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# Implications of a dynamic vertical root distribution for modelled water and carbon fluxes across selected ecosystems

Incorporating a novel rooting scheme into LPJ-GUESS

## Lasse Keetz

2019 Department of Physical Geography and Ecosystem Science Lund University Sölvegatan 12 S-223 62 Lund Sweden



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# Implications of a dynamic vertical root distribution for modelled water and carbon fluxes across selected ecosystems

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Lasse Keetz

Master thesis, 30 credits, in Physical Geography and Ecosystem Science

Paul Miller Lund University

David Wårlind Lund University

Exam committee: Veiko Lehsten, Lund University Mats Lindeskog, Lund University

## Abstract

Roots play a key role in terrestrial carbon and water cycles, and therefore for the global climate system. They mediate plant evapotranspiration, influence photosynthetic processes and are responsible for atmospheric carbon transport into the pedosphere. Fine roots in particular are chiefly regulating water and nutrient uptake. Recent research has suggested that the representation of fine roots in ecosystem models may be too simplistic to accurately represent vegetation responses to predicted environmental changes. Hence, this thesis explores the implications of incorporating a dynamic vertical root distribution into a global dynamic vegetation model (LPJ-GUESS) for the modelled water and carbon fluxes. In contrast to the current static root representation in LPJ-GUESS, root fractions per soil layers dynamically adapt to permafrost, and to soil water conditions if plants are under water stress. The different scheme outputs are contrasted and compared to observational data for gross primary production (GPP) and actual evapotranspiration (AET) from 15 FLUXNET sites representing a selected set of (Sub-)Arctic, water limited, and non-water limited ecosystems. Furthermore, the sensitivity of the new scheme to precipitation input and root reallocation rate is examined. It was found that the new rooting scheme leads to differences in both modelled fluxes and can locally improve model accuracy with regards to the observational data. The total root-mean-square error (RMSE) for mean annual fluxes is reduced using the new scheme (GPP: 0.62 vs. 0.58 kg C m-2 year-1 and AET: 144 vs. 138 mm year-1). However, other sites and biomes were better represented by the static scheme. It is therefore crucial to analyse local results carefully as many input factors not directly determined by the root representation influence the accuracy of modelled fluxes (e.g. dominating plant functional types). It must also be distinguished between monthly and annual flux model accuracy. In Arctic sites with low plant productivity, the new initial root distribution and dynamic adaptation to permafrost do not considerably change modelled fluxes. Moreover, a dynamic adaptation due to water stress and availability alone may be too simplistic. Further development of the novel rooting scheme is therefore needed which is aggravated by limited data availability.

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# **1** Introduction

## 1.1 Background

## 1.1.1 Roots and the rhizosphere

Belowground vegetation processes are often overlooked. In addition to the obvious sense that they are usually hidden from sight, for a long time they have also received relatively low attention from the scientific community in comparison to aboveground plant properties and mechanisms (Jochen Schenk 2005), especially in terms of their representation in ecosystem models (Warren et al. 2015). Over recent years, however, the importance of roots and their interactions with the environment, both above- and belowground, is increasingly recognized (Warren et al. 2015). The domain within soils where roots and their surroundings closely interact is referred to as the rhizosphere (Iversen et al. 2015). Accordingly, it is the region within soils where most biological and chemical processes take place (Schenk and Jackson 2005). There are various different types and functional or structural definitions of roots. In the most broad sense, they are often categorized as 'coarse' (cross-cut larger than 2 mm) and 'fine' (cross-cut smaller than 2 mm) (Blume-Werry et al. 2016). The former's main function is stabilization and storage, while the latter are short lived (*i.e.* frequently replaced ih a process called root turnover) and mainly responsible for resource acquisition (Iversen et al. 2015). Consequently, roots regulate plant water and nutrient uptake, fuel microbial activity, and alter soil structure (Schenk and Jackson 2005). Through root litter and exudates, photosynthetically assimilated carbon (C) is transported into the soil (Blume-Werry et al. 2016). Hence, roots also directly and indirectly affect atmospheric processes: they mediate plant evapotranspiration which chiefly regulates land surface energy and water balances (Warren et al. 2015). Moreover, they sequester C in soils and control a plant's ability to photosynthesize, therefore substantially influencing the atmospheric C balance (Iversen et al. 2015). Thus, there is also a direct link to recently observed climatic changes and reciprocal effects on the biosphere (IPCC 2014).

## 1.1.2 Relevance of roots for the climate system

To illustrate the importance of root-atmosphere interactions for the global C cycle, the relationship can be exemplified in northern high latitude ecosystems. There are various ways to classify the ecosystems in this region (Walker et al. 2005). In this the-

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sis, a rather broad definition is used: 'Arctic' refers to regions north of 70°N where arctic tundra vegetation is the dominant land cover and 'Subarctic' refers to regions between 50°N and 70°N where the land cover is dominated by boreal forests or taiga vegetation (Walker et al. 2005, and references therein). Accordingly, approximately 8% of the global land cover can be classified as Arctic tundra vegetation, even though exact definitions of the spatial extent vary among studies (McGuire et al. 2012). This biome is mostly comprised of short-statured flora growing on periodically frozen soil, frequently situated on permafrost (Walker et al. 2005). Permafrost by definition is ground that has a temperature at or below 0°C for at least two consecutive years. The thin soil layer that gets unfrozen in the summer is called the active layer, and the depth it extends into the soil is referred to as active layer depth (ALD) (see Hugelius et al. 2014). Accordingly, it was shown that an increase in active layer depth could alter vegetation compositions, *e.g.* deep rooted species such as gramminoids could get a competitive advantage and reach nutrients in currently frozen soil layers (Wang et al. 2016a).

A large portion of the biomass of Arctic tundra plant communities is located belowground - often more than 80% of the total plant biomass can be ascribed to roots. In boreal forests on the other hand, the fraction is 30% (Blume-Werry et al. 2016). Accordingly, a substantial amount of total terrestrial soil organic C – approximately 50% - is stored in the Arctic tundra pedosphere, which corresponds to roughly twice the current amount of C in the atmosphere (Iversen et al. 2015; Bradley-Cook and Virginia 2018). A recently observed warming in the Arctic, increasing atmospheric carbon dioxide (CO<sub>2</sub>) concentrations and coinciding permafrost degradation, trends which are predicted to exacerbate in the future (IPCC 2014), therefore illustrate the importance to understand and predict interactions between the biosphere, the rhizosphere and the climate. Increased temperatures and elevated CO<sub>2</sub> levels have direct and indirect effects on ecosystem processes relevant for the regional C cycles such as plant productivity, respiration rates, previously frozen soil C that becomes available for microbial decomposition through thawing permafrost, and nutrient cycling (Schuur et al. 2008). However, large quantitative uncertainties about the interconnection of these processes and how they will react to future developments remain (McGuire et al. 2012).

This thesis therefore aims at reducing this knowledge gap on a more global scale. More precisely, it will try to improve the representation of root structure and dynamics in an ecosystem model. Consequently, the mechanistic understanding of processes related to roots, and the ability to make future predictions about vegetation responses to environmental changes could be enhanced. The following sections will explain this in more detail.

## 1.2 Ecosystem modelling

One approach to study vegetation dynamics and ecosystem reactions to environmental parameters are process-based ecosystem models. The complexity and applications of available models vary considerably (Iversen et al. 2015; Warren et al. 2015), but they all share the same underlying principle to accurately represent ecosystem processes using mathematical approximations. For instance, plants annually cycle more than one third of atmospheric  $CO_2$  of which approximately 50% is assimilated through photosynthesis and are therefore an important driver of the global carbon cycle (Sitch et al. 2003). The growth of plants (through photosynthesis) and corresponding C uptake, transport to the soil and release through respiration can be estimated derived from experiment, theory or both. One sophisticated type of ecosystem model to study vegetation dynamics on large temporal and spatial scales are process-based dynamic global vegetation models (DGVM). They couple mathematical abstractions of biogeochemical processes and vegetation structure and -composition to *e.g.* simulate plant growth and competition for resources over time (Sitch et al. 2003).

## 1.2.1 LPJ-GUESS

The ecosystem model used in this thesis is the latest version of the Lund-Potsdam-Jena General Ecosystem Simulator (LPJ-GUESS r7539) (Smith et al. 2001, 2014). The dynamic vegetation model is designed to provide optimized results for studies on global and regional scales. A description of the updated version including various modifications such as a new set of plant functional types (PFT) can be found in Ahlström et al. (2012). Moreover, the model incorporates a scheme for soil water freezing (Zhang et al. 2013). A PFT is a group of plant species which share similar structural, life-strategy and biogeochemical features. For example, PFTs differ in the following attributes: growth form, phenology, photosynthetic pathway ( $C_3$  or  $C_4$ ), bioclimatic limitations for establishment and survival, and, in case of woody PFTs, allometry. In LPJ-GUESS, vegetation dynamics and corresponding ecosystem processes are represented as follows: a modifiable number of *n* **patches** (area of 0.1 ha) is

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assigned to a stand (area of 10ha - 2500 km<sup>2</sup>) which represents the overall vegetation composition in a specific grid cell location. Each patch therefore depicts a 'random sample' of the locality, i.e. a number of PFTs that are able to grow in the given conditions in order to account for effects of local disturbances and differences in stand age (Figure 1). In this thesis, the 'cohort' mode of LPJ-GUESS is used. Here, in the case of woody PFTs, one average single individual represents an entire cohort of individuals growing in the same patch. Primary production and plant growth are simulated according to the approach of LPJ-DGVM (Sitch et al. 2003) that was extended by the implementation of nitrogen cycling (Smith et al. 2014). The net primary production (NPP) that is simulated for each average individual is partitioned to leaves, fine roots and, for woody PFTs, sapwood. Here, each PFT has its own set of allometric relationships that determine biomass acquisition, height and diameter growth (Sitch et al. 2003, see Figure 1). Plant recruitment and mortality (i.e. population dynamics) are stochastic processes, influenced by current resource availability, plant age and the life history characteristics of each PFT. Furthermore, vegetation composition is determined by the plants' competition for resources (e.g. incoming radiation based on canopy properties). Figure 1 depicts a schematic representation of the most important principles.

## 1.2.2 Motivation for a new rooting scheme

A growing body of research over recent years suggests that various current mechanistic vegetation models do not capture key processes related to roots (Iversen et al. 2015) and are therefore limited to make predictions for future, possibly more stressful, environments (Warren et al. 2015). For instance, Warren et al. (2015) suggest to incorporate spatial and temporal dynamics for root productivity based on specific root traits and environmental conditions in the soil. Wang et al. (2016b) conclude that accurate implementation of vertical root distribution is crucial for hydrological, ecological and climatic simulations.

