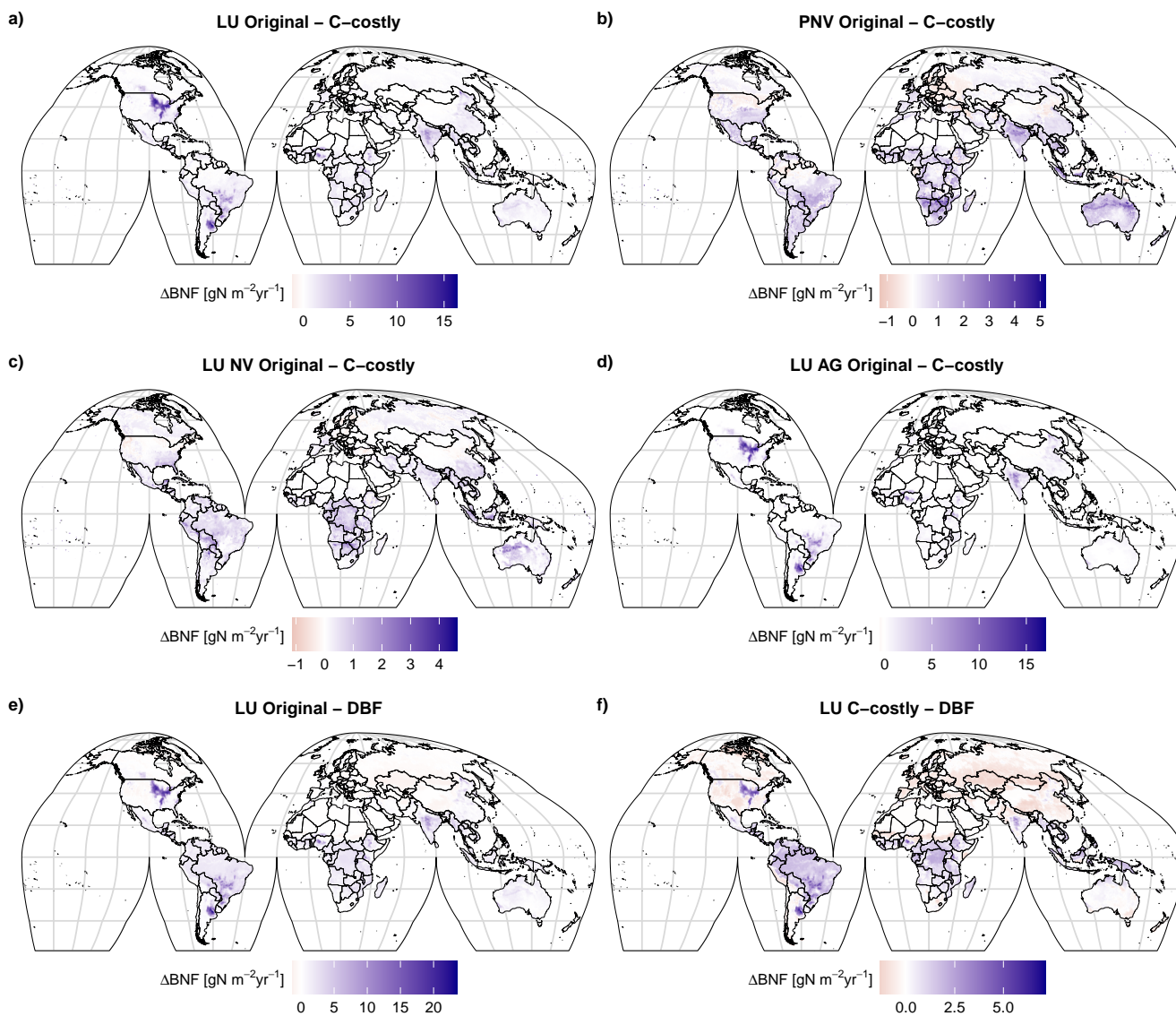
Figure B4. Difference between 2001 to 2010 average BNF in $\text{gNm}^{-2}yr^{-1}$ between the two approaches (a-d) for the dynamic land-use (LU) simulations (a), the potential natural vegetation simulations (PNV) (b), for the area fractions of natural vegetation (NV) (c) and managed land (AG) (e) of the dynamic land-use simulations and difference to the data from Davis-Barnard & Friedlingstein 2002 (DBF) (e,f).