In its current implementation, LPJ-GUESS utilizes a static rooting scheme. In general, a PFT specific amount of totally assimilated plant C is assigned to root growth. The investment of C to fine roots while growing is mainly constrained by water and nitrogen stress and a maximum leaf-to-root mass ratio. Moreover, fine roots can act as a C reserve for leaves in times of stress. For more details refer to Sitch et al. (2003). The amount of water that is taken up by the plants is thereby determined by the

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Figure 1: Vegetation representation in LPJ-GUESS cohort mode. This scheme represents an earlier version of the model which only used two soil layers (15 in the one used in this thesis). Adapted from Smith et al. (2014).

availability per soil layer and the fraction of fine roots in those layers. The root fraction distributions per soil layer in the static rooting scheme employed in this thesis only vary among three different plant functional groups: shrubs and trees, grass and low shrubs (Figure 2). The respective fractions are identical in the soil layers from 0-50 cm and 50-150 cm, respectively, as earlier versions of LPJ-GUESS represented soil dynamics with only two layers. Plus, they remain constant even under changing environmental conditions. For instance, they can be assigned to permanently frozen soil layers. Therefore, the new rooting scheme that is developed in this thesis aims at incorporating a more sophisticated root representation. It follows a similar mathematical approach as proposed by Wang et al. (2016b, 2018) which was developed for the Community Land Model (CLM). In their concept, fine roots are dynamically redistributed based on resource availability, more precisely on a compromise between water and nitrogen occurrence per soil layer (Wang et al. 2018). However, in contrast to CLM 4.5, LPJ-GUESS does currently not incorporate vertical distribution of nitrogen in the soil and root growth takes place annually as opposed to daily. Therefore, the dynamic root fraction reallocation was adapted to the LPJ-GUESS framework: the vertical root distribution is determined by water stress and water availability, and a

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standard root distribution based on empirical studies (Zeng 2001) if water conditions are not limiting. Thus, if an individual is under water stress conditions, a larger fraction of the roots is allocated in soil layers with higher water availability. The current, static implementation will henceforth be referred to as *SI*, the new, dynamic implementation will be referred to as *DI*.

Water availability is the most limiting factor in various ecosystems and strongly correlates with plant growth and survival. It is mainly determined by precipitation and evapotranspiration, and locally by soil characteristics and topography (Olmo et al. 2014, and references therein). Consequently, water availability in a specific location can also vary substantially over time, for instance with changes in mean annual precipitation (MAT). Plants and vegetation compositions will therefore be affected by future changes in precipitation patterns (Olmo et al. 2014). According to IPCC (2014), while average annual rainfall is expected to increase in the majority of locations in the future, especially mid-latitude and subtropical dry regions will likely deal with a significant decrease in precipitation. Aridity may furthermore increase in some places due to projected rises in temperature alone, independent of changes in precipitation (IPCC 2014). Many plant species react to aridity and drought by relatively higher investment in root biomass as opposed to shoot biomass. Thus, transpiration rates are reduced while simultaneously soil exploration and water acquisition are enhanced (Olmo et al. 2014). This has also been shown to influence the vertical distribution of roots. In times of drought, evapotranspiration causes a reduction of soil water in upper soil layers. Numerous species react by enhanced root growth in wetter soil layers (Cattivelli et al. 2008). For instance, Olmo et al. (2014) showed that 10 woody species shifted their vertical root distribution towards higher proportions in deeper soil layers under experimental drought conditions and Tsutsumi et al. (2002) illustrate a strong response of vertical root structure to punctual irrigation for Glycine max (soybean).

The aforementioned findings provide the theoretical basis for the new root representation. According to the presented physiological functions of roots and their representation in LPJ-GUESS, it is furthermore hypothesized that a change in vertical root distribution will have an impact on modelled C and water fluxes. This may have significant effects on a global scale - therefore, the implications of the new rooting scheme are tested across several selected ecosystems with a special focus on (Sub-)Arctic and water limited sites. For a schematic representation of the approach refer

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to Figure 3. All relevant assumptions and equations, including a description how water stress is determined, are presented in the methods.

## 1.3 Aim and justification

To summarize, this thesis aims at exploring the potential benefits of including a dynamic root redistribution in response to environmental change in an ecosystem model (LPJ-GUESS) as *e.g.* discussed by Iversen et al. (2015). It depicts an exploratory attempt at addressing the following questions:

- 1. How can a dynamic vertical root redistribution based on water stress and water availability affect carbon and water fluxes across various biomes with a special focus on water limited locations?
- 2. How does this new rooting scheme affect the performance of modelled gross primary production (GPP) and actual evapotranspiration (AET) fluxes in relation to observational field data?
- 3. How does a dynamic adaptation of the vertical root distribution to frozen soil and permafrost affect carbon and water fluxes in Subarctic and Arctic locations?

Tackling these questions is crucial as recent research has indicated that the representation of roots in current ecosystem models, and in LPJ-GUESS in particular, may be too simplistic for the more stressful environmental conditions projected for the future (IPCC 2014; Iversen et al. 2015; Wang et al. 2018). Moreover, in earlier versions of LPJ-GUESS, the vertical rooting profile of a PFT is based on a categorization into one of three plant functional groups with fixed root fractions per soil layer. However, empirical studies are available that provide parameter based root distributions for a wider set of PFT and soil layers. It was shown that incorporating these findings can improve model accuracy (Zeng 2001). Enhancing the performance of ecosystem models through improving root representation could ultimately lead to more robust predictions of the C balance between the biosphere and the atmosphere. As a consequence, projections for future climate scenarios would become more accurate (Iversen et al. 2015). Furthermore, in the current implementation of LPJ-GUESS, vertical root distribution is not affected by permafrost. A dynamic adaptation is hypothesized increase the root fractions in the (active) upper soil layers which may affect model performance in Arctic regions, which are of special importance for the global climate

system due to the large amount of C stored in the soils (Bradley-Cook and Virginia 2018).

## 2 Methods

## 2.1 Novel dynamic rooting scheme

## 2.1.1 Initial vertical root distribution

The static rooting scheme in the version of LPJ-GUESS used in this thesis assigns fixed root fractions to individuals in each of the 15 soil layers. In this case, there are different distributions for three plant functional groups (PFG): Shrubs and trees, grass and low shrubs (Figure 2, see Table S1 for corresponding PFTs in the model), but different root fraction assignments have also been utilized (see e.g. Sitch et al. 2003). As in previous model versions the soil and hydrological processes were represented using only two layers, the first two mentioned PFGs have identical fractions in soil depths from 0 to 0.5 m and 0.6 to 1.5 m, respectively. A more advanced approach was implemented for low shrubs. Refer to (Sitch et al. 2003) for a detailed description of root and soil dynamics in the model.



Figure 2: Current static root fractions (a) and the initial root fractions of the new dynamic rooting scheme (b) per current model version soil layer (15 layers, each with a depth of 10 cm) for different plant functional groups in LPJ-GUESS. Refer to the appendix (Table S1) for corresponding plant functional types.

The initial vertical root distribution and, accordingly, the distribution under no water stress of the new dynamic scheme follows a more advanced approach as proposed

by Zeng (2001). It builds upon an empirical global root distribution model from Jackson et al. (1996) and was shown to more accurately capture the maximum rooting depths of plants while maintaining the same root fractions in the upper soil layer (*i.e.* both mentioned models have identical root fractions up to a depth of 0.1 m which corresponds to the top layer in LPJ-GUESS). Consequently, the performance of land surface models in various biomes could be improved (Zeng, 2001). The function to calculate the cumulative root fraction  $Rf_Z(d)$  is given as:

$$Rf_Z(d) = 1 - \frac{1}{2}(e^{-ad} + e^{-bd})$$
(2.1)

where *d* is the soil depth in meters, and *a* and *b* are PFT specific parameters (Zeng 2001, see Table S1). To obtain the respective non-cumulative fraction in each soil layer  $Rf_{Z,i}(d)$ , the following formula is used:

$$Rf_{Z,i}(d_i) = Rf_Z(d_i) - Rf_Z(d_{i-1})$$
(2.2)

where *i* is the soil layer under the constraint that  $Rf_{Z,i}(d_i) = Rf_Z(d_i)$  for i = 1. If the maximum rooting depth of a PFT exceeds the maximum soil layer depth of LPJ-GUESS (in this version: 1.5 m), the root fractions are normalized as follows so that they sum to 1:

$$Rf_{Z,i,normalized} = \frac{Rf_{Z,i}(d_i)}{\sum_{i=1}^{n} Rf_{Z,i}(d_i)}$$
(2.3)

where *n* is the total amount of soil layers. As a consequence, the differences between PFT root distributions are somewhat smaller compared to Zeng (2001). However, maximum rooting depths are flexible regarding possible future model updates with deeper soil layers.  $Rf_{Z,i,normalized}$  and  $Rf_{Z,i}$  will hereafter be used interchangeably.

#### 2.1.2 Water stress

In accordance with Wang et al. (2016b), a factor  $\beta_t$  is utilized to approximate water stress for plants. In this case, it is based on the ratio of leaf intercellular to ambient  $CO_2$  concentration, which is utilized as a proxy for the daily water stress (Sitch et al. 2003). More precisely, it builds upon the fact that stomatal conductance strongly correlates with a deficit of water vapor pressure, which can also be linked to changes in the mentioned ratio (Tan et al. 2017). A  $\lambda_{max}$  (0.8 for C<sub>3</sub> plants and 0.4 for C<sub>4</sub> plants, *i.e.* 

according to their respective photosynthetic pathway) value is assigned to each PFT which denotes the optimal partial pressure ratio under no water stress. Subsequently, a daily partial pressure value  $\lambda$  ( $0 \le \lambda \le \lambda_{max}$ ) is determined based on hydrological conditions during the growing season (see next subsection). The growing season water stress value used for the new rooting scheme is therefore calculated at the end of each simulation year as:

$$\beta_t = \frac{\sum \lambda \ GPP_{ns} / \sum GPP_{ns}}{\lambda_{max}}$$
(2.4)

where  $\sum \lambda \ GPP_{ns}$  is the annual sum of daily  $\lambda$  times the potential GPP under no water stress condition ( $\lambda$ ) and  $\sum GPP_{ns}$  is the potential GPP that would be obtained without taking water stress into account (*i.e.*  $\sum \lambda \ GPP_{ns} \leq 0.8 \sum GPP_{ns}$  for C3 plants and  $\sum \lambda \ GPP_{ns} \leq 0.4 \sum GPP_{ns}$  for C4 plants). Therefore,  $0 \leq \beta_t \leq 1$  is the water stress scalar over the growing season with a higher  $\beta_t$  denoting higher water availability and thus better growing conditions for the plant.

## 2.1.3 Water availability per soil layer

An annual mean water content for the growing season  $w_{gs,i}$  (hereafter also referred to as GSWC) is calculated for each of the 15 soil layers. Here, *w* denotes the water content as a fraction of available water holding capacity (see Sitch et al. 2003). Accordingly, the more a plant is under water stress, the more proportion of C is assigned to root layers where relative water availability during the growing season was high. A growing season day is defined as a day with ambient air temperature  $T > 5^{\circ}C$ where root redistribution is assumed to occur. Mean growing season water content is therefore calculated as:

$$w_{gs,i} = \begin{cases} \frac{1}{d_{gs}} \sum_{k=1}^{d_{gs}} w_{d,i} & , d_{gs} > 0\\ 0 & , d_{gs} = 0 \end{cases}$$
(2.5)

with *i* being the respective soil layer, *k* being individual growing season days,  $d_{gs}$  being the total amount of growing season days and  $w_{d,i}$  being the daily water content on a growing season day in the corresponding soil layer. Consequently,  $0 \le w_{gs,i} \le 1$ .

#### 2.1.4 Dynamic root allocation

Fine root growth takes place at the end of each simulation year. To take the vertical distribution of the previous year into account, it is assumed that fine root longevity

(see Sitch et al. 2003) partly determines the new year's root distribution, unless root longevity is shorter than 1 year. The amount of C associated with the roots is therefore divided into two variables: one denoting this year's root growth ( $C_{inc}$ ) and one containing the total root C ( $C_{tot}$ ; new growth plus remaining C from previous years). The updated fraction of C in a soil layer  $C_{fr,i}$  is calculated as follows:

$$C_{fr,i} = \left[ (1 - \beta_t) \frac{w_{gs,i} \Delta z_i}{\sum_{i=1}^n w_{gs,i} \Delta z_i} + \beta_t R f_{Z,i}(d_i) \right] \cdot C_{inc} + \left[ (C_{tot} - C_{inc}) \cdot R f_i \right]$$
(2.6)

where  $\Delta z_i$  is the difference of the depths of soil layer *i* and soil layer *i* – 1 (in meters) to account for possible differences in soil layer depth of future releases, n is the number of soil layers and  $Rf_i$  is the root fraction of layer *i* in the previous year. Therefore, if a plant is under water stress ( $\beta_t < 1$ ), the fraction of available soil water in a soil layer (in relation to the sum of GSWC in all layers) will partly determine the fraction of roots that is assigned to that layer. For instance, during drought conditions when the top layers' water content is depleted (Olmo et al. 2014), the weighting ratio for water availability (as per fractional GSWC) will be higher in lower layers and a higher root fraction will be assigned here. Consequently,  $\beta_t$  acts as a weighting factor that determines whether root fraction allocation will be determined by soil water availability or the standard root distribution. Thus, on the contrary, the less a plant is water limited, the more the resulting distribution will be determined by the initial (optimum) Zeng (2001) distribution  $Rf_{Z,i}(d_i)$  per soil layer. Additionally, in order to avoid root growth in frozen soil, one additional constraint was implemented which affects the dynamic reallocation independent of water stress. For all layers  $d_i$  with a depth *i* situated below the active layer depth (ALD), the root fraction becomes zero:

$$\forall Rf_i \mid i > ALD : Rf_i = 0 \tag{2.7}$$

If at least one soil layer was permanently frozen over the year, the fractions in the other ones are normalized based on the proportion of total C in the unfrozen layers (Equation 2.8). Finally, the new root fractions in each soil layer are updated as follows:

$$Rf_{i} = \frac{C_{fr,i}}{\sum_{i=1}^{n} C_{fr,i}}$$
(2.8)

Refer to Figure 3 for a schematic representation of the assumptions and principles of the new rooting scheme.





Figure 3: Schematic representation of the novel root distribution algorithm DI.

## 2.2 Model setup and adaptations

This section briefly describes utilized important run options for LPJ-GUESS and the adaptations that were made for the implementation and output of the novel rooting scheme. For more details refer to (Smith et al. 2014). All simulations were executed for n = 10 patches using the cohort mode of LPJ-GUESS (Smith et al. 2001). The model spin-up phase was 500 years. Here, a 30 year climate input obtained from the beginning of the historic simulation period is cycled repeatedly. During this period, vegetation C and nitrogen (N) pools are established and reach an equilibrium state with the climate at the beginning of the historic simulation period (year 1900). The dynamic root reallocation only takes place after the spin-up phase of the model. Simulations included fire and random disturbances, *i.e.* generic patch-destroying events that eliminate all living vegetation while litter remains. The vegetation water uptake

in the model is based on patch PFT properties, therefore a mean patch PFT root fraction (*i.e.* of all individuals belonging to the same PFT in a patch) per soil layer is calculated. The adapted model output for each simulation year includes the water stress factor  $\beta_t$ , and for each soil layer: mean root fractions per PFT, a total mean root fraction (arithmetic mean of PFT root fractions; used for analysis in this thesis) and a mean GSWC across patches.

## 2.3 Data

This section describes the data and the preprocessing that was used to drive the model and to evaluate the model output. For a more detailed description of the data used for processes in LPJ-GUESS refer to Smith et al. (2014) and Sitch et al. (2003).

## 2.3.1 Climate forcing data

LPJ-GUESS requires climate forcing input data to drive ecosystem processes. The data sources and handling of the annual atmospheric CO<sub>2</sub> concentrations (derived from observations) and the monthly N deposition rates are described in Smith et al. (2014). The input for monthly precipitation, temperature and radiation in this thesis, however, combines a global data set and regional input for the chosen observational data sites. The CRUNCEP data set (Viovy 2018) spans the entire ice-free global land surface on a  $0.5^{\circ} \times 0.5^{\circ}$  (latitude, longitude) grid. It merges meteorological information of the CRU (mean monthly values at  $0.5^{\circ} \times 0.5^{\circ}$  resolution) and the NCEP (6-hourly values at  $2.5^{\circ} \times 2.5^{\circ}$  resolution) data sets and is therefore widely used for modelling purposes (e.g. Wang et al. 2016b). Moreover, the FLUXNET sites used in this thesis (see subsection 2.3.2) provide climatic data measured in situ. This locally optimized information is used to bias correct the input of the nearest CRUNCEP grid cell as follows: a mean error between the FLUXNET and the CRUNCEP data is calculated for the available observational period. Subsequently, this mean error is uniformly subtracted from the CRUNCEP input of the entire historical model simulation period (1900-2015). This assumption therefore aims at improving the climate input parameters for each site individually.

### 2.3.2 Carbon and water flux data

The FLUXNET2015 data set (freely available at https://fluxnet.fluxdata.org (accessed 05-10-2019), see Baldocchi et al. 2001; Pastorello et al. 2017) was utilized to relate the



Figure 4: Locations and identifiers of the utilized FLUXNET data sites.

model output of the different rooting schemes to observational data. FLUXNET is a scientific network measuring atmospheric state variables (e.g. air temperature, humidity, CO<sub>2</sub> fluxes, incoming and outgoing radiation) continuously at more than 900 sites across the globe. This thesis examines the effect of a dynamic root distribution on carbon and water fluxes across biomes with a special focus on water limited and Arctic sites. Hence, sites which fulfill these criteria were identified based on their location (Figure 4), site description, mean annual precipitation (MAP) and mean annual temperature (MAT). Additionally, some sites without water limitation were added to explore the influence of the new rooting scheme on other biomes (e.g. GF-Guy, see Table 1). Furthermore, sites were selected based on long term data availability (at least 10 years) to improve statistical robustness of the results. One exception to this is the site RU-SkP (Takata et al. 2017) which was added due to the fact that it is the only FLUXNET site where the vegetation is classified as DNF (deciduous needleleaf forest, *i.e.* larch forest) that can also be affected by frozen soil layers during the early growing season. In total, 15 sites were selected. Their names and available meta data are shown in Table 1. To evaluate carbon and water fluxes, the following measured variables were compared to the model output data:

1. Monthly gross primary production (GPP)

Gross primary production (GPP) is defined as the total amount of C that is assimilated by plants through photosynthesis (Hatfield and Dold 2019). GPP can therefore be expressed as the difference between net ecosystem exchange (NEE, *i.e.* net C flux from the biosphere to the atmosphere) and ecosystem respiration

 Table 1: Meta data for the FLUXNET sites used in this thesis (NA = data not available). For details refer to Pastorello et al. (2017). IGBP denotes respective vegetation land cover classification (Loveland and Belward 1997): Savanna (WSA), Evergreen needleleaf forest (ENF), Evergreen broadleaf forest (EBF), Deciduous needleleaf forest (DNF), Grassland (GRA) and Shrubland (OSH).

Site ID	Site name	Data start*	Data end*	Lat [°]	<b>Lon</b> [°]	Elevation [m.a.s.l.]	IGBP	MAT [°C]	MAP [mm yr <sup>-1</sup> ]
(Sub-)Arctic									
CA-Obs	Saskatchewan - Western Boreal Mature Black Spruce	Tier2: 1997	Tier2: 2010	53.99	-105.12	628	ENF	0.79	406
DK-ZaH	Zackenberg Heath	Tier1: 2000	Tier1: 2014	74.47	-20.55	38	GRA	-9	211
FI-Hyy	Hyytiala	Tier1: 1996	Tier1: 2014	61.85	24.29	181	ENF	3.8	709
RU-Cok	Chokurdakh	Tier1: 2003	Tier1: 2014	70.83	147.49	48	OSH	-14.3	232
RU-Fyo	Fyodorovskoye	Tier1: 1998	Tier1: 2014	56.46	32.92	265	ENF	3.9	711
RU-SkP	Yakutsk Spasskaya Pad larch	Tier2: 2012	Tier2: 2014	62.26	129.17	246	DNF	NA	NA
Other									
AU-How	Howard Springs	Tier1: 2001	Tier1: 2014	-12.49	131.16	NA	WSA	NA	NA
FR-Pue	Puechabon	Tier1: 2000	Tier1: 2014	43.74	3.6	270	EBF	13.5	883
GF-Guy	Guyaflux (French Guiana)	Tier1: 2004	Tier1: 2014	5.28	-52.92	48	EBF	25.7	3041
IT-MBo	Monte Bondone	Tier1: 2003	Tier1: 2013	46.01	11.05	1550	GRA	5.1	1214
IT-Ren	Renon	Tier1: 1998	Tier1: 2013	46.57	11.43	1730	ENF	4.7	809
US-SRM	Santa Rita Mesquite	Tier1: 2004	Tier1: 2014	31.82	-110.87	1120	WSA	17.92	380
US-Ton	Tonzi Ranch	Tier1: 2001	Tier1: 2014	38.43	-120.97	177	WSA	15.8	559
US-Var	Vaira Ranch - Ione	Tier1: 2000	Tier1: 2014	38.41	-120.95	129	GRA	15.8	559
US-Wkg	Walnut Gulch Kendall Grasslands	Tier1: 2004	Tier1: 2014	31.74	-109.94	1531	GRA	15.64	407

\*Tier1 and Tier2 refer to different data use policies and indicate which data set was used.