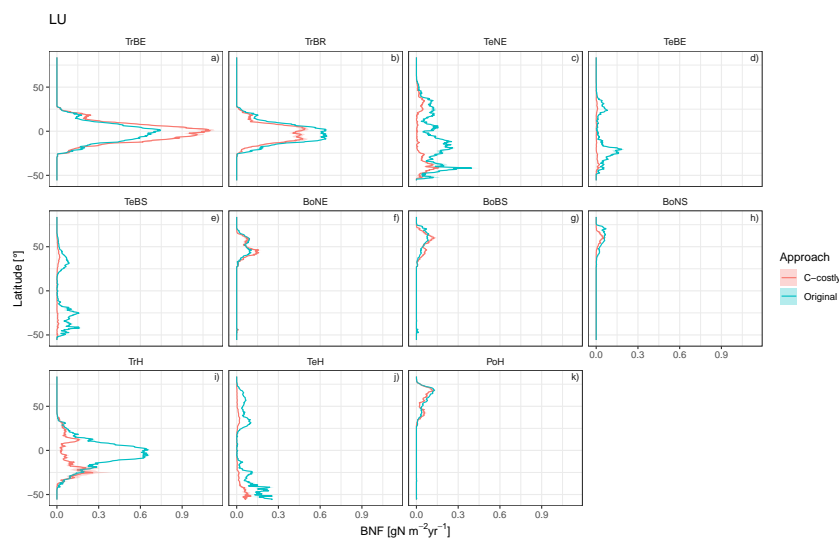
Figure B5. Latitudinal distribution of BNF for each PFT for the dynamic land-use simulations for the *Original* (red) and *C-costly* approach (blue).
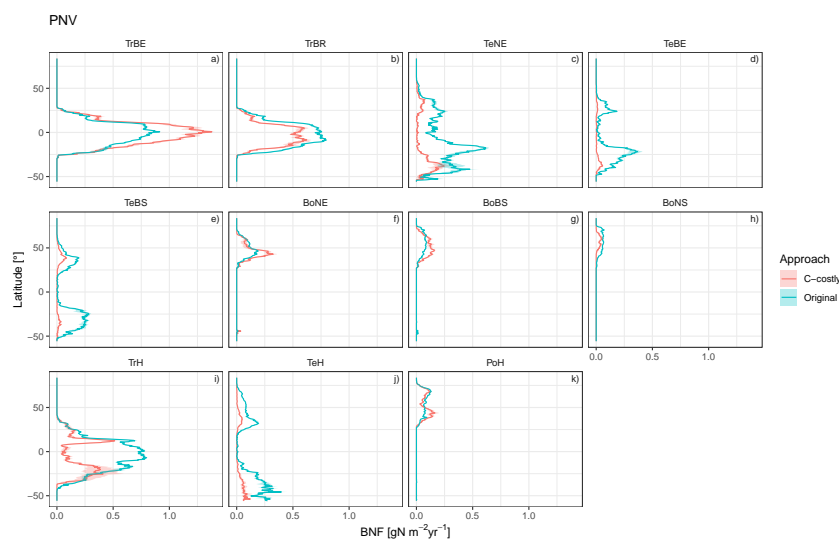
Figure B6. Latitudinal distribution of BNF for each PFT for the potential natural vegetation simulations for the *Original* (red) and *C-costly* approach (blue).
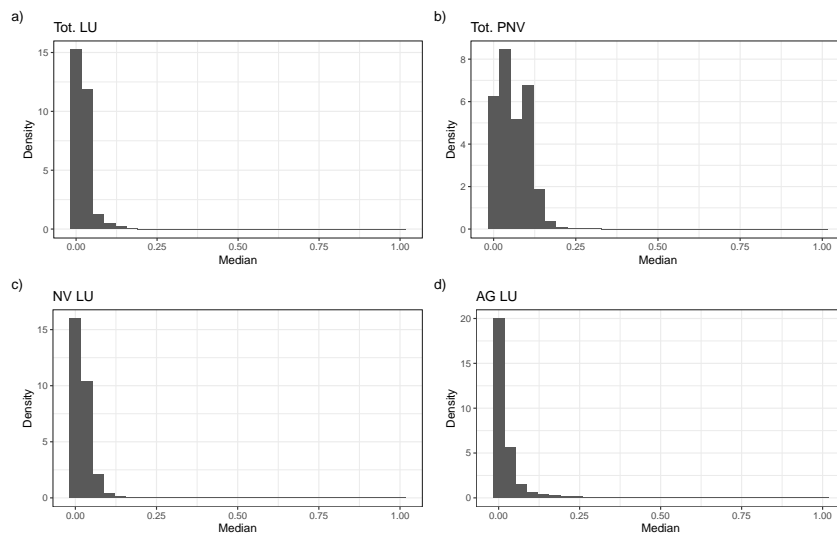
Figure B7. Density distribution of the fraction of BNF of total N uptake for the dynamic land-use (a), potential natural vegetation (b) and for the area fractions of natural vegetation (NV) (c) and managed land (AG) (d) of the dynamic land-use simulations.