(RECO, *i.e.* heterotrophic respiration, *e.g.* from soil organisms, plus autotrophic respiration from plants). By convention, a positive NEE means net C flux from the atmosphere to the biosphere, while a negative NEE means the C flux to the atmosphere through respiration is higher than C assimilation by the biosphere (Hatfield and Dold 2019). In the case of the employed FLUXNET data, a night-time model (Reichstein et al. 2005) is used to calculate GPP from NEE flux tower measurements based on nighttime data that is used to estimate RECO. This explains why the data includes several negative values for GPP which is technically not consistent with its definition. The FLUXNET GPP data (*GPP<sub>FLUX</sub>*) is

given in *g*  $C m^{-2} day^{-1}$ . To convert it to the output data for GPP of LPJ-GUESS (*GPP*<sub>LPJ</sub>) which is given in *kg*  $C m^{-2} month^{-1}$ , the following formula is used:

$$GPP_{LPI} \stackrel{\circ}{=} (GPP_{FLUX}/1000) \cdot 30.416 \tag{2.9}$$

### 2. Monthly evapotranspiration

The term evapotranspiration (ET) refers to the process where liquid water is transformed into water vapour through the addition of energy. The required energy chiefly stems from direct solar radiation and, to a smaller degree, from the ambient air temperature. ET is the sum of evaporation from the soil surface and transpiration, *i.e.* the vaporization of water within plant tissues. Therefore, both the soil and the plants lose water to the atmosphere through ET (Allen 1998). It is distinguished between potential ET (PET) and actual ET (AET), where the former refers to the physical potential of the atmosphere to remove water through ET assuming no limitation on water supply and the latter to the ET that is actually measured. Hence, plant water usage can be estimated by the difference between PET and AET. In FLUXNET sites, AET is measured using the latent heat (LE) energy flux ( $LE_{FLUX}$ ), given in  $W m^{-2}$ , using eddy co-variance techniques. LE is linearly correlated to the amount of evaporated water (Allen 1998). It can therefore be converted to  $mm month^{-1}$ , which in LPJ-GUESS is used as the unit of the AET output  $(AET_{LPI})$  following an adaptation of the conversion formula given by Allen (1998):

$$AET_{LPI} \stackrel{\scriptscriptstyle\frown}{=} LE_{FLUX} \cdot 0.933 \tag{2.10}$$

Note that this approximation assumes water with a density of  $1000 \text{ kg m}^{-3}$  that has a temperature of  $20^{\circ}C$ .

## 2.4 Evaluation metrics

This sections presents the statistical methods used to compare the different algorithms, to evaluate the model performance and to quantify the variation within data. One aim was to employ commonly utilized metrics in order to facilitate comparability to other modelling studies (see e.g. Morales et al. 2005). Subsequent equations denote observed values as  $O_i$ , modelled or predicted values as  $P_i$ , generic input values as  $X_i$ , mean values as a bar above the corresponding measure (*e.g.*  $\overline{O}$ ) and *n* as

the total amount of values in a population. Firstly, the coefficient of determination  $(r^2)$  was used to quantify the linear relationship between two variables. The value ranges between 0 and 1, where 1 indicates a perfect linear agreement and 0 indicates no linear relationship. It is calculated as follows:

$$r^{2} = \left(\frac{\sum_{i=1}^{n} (O_{i} - \bar{O})(P_{i} - \bar{P})}{\left(\sum_{i=1}^{n} (O_{i} - \bar{O})^{2} \sum_{i=1}^{n} (P_{i} - \bar{P})^{2}\right)^{0.5}}\right)^{2}$$
(2.11)

The average error of the model in relation to the observations was quantified by calculating the root-mean-square error (RMSE). One major advantage of the metric is that it has the same unit as the input variables which facilitates interpretation. On the other hand, one must consider the units when comparing different RMSE values. It is calculated as follows:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (P_i - O_i)^2}{n}}$$
(2.12)

In order to quantify the variation within data sets (*e.g.* for mean values of a time series), the standard deviation (SD) was calculated for some analyses. It indicates the dispersion of data around their mean value (Reeuwijk 1998) and is calculated as:

$$SD = \sqrt{\frac{\sum_{i=1}^{n} (X_i - \bar{X})^2}{n}}$$
 (2.13)

More sophisticated statistical tests to examine significant differences and trends between flux outputs of the two rooting schemes were considered (*e.g.* a two-paired t-test and various non-parametric tests). However, due to the non-trivial nature of the data (repeated, cyclical measurements; differences of the outputs not normally distributed) and given time constraints, a more detailed statistical analysis was not carried out in this thesis and is suggested before a possible future development of the scheme.

# **3 Experiments**

The functionality of the novel rooting scheme was tested in different scenarios and applications. This section describes the experimental setups chosen to examine how water stress and vertical root structure are interconnected using the new algorithm, how annual and monthly water and carbon fluxes differ using the different rooting schemes, how the permafrost adaptation affects modelling results in grid cells with frozen soils and how the model performance in relation to observational data is affected.

## 3.1 General performance and influence of permafrost

The first experiment aims at verifying whether the novel root redistribution algorithm DI results in the desired behaviour, *i.e.* distribution shifts towards available soil water if  $\beta_t$  is low and there are no root fractions in frozen soil layers. The simulations were executed for LPJ-GUESS grid cells corresponding to the chosen FLUXNET sites to make use of the locally optimized climate input and to facilitate interpretation regarding prevalent ecosystems. Therefore, the mean root fraction Mean  $Rf_i$  of all individuals in the model grid cell is determined for each soil layer (see subsection 2.2.1) for both SI and DI runs and subsequently plotted together with the mean GSWC per soil layer. The values were averaged over the available observational data period (see Table 1). Additionally, the same procedure is executed using only the initial root distribution of DI without dynamic reallocation of roots (henceforth called Zeng, see subsection 2.2.1 and Table 2). This is done to illustrate how Mean  $Rf_i$  using DI deviates from the initial conditions due to the reallocation and simultaneously to evaluate how the model output is affected by the new initial root distribution alone. An average value over all individuals and the corresponding time period of  $\beta_t$  for DI and Zeng is given to compare differences in water stress. Note that due to the current model implementation,  $\beta_t$  is not calculated for SI. Moreover, the model outputs of GPP and AET using SI, DI and Zeng are examined by adding the mean annual fluxes of the given period to the plot. For corresponding standard deviations and modelled PFTs, refer to Table 3 and Table 4. The modelled maximum active layer depth (henceforth referred to as Max ALD) during the entire time series is depicted to illustrate how it affects the vertical root distribution and consequently AET and GPP in plots with continuously frozen soil layers.

## 3.2 Model output sensitivity

For the novel rooting scheme (*DI*) it was hypothesized that the dynamic reallocation of roots can play an important role for GPP and AET fluxes under water limited growing conditions. Therefore, the different schemes were compared regarding the

Abbreviation	Full notation	Description				
SI	Static rooting scheme	Fixed root fractions per soil layer, 90% in top 50 cm soil depth, 10% in 60-150 cm soil depth. Differ- ent parametrization for three plant functional groups (Shrubs and trees, Grass, Low shrubs; see Figure 2a).				
Zeng	Root distribution according to Zeng (2001)	Fixed root fractions for 8 plant functional groups (see Figure 2b and Table S1) which are based on model fitting to empirical global rooting depth data. Root fractions can be assigned to generic soil depths based on PFT specific parameters according to Equation 2.1.				
DI	Dynamic rooting scheme	Dynamically reallocates root fractions based on wa- ter stress and availability, and permafrost at the end of each simulation year (Equation 2.6). Uses same ini- tial root distribution as <i>Zeng</i> and strives towards this distribution if water conditions are not limiting.				

Table 2: Description of the different rooting schemes.

relationships of these fluxes and the precipitation input, as well as the factor which determines the rate of reallocation  $\beta_t$  in two separate experiments. Both were limited to one identical grid cell. It corresponds to the FLUXNET site *US-Var* (Vaira Ranch - Ione, USA, see Table 1) and was chosen for the following reasons: here, as expected based on the meta data, the model indicates a moderate water limitation for the plants (see section 4). Moreover, the dominant IGBP vegetation cover classification is savanna, an ecosystem which is considered appropriate for testing the algorithm due to frequently occurring water stress. The ecosystem productivity is highly dependent on precipitation events and the wet season (Grant et al. 2012). Moreover, the modelled vegetation composition is relatively homogeneous and mostly dominated by C3 grass (Table 3). This minimizes additional external influences (*e.g.* competition between woody and herbaceous PFTs). The individual experiments are described below.

## 3.2.1 Sensitivity to precipitation input

The bias corrected precipitation input was artificially altered during the available observational data period (2000-2014) by multiplying all daily values by a factor  $p_f$ 

ranging from 0.25 to 2 in 0.25 steps. Hence, 8 different scenarios for each rooting scheme were simulated. For instance, if daily precipitation is 4 mm and  $p_f = 0.5$  then the manipulated daily precipitation input is 2 mm. To analyze the effects on modelled GPP and AET, their mean annual values were plotted against  $p_f$ . However, the analysis of annual fluxes includes only the last 5 years of the manipulation experiment to allow the ecosystem to adjust to the new environmental conditions and thus to reduce variation in the output values. Therefore, for low  $p_f$  this experiment illustrates how the different rooting schemes affect ecosystem productivity under long lasting drought conditions, which might be relevant according to projected climatic conditions in this site location (IPCC 2014). Differences in fluxes are examined both in absolute and relative terms.

### **3.2.2** Sensitivity to reallocation factor $\beta_t$

The reallocation rate of root fractions in *DI* due to water stress and availability is, at the current state, mainly based on theoretical assumptions and limited observations, and not supported by extensive empirical data (see subsection 1.2.2). Therefore, the influence of the water stress factor  $\beta_t$  on GPP and AET fluxes was tested by adding a weighting factor  $\Phi$  to Equation 2.6 as follows:

$$C_{fr,i} = \left[ (1 - \beta_t^{\Phi}) \frac{w_{gs,i} \Delta z_i}{\sum_{i=1}^n w_{gs,i} \Delta z_i} + \beta_t^{\Phi} R f_{Z,i}(d_i) \right] \cdot C_{inc} + \dots$$
(3.1)

and  $0.125 \le \Phi \le 8$  (value doubled for a total of 7 runs). Therefore,  $\Phi < 1$  results in a relatively lower root fraction reallocation due to water stress (*i.e.* low  $\beta_t$ ) and *vice versa* for  $\Phi > 1$ . Climate parameters remain unaltered for all runs and the analysis was carried out for the available observational data period. Results for mean annual AET and GPP output were plotted for the different  $\Phi$  values and bars indicating observational data and the results for *SI* are added as a reference.

## 3.3 Comparison to observational data

To assess the model performance for monthly AET and GPP using the different rooting schemes, seperate simulations were carried out for all 15 FLUXNET sites. Subsequently, the time series of all respective monthly fluxes were plotted against the observed values and relationships were quantified by determining  $r^2$ , *RMSE* and linear regression equations. The results are displayed in a table that also take modelled

PFT, the mean total leaf area index (LAI; one-sided green leaf area per unit ground surface area which is used as a proxy for vegetation density) and the water stress factor  $\beta_t$  into account. Moreover, the total mean annual AET and GPP values of the different rooting schemes were determined and plotted against observations for each site to illustrate the overall model performance.

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Figure 5: Comparison of mean root fractions (Mean  $Rf_i$ ), mean growing season water content (GSWC), mean plant water stress ( $\beta_t$ ), maximum active layer depth (Max ALD) and modelled mean annual GPP/AET fluxes for the different rooting schemes (SI = Static, DI = Dynamic, Zeng (2001) = Zeng) for selected FLUXNET data sites. Values are averaged over the available observational data period. Units:  $\beta_t$  [ratio], GPP [kg C m<sup>-2</sup> year<sup>-1</sup>], AET [mm year<sup>-1</sup>].

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## 4.1 General performance and influence of permafrost

To illustrate the most important findings, the analysis result figures for four sites (*RU-SkP, FI-Hyy, RU-Cok, US-Var*) are presented in this section (Figure 5). Refer to the appendix (A.3) for analysis result figures for the remaining sites. In most cases, the modelled fluxes using the novel dynamic rooting scheme *DI* clearly differ from the corresponding static rooting scheme *SI* output for GPP (see *AU-How, CA-Obs, Fi-Hyy, FR-Pue, GF-Guy, IT-Ren, RU-Cok, RU-Fyo, US-SRM, US-Var, US-Wkg*) and AET (see

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AU-How, Fi-Hyy, FR-Pue, GF-Guy, IT-Ren, IT-MBo, RU-Cok, RU-Fyo, US-SRM, US-Var, US-Wkg, subsection A.3).

The vertical root structure of sites with relatively high modelled water limitation (approx.  $\beta_t < 0.7$ ) is often clearly distinguishable from its initial *Zeng* distribution (*e.g.* Figure 5a). Accordingly, *Zeng* and *DI* mean root fractions per soil layer in sites with a relatively high  $\beta_t$  are more similar (*e.g.* Figure 5b). It is also evident that the different rooting schemes can strongly impact the available water per soil layer and can therefore lead to distinct vertical GSWC profiles (*e.g.* Figure 5d). Moreover, the mean plant water stress ( $\beta_t$ ) when comparing *DI* and *Zeng* can vary - differences range from 0 (Figure 5d) to 0.1 (*AU-How*, Figure S1 a).

The modelled annual GPP and AET fluxes in cold Arctic and Subarctic sites are relatively low in comparison to the other sites (*e.g.* RU-SkP GPP =  $0.05 \text{ kg C} m^{-2} \text{ year}^{-1}$ , Figure 5a) and vary only slightly among the different rooting schemes despite differences in vertical root structure (Figure 5a). There are no root fractions in permanently frozen soil using *DI* (Figure 5c).

## 4.2 Model output sensitivity

The modelled GPP and AET fluxes at the site chosen to examine model sensitivity, *US-Var*, are sensitive to changes in precipitation input for both rooting schemes. Higher water influx leads to higher plant productivity and evapotranspiration, and *vice versa*. *DI* and *SI* output results, however, are affected by changes in different ways (Figure 6).

For the standard precipitation input  $p_f = 1$ , DI in comparison to SI has higher modelled GPP (1.11±0.2 kg C m<sup>-2</sup> year<sup>-1</sup> versus 1.05±0.23 kg C m<sup>-2</sup> year<sup>-1</sup>, Figure 6a) and AET (390±82 mm year<sup>-1</sup> versus 360±82 mm year<sup>-1</sup>, Figure 6b). However, for descending  $p_f < 1$  both fluxes steadily decline, but at a higher rate for DI. Thus, for  $p_f = 0.25$  it results in lower absolute values for both GPP (0.41±0.09 kg C m<sup>-2</sup> year<sup>-1</sup> versus 0.51±0.17 kg C m<sup>-2</sup> year<sup>-1</sup>) and AET (129±36 mm year<sup>-1</sup> versus 133±39 mm year<sup>-1</sup>). In relative terms, a decrease in precipitation by 75% ( $p_f = 0.25$ ) for DI results in a reduction of GPP by 63% and of AET by 67%, and for SI in a reduction of GPP by 49% and of AET by 63% (Figure 6 c,d). For ascending  $p_f > 1$ , GPP and AET also increase steadily for both DI and SI. A 75% increase in





Figure 6: Comparison of the sensitivity of modelled GPP (a, c) and AET (b, d) using DI and SI to changes in precipitation input. The daily precipitation during the observational data period (2000-2014) for the FLUXNET site US-Var was multiplied by factor  $p_f$ . Figures show averages of the last 5 years of the manipulation period. For the relative figures (c, d),  $p_f = 1$  denotes the reference value of the respective rooting scheme. Error bars indicate one SD (a,b) or one relative SD (c,d; respective SD divided by mean annual AET/GPP values).

precipitation ( $p_f = 1.75$ ) results in an increase of GPP by 14% and of AET by 18% for *DI*, and of GPP by 14% and of AET by 22% for *SI*.

Modelled GPP and AET fluxes using *DI* are furthermore affected by the weighting ( $\Phi$ ) of the root fraction reallocation factor  $\beta_t$  (Equation 3.1) in *US-Var* (Figure 7). GPP is highest for  $\Phi = 1$  (1.08±0.17) and  $\Phi = 0.5$  (1.08±0.2, both in  $kg \ C \ m^{-2} \ year^{-1}$ ) and declines for both higher and lower values of  $\Phi$  (Figure 7). The lowest mean annual GPP was modelled for  $\Phi = 8$  with 0.94±0.15  $kg \ C \ m^{-2} \ year^{-1}$ . A similar distribution is observed for AET - however, here the lowest value was modelled for  $\Phi = 0.125$  and  $\Phi = 2$  with 362±52  $mm \ year^{-1}$  and 362±65  $mm \ year^{-1}$ , respectively.

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Figure 7: Sensitivity of modelled mean annual GPP and AET to the water stress ( $\beta_t$ ) weighting factor  $\Phi$  for the grid cell corresponding to the FLUXNET site US-Var using the new dynamic rooting scheme. Values were averaged over the observational data period (2000-2014), and corresponding observational (Obs) and modelled static scheme (Stat) values are added as a reference. Error bars indicate standard deviations.

## 4.3 Comparison to observational data

The results for evaluation metrics of *DI* in comparison to *SI* with regards to relating modelled AET and GPP to the FLUXNET data are substantially site dependent. A full summary for each site ( $r^2$ , *RMSE*, comparison of total annual output, modelled leaf area index, modelled PFT, mean  $\beta_t$ ) can be obtained from Table 3 and Table 4. Additionally, time series scatter plots for monthly GPP and AET, and corresponding 1:1 representations including linear regressions for each site can be found in the appendix (A.3). One such set of plots for the site *FI-Hyy* is included here to illustrate commonly observed patterns (Figure 8).

Vegetation in *FI-Hyy* has relatively low water stress (mean  $\beta_t = 0.93$ ). However, the new standard root distribution results in different patterns for modelled monthly GPP and AET. While the GPP curves are somewhat identical for most of the annual cycle and in high agreement with observations ( $r^2 = 0.9$ , *RMSE* =  $0.03 kg C m^{-2} year^{-1}$  for both schemes), *DI* results in a consistently lower peak (annual maximum value) during the growing season (Figure 8a). In some years, the observations are there-

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Figure 8: Time series of modelled monthly GPP (a) and AET (b) against observations in the FLUXNET site FI-Hyy (Finland, Hyytiälä) and corresponding 1:1 plots (c) and (d), respectively.
fore more accurately represented by DI (e.g. 2007, 2010) whereas in other years, the higher growing season peak of SI is closer to observed values (e.g. 2001, 2011). The mean total annual GPP for DI is  $1 \pm 0.1$ , for SI is  $1.11 \pm 0.1$  and respective observations were  $1.1 \pm 0.2$  (all in kg C  $m^{-2}$  year<sup>-1</sup>). The same lower growing season peak can be observed for the modelled AET time series (Figure 8b). However, here the agreement of DI is slightly higher (SI:  $r^2 = 0.93$ , RMSE = 7 mm month<sup>-1</sup>; DI:  $r^2 = 0.94$ ,  $RMSE = 6 mm month^{-1}$ ). Moreover, observed AET in the winter time is underestimated by both schemes in some years (e.g. 2009). The same general trend of lower modelled AET and GPP during the growing season peak can be observed in the following sites (dominant PFT based on mean LAI in parentheses): IT-MBo (BNE, BINE), IT-Ren (BNE, BINE), RU-Fyo (IBS, TeBS), US-SRM (C3G, BLSE), US-Ton (C3G, TeBE) and US-Wkg (C3G, BLSE). To the contrary, in GF-Guy (TrBE, TrIBE), DI results in higher growing season peaks for both AET and GPP. In AU-How (TrIBE, TrBE), modelled monthly GPP using DI is in overall higher during the growing season, but lower between growing seasons. Simultaneously, monthly AET on average is lower during and between growing season compared to SI. Both schemes underestimate observed GPP and AET in this site.

In unproductive Arctic and Subarctic sites (*i.e.* sites where modelled PFT are grasses and shrubs with mean total LAI < 1, see Table 3) the monthly GPP and AET time series curves for *DI* and *SI* are hardly discernible and they both consistently underestimate the two variables (*e.g.* Total annual mean AET in *RU-Cok - SI*:  $37 \pm 8 mm$  year, *DI*:  $40 \pm 8 mm$  year, Observed:  $245 \pm 99 mm$  year). Moreover, in *DK-ZaH*, there is no vegetation establishment in some years (GPP = 0, see Figure S4).

For most sites, the differences in model performance regarding monthly GPP expressed as  $r^2$  and *RMSE* using *DI* versus *SI* are relatively small. Differences in respective  $r^2$  are 0.02 or smaller for 10 out of 15 sites (Table 3 and Table 4). Above this threshold, *SI* has higher  $r^2$  in *FR-Pue* (0.51 versus 0.43), *US-SRM* (0.1 versus 0.04) and *US-Wkg* (0.24 versus 0.18). *DI* on the other hand has higher  $r^2$  in US-Ton (0.39 versus 0.25) and US-Var (0.62 versus 0.59). The same trend regarding these mentioned sites account for differences of  $r^2$  in monthly AET (refer to Table 4 for respective values). Additionally, here the  $r^2$  of *DI* is higher in *RU-SkP* (0.43 versus 0.38) and *DK-ZaH* (0.13 versus 0.08).