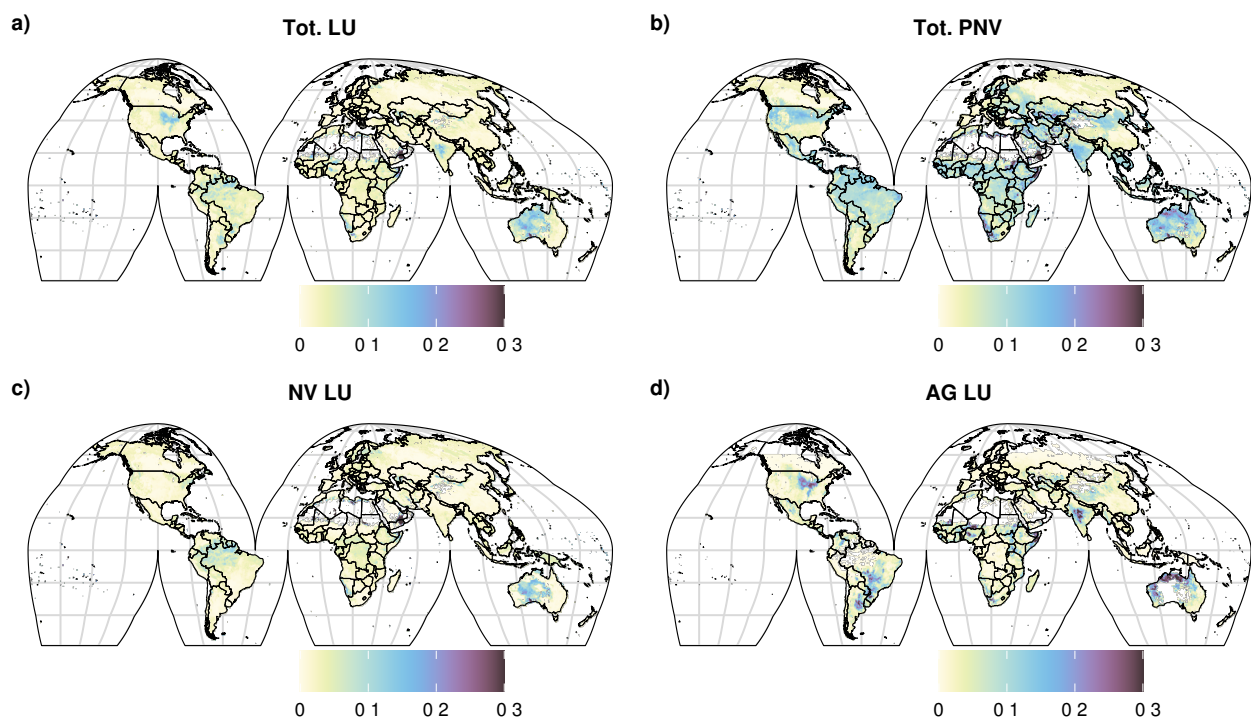
Figure B8. Global distribution of the fraction of BNF of total N uptake for the dynamic land-use (a) and potential natural vegetation simulations (b) and the natural vegetation (c) and managed land (d) fraction of the dynamic land-use simulation.

Author contributions. SBW, CM, FS, SR, Ssch and WvB designed the study. SBW designed and conducted the model implementation with inputs from CM, JB, SR, Ssch and WvB. All authors contributed to general model development and evaluation. SBW conducted the model simulations and wrote the original draft of the manuscript with inputs from CM, FS, SR, Ssch and WvB. All authors discussed the simulation results and the original draft, reviewed and edited the manuscript.

350 *Competing interests.* At least one of the (co-)authors is a member of the editorial board of Geoscientific model development.

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