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Table 3: Evaluation metrics to compare monthly gross primary production (GPP) LPJ-GUESS output (n patches = 10) using SI and DI with selected FLUXNET data sites. IGBP\* denotes respective vegetation land cover classification. Total leaf Area Index (LAI), mean water stress ( $\beta_t$ ) and total annual GPP values were averaged over the observational data period as given in Table 1. LPJ-PFT denotes the two most dominant PFT in the respective LPJ-GUESS grid cell (based on highest LAI; for a list of PFT, refer to Table S1).

					r <sup>2</sup>		RMSE		Total GPP ( $\pm$ SD)		
Site ID	IGBP*	LPJ-PFT	LAI	$\beta_t$	SI I	DI	SI	DI	SI	DI	Obs
(Sub-)Arctic											
CA-Obs	ENF	C3G,IBS	0.2	0.45	0.59	0.58	0	0	0.07 (±0)	0.07 (±0)	0.8 (±0.07)
DK-ZaH	GRA	C3G	0	0.68	0.01	0.01	0	0	0 (±0)	0 (±0)	0.1 (±0.05)
FI-Hyy	ENF	IBS,TeBS	2.8	0.93	0.9	0.9	0.03	0.03	1.11 (±0.1)	1 (±0.1)	1.1 (±0.19)
RU-Cok	OSH	C3G,BLSE	0.8	0.97	0.58	0.58	0.02	0.02	0.17 (±0)	0.18 (±0)	0.4 (±0.18)
RU-Fyo	ENF	TeBS,IBS	3.6	0.86	0.88	0.87	0.04	0.04	1.27 (±0.1)	1.21 (±0.1)	1.5 (±0.2)
RU-SkP	DNF	C3G,BNS	0.1	0.49	0.24	0.24	0	0	0.05 (±0)	0.05 (±0)	0.1 (±0.19)
Other											
AU-How	WSA	TrIBE,TrBE	3.7	0.55	0.5	0.5	0.05	0.06	1.16 (±0.1)	1.26 (±0.2)	$1.8 (\pm 0.45)$
FR-Pue	EBF	TeBE,TrBR	3	0.65	0.51	0.43	0.07	0.06	1.97 (±0.1)	1.74 (±0.2)	1.2 (±0.24)
GF-Guy	EBF	TrBE,TrIBE	5.8	0.96	0.06	0.07	0.07	0.07	1.74 (±0.1)	1.81 (±0.1)	3.4 (±1.09)
IT-MBo	GRA	BNE,BINE	4.3	0.91	0.84	0.82	0.06	0.06	1.99 (±0.2)	1.99 (±0.2)	1.3 (±0.42)
IT-Ren	ENF	BNE,BINE	4.1	0.95	0.59	0.58	0.08	0.08	1.7 (±0.1)	1.65 (±0.1)	1.1 (±0.61)
US-SRM	WSA	C3G,BLSE	2.2	0.63	0.1	0.04	0.04	0.03	0.68 (±0.2)	0.53 (±0.1)	0.3 (±0.11)
US-Ton	WSA	C3G,TeBE	2.4	0.56	0.25	0.39	0.06	0.05	1.04 (±0.2)	1.05 (±0.2)	0.9 (±0.17)
US-Var	GRA	C3G,TeBE	2.7	0.58	0.59	0.62	0.04	0.04	1.02 (±0.2)	1.08 (±0.2)	0.7 (±0.2)
US-Wkg	GRA	C3G,BLSE	2.2	0.6	0.24	0.18	0.05	0.04	0.76 (±0.2)	0.66 (±0.1)	0.2 (±0.11)

\*Savanna (WSA), Forest (ENF,EBF,DNF), Grassland (GRA), Shrubland (OSH). Refer to Loveland and Belward (1997).

Accordingly, the accuracy for modelled mean annual GPP and AET fluxes is site dependant. Figure 9 shows the average values for each site with regards to observations. The *RMSE* regarding GPP for *SI* is 0.62 [*kg* C  $m^{-2}$  year<sup>-1</sup>] and for AET is 144 [*mm* year<sup>-1</sup>], and for *DI* 0.58 [*kg* C  $m^{-2}$  year<sup>-1</sup>] and 138 [*mm* year<sup>-1</sup>], respectively. It is important to note that both the highest mean annual AET and GPP values were simulated for *GF-Guy*, a neotropical rain forest ecosystem site (Bonal et al. 2008) with low modelled water limitation and  $r^2 = 0.06$  for both rooting schemes (Table 3). The annual fluxes in sites classified as Arctic or Subarctic with low productivity and vegetation cover (*i.e.* MAT < 1°C and/or mean LAI < 1) are consistently underestimated (*e.g.* mean annual AET in RU-Cok: *SI* = 37(±8), *DI* = 37(±8), Observed = 245(±99), all in *mm* year<sup>-1</sup>).

				,	5		1		,		
					r <sup>2</sup>		RMSE		Total AET ( $\pm$ SD)		
Site ID	IGBP*	LPJ-PFT	LAI	$\beta_t$	SI	DI	SI	DI	SI	DI	Obs
(Sub-)Arctic											
CA-Obs	ENF	C3G,IBS	0.2	0.45	0.52	0.52	1.16	1.15	16 (±3)	16 (±3)	283 (±42)
DK-ZaH	GRA	C3G	0	0.68	0.08	0.13	0.01	0	0 (±0)	0 (±0)	111 (±28)
FI-Hyy	ENF	IBS,TeBS	2.8	0.93	0.93	0.94	6.79	5.73	249 (±25)	225 (±19)	272 (±40)
RU-Cok	OSH	C3G,BLSE	0.8	0.49	0.33	0.34	4.79	5.07	37 (±8)	40 (±8)	245 (±99)
RU-Fyo	ENF	TeBS,IBS	3.6	0.97	0.77	0.77	17.25	15.99	357 (±33)	341 (±27)	336 (±76)
RU-SkP	DNF	C3G,BNS	0.1	0.86	0.38	0.43	1.24	1.16	14 (±1)	14 (±1)	66 (±120)
Other											
AU-How	WSA	TrIBE,TrBE	3.7	0.55	0.52	0.52	31.41	31.57	828 (±83)	797 (±84)	948 (±162)
FR-Pue	EBF	TeBE,TrBR	3	0.51	0.54	0.51	18.93	19.63	493 (±27)	502 (±28)	343 (±79)
GF-Guy	EBF	TrBE,TrIBE	5.8	0.96	0.06	0.06	43.46	48.6	785 (±39)	880 (±29)	1132 (±360)
IT-MBo	GRA	BNE,BINE	4.3	0.91	0.91	0.89	11.11	12.31	481 (±30)	502 (±27)	375 (±122)
IT-Ren	ENF	BNE,BINE	4.1	0.95	0.54	0.55	21.3	18.97	422 (±28)	384 (±26)	427 (±203)
US-SRM	WSA	C3G,BLSE	2.2	0.63	0.44	0.36	14.6	10.06	272 (±51)	179 (±46)	256 (±87)
US-Ton	WSA	C3G,TeBE	2.4	0.56	0.45	0.63	16.75	13.97	352 (±96)	367 (±65)	325 (±53)
US-Var	GRA	C3G,TeBE	2.7	0.58	0.7	0.77	12.47	12.14	357 (±73)	392 (±74)	263 (±34)
US-Wkg	GRA	C3G,BLSE	2.2	0.6	0.53	0.51	15.03	11.23	283 (±44)	235 (±45)	220 (±82)

Table 4: Same as Table 3, but for actual evapotranspiration (AET).

\*Savanna (WSA), Forest (ENF,EBF,DNF), Grassland (GRA), Shrubland (OSH). Refer to Loveland and Belward (1997).

## **5** Discussion

### 5.1 General assessment

Firstly, it can be stated that the dynamic root reallocation of the new rooting scheme works as intended and can alter the vertical root structure in response to soil water conditions. In sites with a relatively low  $\beta_t$  (approx. < 0.7), the vertical root distribution of *DI* is clearly discernible from the initially assigned fractions as indicated by the *Zeng* curves in Figure 5. Accordingly, in sites with  $\beta_t$  values close to 1, root fractions per soil layer hardly deviate from their initial state (*Zeng*). The *DI* root distribution under water stress conditions in some cases seems to converge to the *SI* distribution (*e.g. RU-SkP*, Figure 5), *i.e.* an abrupt decrease in fractions at 60 cm as opposed to 50 cm soil depth is observed. This can be explained by the fact that LPJ-GUESS uses a leaky bucket model with two buckets (bucket 1: 10-50 cm depth, bucket 2: 60-150 cm depth) to represent soil hydrology (for details refer to Sitch et al. 2003). Accordingly, soil water frequently accumulates at the bottom of the first bucket which in turn attracts root growth under water stress conditions (Equation 2.6). This can therefore be understood as a validation of the intended behaviour of the algorithm. Moreover, there seems to be agreement between low  $\beta_t$  values and sites where water stress



Figure 9: Evaluation of model performance in terms of modelled mean annual GPP (a) and AET (b) output of DI (Dynamic) and SI (Static) against corresponding observations of all 15 utilized FLUXNET sites (names omitted for readability, refer to Table 3 and Table 4). Values are averaged over the respective available data collection periods (see Table 1), error bars indicate standard deviations. For the unit of RMSE refer to the respective axis.

would be expected according to dominant vegetation cover and MAT/MAP values (Table 1), for instance, in all of the southwestern US grassland/savanna sites, *i.e.* US-SRM, US-Ton, US-Var and US-Wkg (see Grant et al. 2012). This could indicate that  $\beta_t$  is in principle a suitable metric to determine water stress during the growing season and consequently structural root adaptation caused by it.

One limitation of the current implementation of *DI* is the assumption that all PFTs react to water stress by shifting their vertical fine root distribution at the same rate. Many studies have shown that, for certain species, drought leads to a shift of root fractions to deeper soil layers or an increase in rooting depth (e.g. Persson et al. 1995; Tsutsumi et al. 2002; Padilla and Pugnaire 2007; Olmo et al. 2014). This research is often carried out under laboratory conditions or on plants in early life stages. On the other hand, however, a study on the response of fine root biomass to irrigation in the upper soil layer of a water limited pine forest site found no significant differences between irrigated and control plots (Brunner et al. 2009). Generally, Equation 2.8 and the results shown in Figure 7 show that modelled fluxes of the new rooting scheme can be influenced by the weighting of water stress reallocation. The general lack of available data can conceivably partly be owed to the difficult nature of measuring belowground processes (Warren et al. 2015). The Fine-Root Ecology Database (FRED; http://roots.ornl.gov [accessed 12-05-2019], see Iversen et al. (2017)) for ex-

ample contains more than 70 000 fine root trait observations merged from different data sets. Here, one of the main goals is to relate root variables to environmental variables (Iversen et al. 2017). However, it does not provide data that could be used to link the relationship of vertical root structure on a high spatial (vertical soil profile) resolution to corresponding soil moisture measurements or water stress changes over time. Generally, the analysis for the current implementation of *DI* revealed, however, that modelled plant productivity (GPP) and water fluxes (AET) are sensitive to the reallocation weighting factor  $\beta_t$  (subsection 3.2.2). Further data collection is therefore needed to parameterize a dynamic and PFT specific root adaptation to water stress. In any case, a redistribution based on water availability and stress alone is too simplistic to accurately capture fine root dynamics (e.g. Persson et al. 1995; Warren et al. 2015). Another limitation that should be noted is that due to the setup of LPJ-GUESS, the root redistribution is lagging one year behind the climate data, *i.e.* a current year's root distribution is determined by the previous year's soil water conditions. The implications on model output are however estimated to be small over long time periods.

Moreover, it is evident that the new rooting scheme can have substantial effects on the soil water profile (Figure 5). This could in combination with the observed changes in AET have strong implications for the model results of global and regional water balances and climatic variables not considered in this thesis (*e.g.* runoff, air temperature). Wang et al. (2018) for example showed that their implementation of a dynamic rooting scheme in a global simulation had significant effects on, among others, local wind patterns and air temperatures.

It was further demonstrated that *DI* in relation to *SI* can lead to different C and water flux responses to changes in precipitation input at a site with continuous relatively high modelled water limitation (Mean  $\beta_t = 0.58$ ; Figure 6). Here, absolute GPP was lower for *DI* in comparison to *SI* with a drastic decrease in precipitation ( $p_f = 0.25$ ) despite being higher under unaltered conditions (Figure 6). As the average of the last 5 years out of a 14 year artificial drought period was analyzed, this could therefore be explained by a faster and/or more efficient depletion of available soil water reserves in the beginning of the simulated drought. However, due to time constraints this could not be analyzed in detail and the counter intuitive lower productivity despite the expected improved use of water resources must be further evaluated in the future. Generally, the possibility to adequately capture plant responses to drought in some sites might be hampered by the fact that the current model version of LPJ-GUESS has a maximum soil depth of 1.5 m. Even though on a global mean level 95% of roots for all PFTs can indeed roughly be ascribed to the top 1.5 m (Schenk and Jackson 2002), roots in *e.g.* tropical forest sites with a dry season can extend to as far as 18 m down in the soil (Lindh et al. 2014).

Finally, the influence of permafrost on vertical root structure is captured more accurately using *DI* over *SI*, as roots no longer grow in permanently frozen soil layers (Figure 5c). The redistribution of fine roots from permanently frozen soil to the active layer in theory allows roots to take up more water and nutrients (Blume-Werry et al. 2016). Nevertheless, neither considerably higher plant productivity (GPP) nor higher water fluxes (AET) could be shown for affected sites with the current model setup (Figure 5a and site *DK-ZaH* in Figure S4; this will be further discussed in subsection 5.2). Additionally, with a dynamic root fraction adaptation to the active layer depth using *DI*, vegetation composition in Arctic biomes could be affected. Wang et al. (2016a) showed for instance that deep-rooted graminoids may get a competitive advantage over shrubs in tundra biomes with thawing permafrost due to their ability to reach nutrients in deeper soil layers. The new rooting scheme could therefore ultimately be a groundwork for improving the process-based representation of Arctic vegetation dynamics.

## 5.2 Model performance

This section examines the most important findings and trends for model performance regarding the different FLUXNET site ecosystems, often summarized by their given vegetation land cover classification (Table 1). It is however important to note that each site has a unique set of properties and environmental conditions which can all influence observations and model outcome. A detailed individual analysis is therefore beyond the scope of this thesis which aims at evaluating general implications of the new rooting scheme rather than trying to locally optimize or explain model results. The same therefore accounts for an extensive relation to all the different ecosystem properties and characteristics. For more insights about each site and ecosystem refer to their citations as given by the FLUXNET network (Baldocchi et al. 2001).

Overall, it cannot be stated that the current implementation of the new rooting scheme *DI* generally improved the model performance for modelled water and carbon fluxes in relation to the utilized FLUXNET sites (Table 3, Table 4), even though the total

RMSE for both modelled mean annual fluxes was lower using DI (Figure 9). First, it must be clearly distinguished between the model agreement in terms of mean annual and monthly fluxes. For instance, at the site GF-Guy, the error for annual mean AET and GPP was decreased using DI over SI (Figure 9, highest measured values). However, analysis of the monthly AET fluxes (GF-Guy, Figure S7b,d), for example, reveals that the reduction in total error stems from the fact that DI leads to an overestimation of values at the modelled peak of plant productivity during the growing season. At the same time, between growing seasons, the models severely underestimate AET. Both schemes each year simulate minimum values of approx. 10 mm month<sup>-1</sup>, while the observations year round constantly fluctuate around approx.  $100(\pm 25)$  mm month<sup>-1</sup>. Accordingly, the RMSE for monthly AET for DI is higher than for SI (Table 4). This is crucial when evaluating results on a global scale as the high fluxes in tropic ecosystem are an important driver of global climate and C balance (Bonal et al. 2008; Wang et al. 2018) which should motivate further model assessment of LPJ-GUESS in tropical ecosystems. These results are nevertheless consistent with Wang et al. (2018) who also found a total reduction of annual GPP and ET underestimation in tropical sites. Here, the strongest effects of a dynamic rooting scheme on climatic parameters such as local wind patterns were furthermore observed in (sub-)tropical regions. In the context of this thesis it is therefore important to note that the new rooting scheme can substantially affect fluxes in ecosystems without modelled water limitation. Accordingly, Zeng et al. (1998) summarize that root distribution mainly influences modelled AET and soil water content in tropical and midlatitudinal regions.

#### Grasslands and savannas

One striking outcome is the improvement of  $r^2$ , both for AET and GPP for the sites *US-Var* and *US-Ton* (Table 3 and Table 4; henceforth summarized as US1) which have a mean  $\beta_t$  of 0.56 and 0.58, respectively. The distance between these two sites is only roughly 2.5 km (Table 1; Figure 4) and they hence utilize the same LPJ-GUESS CRUNCEP climate input. The IGBP vegetation cover is nevertheless different, *US-Ton* is classified as savanna, and *US-Var* as grassland. The modelled dominant PFTs are identical (C3G, TeBE in that order as per mean LAI; Table 3, Table S1). The C fluxes in seasonally dry grasslands were shown to be correlated to the timing of precipitation events (Grant et al. 2012). An analysis of the corresponding monthly fluxes at both sites (*US-Ton* Figure S14, *US-Var* Figure S15) shows that model results are hampered by the fact that there are modelled distinct peaks in AET and GPP at the

beginning of each growing season which in their magnitude are not consistent with observations. This could, therefore, be partly explained by the resolution or quality of the bias corrected climate data. Especially at *US-Ton*, *DI* more accurately captures observations. Here, additionally to higher  $r^2$ , RMSE is lower for both GPP (Table 3) and AET (Table 4). At the same time, however, model agreement in terms of  $r^2$  at the sites *US-SRM* and *US-Wkg* (henceforth summarized as US2) is lower for *DI* in comparison to *SI*. US2 are also in close proximity and classified as savanna and grassland (Table 3), but are at a higher elevation and substantially drier than US1 (MAP approx.  $400 \text{ mm year}^{-1}$  versus approx.  $560 \text{ mm year}^{-1}$ ).

Interestingly, when comparing US1 to US2, the modelled water limitation is higher for US1, even though measured MAT and MAP would suggest otherwise (Table 1). Reasons for this could be multifarious: differences in soil properties, climate data quality, or the modelled occurrence of BLSE as second most dominant PFT (as per mean LAI) at both US2 sites. BLSE stands for arctic evergreen low shrubs which have a distinct vertical root distribution according to "Low shrubs" (Figure 2, also see vertical root distribution for SI in the figures in Figure S1 l,m), high drought tolerance and should not occur in non-Arctic sites. This stresses the importance of the LPJ-GUESS model setup and conditions regardless of root distribution when comparing results. At the savanna site AU-How, DI leads to higher modelled GPP and lower AET during the growing season which in both cases seems to be generally in higher agreement with observations, while both fluxes get underestimated to a higher degree in comparison to SI between growing seasons. As a consequence, model performance in terms of  $r^2$  and *RMSE* is hardly affected. Finally, the fluxes and model agreement in the site *IT-MBo* with low water limitation ( $\beta_t = 0.91$ ) are hardly affected by the different schemes. To summarize, DI leads to varying patterns in modelled AET and GPP fluxes for different savanna and grassland sites in relation to both observations and DI, but was shown to be locally able to improve monthly flux model agreement while at the same time increasing mean annual flux error due to simulation bias effects. This must, however, be further evaluated and a more sophisticated statistical analysis that takes different model parameters and more site-specific configurations into account is required.

#### **Mid-latitudinal forests**

The *RMSE* for annual GPP at the two sites that represent forests in southern Europe, one evergreen broadleaf forest (*FR-Pue* and one mountainous evergreen needleleaf

forest (*IT-Ren*), was reduced using *DI* despite lower  $r^2$  values (Table 3). However, GPP is still overestimated by both schemes. In the case of *IT-Ren*, the results should be treated with caution as the observational data shows irregularities in some years with close to zero productivity, which might explain the magnitude of overestimation (Figure S9 and Table 3). When comparing the two sites, *DI* in relation to *SI* leads to larger variation at *IT-Ren* in AET and at *FR-Pue* in GPP, which could motivate a more detailed analysis of the different effects on the two different forest types. Hence, in summary, modelled annual GPP using *DI* is lower for both temperate forest sites which is in both cases reducing bias despite lower  $r^2$  with regards to the monthly observations. A detailed assessment of the performance of LPJ-GUESS in European forest flux sites (using the static rooting scheme) can be found in Morales et al. (2005).

#### Arctic and subarctic locations

The Arctic and Subarctic locations can be roughly partitioned into three groups: cold and unproductive high Arctic grassland and shrubland with MAT < 0°C (DK-ZaH, RU-Cok; henceforth referred to as AC1), the subarctic evergreen needle leaf forests with MAT >  $0^{\circ}C$  (CA-Obs, Fi-Hyy, RU-Fyo; henceforth referred to as AC2) and the deciduous larch forest in subarctic Russia (RU-SkP). Firstly, it can be stated that at AC1 and RU-SkP both AET and GPP are consistently underestimated, for both rooting schemes. Moreover, the modelled monthly and annual fluxes for DI and SI are almost identical (*RMSE* and  $r^2$  in Table 3, Table 4 and respective site figures in A.3). This shows that, even though the modelled PFT seem to be in agreement with the given land cover classification in all locations (Table 3), LPJ-GUESS does currently not capture the relatively low plant productivity and the seasonal magnitudes of fluxes at these Arctic and Subarctic sites. Although in absolute numbers this may appear of minor importance at first glance, the fact that a large fraction of total land cover is populated by these biomes can lead to significant consequences for modelling C and water fluxes on a global scale (Schuur et al. 2008; Blume-Werry et al. 2016). The new rooting scheme with a dynamic adaptation to the maximum active layer depth could despite higher total amount of root fractions in unfrozen top layers not help to reduce the underestimation. One way to tackle this could be to test the new rooting scheme with the Arctic version of LPJ-GUESS which incorporates additional ecosystem processes and PFTs optimized for applications in the Arctic (Miller and Smith 2012). It was not used for this thesis to ensure comparability of the model output. Moreover, water limitation plays generally a subsidiary role in many Arctic ecosystems where vegetation composition, competition and productivity is often constrained by nutrient

availability and related processes (Iversen et al. 2015). A dynamic root distribution, at least for Arctic tundra, should therefore also incorporate a vertical nitrogen distribution in the soil (see Wang et al. 2018). Moreover, the assumption of Equation 2.6 that GSWC calculation is limited to the growing season with ambient air temperatures higher than 5°C may be inadequate for Arctic tundra, where the below ground growing season was shown to be significantly longer (Blume-Werry et al. 2016).

The same systematic underestimation with constantly low fluxes is observed at the site *CA-Obs* which has a MAT of 0.79°C and, with a MAP of 406 mm, is relatively dry (accordingly,  $\beta_t = 0.45$ ). The dominant modelled PFTs here are C3 grass and, to a lesser extent, summergreen broadleaf trees as opposed to evergreen needleleaf forest as given by the IGBP landcover classification (Table 1) which might explain the underestimation. The fluxes at the other AC2 sites, on the other hand, are very well captured by the model. Here, DI consistently leads to lower modelled GPP and AET values at the peak of the growing season. As a consequence, annual GPP fluxes are underestimated, even though in some years the monthly flux curves agree better with observations (Figure S5, Figure S11). At RU-Fyo, the RMSE of AET could on the other hand be reduced by using DI (see Table 4). Generally it can be concluded that even though differences are relatively small, SI better represents fluxes in subarctic and not evergreen needleleaf sites that are not water limited. As FI-Hyy and RU-Fyo have low water limitation (mean  $\beta_t > 0.85$ ), the root distributions closely follow their initial state (Figure S1 d,j). Possible explanations for the better representation could therefore be inaccuracies of the initial distribution (Zeng 2001) or general parametrization of LPJ-GUESS that might lead to optimized results for the current root distribution.

## 5.3 Future improvements

This section will briefly explore possible adaptations that could be investigated to possibly improve the novel rooting scheme based on the thesis results and literature recommendations. In general, more field data is needed to parameterize a dynamic redistribution of roots with changes in environmental conditions (Warren et al. 2015; Iversen et al. 2017). Results have shown that model performance with regards to the utilized rooting scheme is substantially site dependent. Accordingly, the factor  $\Phi$  that acts as a weighting factor for the reallocation factor  $\beta_t$  (Equation 3.1) could potentially receive unique values for PFTs or PFGs to account for respective differences of plant fine root redistribution as a reaction to water stress. As a first step,

### 6 Conclusions

parameter fitting techniques could be employed with observational flux data as input to assess potential benefits. One major limitation for the algorithm is that LPJ-GUESS currently does not include vertical nitrogen distribution in the soil. In many ecosystems, nutrients are the main factor limiting plant growth and they strongly influence vegetation competition and root architecture (Iversen et al. 2015). The rooting scheme could therefore benefit from the incorporation of a new nitrogen scheme (see also Wang et al. 2018). Finally, additional structural features and traits regarding the rhizosphere could be examined, such as mycorrhizal associations or hydraulic redistribution. For a detailed assessment of general root representation recommendations in ecosystem models refer to Warren et al. (2015).

## 6 Conclusions

A new rooting scheme for LPJ-GUESS was developed in this thesis. Research suggests that the current static rooting scheme may be too simplistic to represent belowground processes in changing environmental conditions and hence could be insufficient to represent vegetation dynamics in future climate scenarios (Warren et al. 2015). The new scheme dynamically adapts the vertical root distribution to soil moisture conditions if a plant is under water stress, as it was observed in several experiments (e.g. Persson et al. 1995; Olmo et al. 2014). Building on previous studies and theory (Sitch et al. 2003; Wang et al. 2016a), it was therefore hypothesized that vertical root structure has an impact on modelled carbon and water fluxes. Accordingly, the changes in model output of two variables (AET and GPP) were analyzed and related to observational data from selected FLUXNET sites. The goal was to assess effects on different ecosystems with a special focus on (Sub-)Arctic (additional dynamic adaptation to permafrost) and water limited sites. The main findings were:

- The algorithm fulfills the desired functionality. The root fraction reallocation per soil layer is affected by soil water content if a plant is under water stress. Mechanistic validity could be improved by making root fractions dynamically adapt to permafrost.
- 2. Utilizing different vertical root structures can change modelled water and carbon fluxes. Even though results are site dependent and no global trend in the change in fluxes could be identified, the static scheme, the dynamic scheme

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including root reallocation, and the updated initial root distribution for the dynamic scheme alone can all lead to differences in modelled GPP and AET fluxes.

- 3. The root fraction reallocation in its current implementation may be too simplistic. General model performance was not improved and using water stress and availability alone to determine root reallocation may not be sufficient (Warren et al. 2015). Moreover, the assumption that all PFTs reallocate roots at the same rate is unrealistic (e.g. Brunner et al. 2009).
- 4. The algorithm is a good framework. The initial distribution is based on empirical data (Zeng 2001) and the scheme can act as a basis to incorporate additional processes (*e.g.* nitrogen availability, deeper soil layers, *etc.*). This is however limited by data availability and knowledge gaps (Iversen et al. 2017).
- 5. The relatively largest impact of root distribution on modelled fluxes was in a non water limited tropical site where annual flux error was reduced, while monthly flux error was simultaneously increased. This stresses the importance of root distribution beyond the scope of water limitation.
- 6. The different rooting schemes lead to different relative responses of the fluxes to drought conditions which must be further analyzed and validated.
- 7. Modelled fluxes in cold and unproductive Arctic sites were hardly affected by the new rooting scheme. The dynamic adaptation of rooting depth to permafrost did not considerably enhance plant productivity and the fluxes of all respective observational sites were underestimated.
- 8. The new scheme could locally improve monthly model agreement to observations in two water limited grassland/savanna sites, but the accuracy was decreased in others. The new scheme performed slightly worse in Subarctic evergreen needleleaf forests. In two southern European forest sites, *RMSE* for AET was reduced but  $r^2$  was lower. Therefore, results with regards to model performance are highly site dependent and must be analyzed in detail due to the amount of influencing factors. Also, additional statistical evaluation is needed.
- 9. The differences between rooting schemes in modelled GPP and AET can have big impacts on global and regional water and carbon cycles and therefore future climate projections.

### 6 Conclusions

A higher degree of attention to belowground processes and a further development of the rooting scheme are therefore well motivated. Additional fundamental research should focus on data collection and hence the quantification of processes and environmental factors that affect vertical root distribution over time. Simultaneously, adequate simplifications are needed that are suitable for large scale modelling applications.

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# **A** Supplementary Materials

## A.1 Additional tables

Table S1: Plant functional types (PFT) in LPJ-GUESS, their corresponding plant functional groups (PFG) according to Zeng (2001) and corresponding PFG in the current static rooting scheme. Parameters a and b are used for initial root distribution according to Equation 2.1. [ST] = shade tolerant, [SI] = shade intolerant, NA = not included.

PFT LPJ-GUESS	PFG Zeng (2001)	PFG in SI	а	b
BNE (Boreal needle leaved	Evergreen needleleaf	Shrubs	6.706	2.175
evergreen tree [ST])	tree	and trees		
BINE (BNE [SI])	Evergreen needleleaf	Shrubs	6.706	2.175
	tree	and trees		
TeNE (Temperate needle leaved	Evergreen needleleaf	Shrubs	6.706	2.175
evergreen tree [SI])	tree	and trees		
BNS (Boreal needle leaved	Deciduous needleleaf	Shrubs	7.066	1.953
summergreen tree [SI])	tree	and trees		
TeBS (Temperate broadleaved	Deciduous broadleaf	Shrubs	5.990	1.955
summergreen tree [ST])	tree	and trees		
IBS (Broadleaved summergreen	Deciduous broadleaf	Shrubs	5.990	1.955
tree [SI])	tree	and trees		
TrBR (Tropical broadleaved	Deciduous broadleaf	Shrubs	5.990	1.955
raingreen tree [SI])	tree	and trees		
TeBE (Temperate broadleaved	Evergreen broadleaf	Shrubs	7.344	1.303
evergreen tree [ST])	tree	and trees		
TrBE (Tropical broadleaved	Evergreen broadleaf	Shrubs	7.344	1.303
evergreen tree [ST])	tree	and trees		
TrIBE (Tropical broadleaved	Evergreen broadleaf	Shrubs	7.344	1.303
evergreen tree [SI])	tree	and trees		
C3G (Cool C3 grass)	Short grass	Grass	10.74	2.608
C4G (Warm C4 grass)	Tall grass	Grass	8.235	1.627
CROP	Crop/mixed farming	NA	5.558	2.614
BLSE (Arctic evergreen low	Evergreen shrub	Low	6.326	1.567
shrub)		shrubs		
BLSS (Arctic summergreen low	Deciduous shrub	Low	6.326	1.567
shrub)		shrubs		

## A.2 Vertical root structure

Comparing differences in modelled vertical root structure and associated variables in the chosen FLUXNET sites using the different rooting schemes. Refer to the figure caption at the end for a more detailed explanation of depicted variables.

1.00

1.00

0.5

GSWC

0

0

0.5

GSWC

0.5

GSWC

0









Figure S1: Mean vertical root distribution ( $Rf_i$ ), mean growing season soil water content (GSWC), maximum active layer depth (Max ALD), mean water stress ( $\beta_t$ ), mean annual gross primary production (GPP) and mean annual actual evapotranspiration (AET) over the indicated period for the different FLUXNET sites, using the different rooting schemes [Static (red), Dynamic (blue) and Zeng (black)].



**AU-How** 



Figure S2: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **AU-How**.

CA-Obs



Figure S3: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **CA-Obs**.

DK-ZaH



Figure S4: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **DK-ZaH**.

**FI-Hyy** 



Figure S5: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **FI-Hyy**.





Figure S6: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **FR-Pue**.





Figure S7: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **GF-Guy**.

IT-MBo



Figure S8: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **IT-MBo**.

IT-Ren



Figure S9: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **IT-Ren**.

**RU-Cok** 



Figure S10: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **RU-Cok**.

**RU-Fyo** 



Figure S11: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **RU-Fyo**.

**RU-SkP** 



Figure S12: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **RU-SkP**.





Figure S13: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **US-SRM**.





Figure S14: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **US-Ton**.





Figure S15: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **US-Var**.




Figure S16: Comparing modelled monthly (a) gross primary production (GPP) and (b) actual evapotranspiration (AET) with respective 1:1 plots (c,d) for the different rooting schemes to observational data from the FLUXNET site **US-Wkg**.