https://doi.org/10.5194/egusphere-2024-1319
Preprint. Discussion started: 28 June 2024
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From hydraulic root architecture models to efficient macroscopic sink terms including perirhizal resistance: Quantifying accuracy and computational speed

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Abstract. Root water uptake strongly affects soil water balance and plant development. It can be described by mechanistic models of soil-root hydraulics based on soil water content, soil and root hydraulic properties, and the dynamic development of the root architecture. Recently, novel upscaling methods have emerged, which enable the application of detailed mechanistic models on a larger scale, particularly for land surface and crop models, by using mathematical upscaling.

In this study, we explore the underlying assumptions and the mathematical fundamentals of different upscaling approaches. Our analysis rigorously investigates the errors introduced in each step during the transition from fine-scale mechanistic models, which considers the nonlinear perirhizal resistance around each root, to more macroscopic representations. Upscaling steps simplify the representation of the root architecture, the perirhizal geometry, and the soil spatial dimension and thus introduces errors compared to the full complex 3D simulations. In order to investigate the extent of these errors, we perform simulation case studies: spring barley as a representative non-row crop and maize as a representative row crop, and using three different soils.

We show that the error introduced by the upscaling steps strongly differs, depending on root architecture and soil type. Furthermore, we identify the individual steps and assumptions that lead to the most important losses in accuracy. An analysis of the trade off between model complexity and accuracy provides valuable guidance for selecting the most suitable approach for specific applications.

1 Introduction

Plant transpiration plays a vital role in the overall soil water balance within the field and is a sensitive process in land surface and crop models (Good et al., 2015). A mechanistic description of how plant transpiration is influenced by soil and root properties helps to unravel the interaction between climate, soil water balance and plant development. Such models can support plant breeding efforts to find root traits aiming for more drought resistant plants in specific pedoclimatic environments and empower decision-makers in optimizing agricultural practices for improved crop water management and sustainable land use (Louarn

https://doi.org/10.5194/egusphere-2024-1319
Preprint. Discussion started: 28 June 2024
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and Song, 2020; Soualiou et al., 2021).

The soil-plant system is a multi-scale hierarchically structured system with typical structures that exist and influence or control processes at different scales. At the smallest scale, water flow in soils depends on the structure of the water filled pore network, i.e. the size of water filled pores, of water films on solid surfaces, and their connectivity. In plants, this scale corresponds to the water flow in cell walls, through cell membranes, through water conducting vessels, i.e. xylem vessels. The arrangement of cells in tissues, the constitution of cell walls and the size of xylem vessels and the pits in their sieve plates control water flow in root system. Using models that solve Navier-Stokes equations, hydraulic properties that define the averaged flow over these smaller scale structures as a function of averaged water potential gradients can be derived. These hydraulic properties can subsequently be used to describe the averaged flow as a function of averaged water potentials using continuum equations.

In this way the flow in the entire rooting zone can be simulated, and a straightforward approach is to represent both the soil and roots as two separate and mutually exclusive domains with different properties. However, the small diameter of roots with respect to their length and size of the root zone would require a very small discretization with respect to the size of the simulation domain to represent the fluxes and water potentials in this system accurately. Therefore, a so-called 1D-3D mixed model approach is used (Koch et al., 2018). In this approach, the flow in the soil is described using a 3D continuum equation, i.e. the Richards equation. This approach will be the starting point of our upscaling.

The flow in the root system is represented by a network of porous pipes with pipe walls representing the root tissues through which water flows radially towards the xylem tissue that represents the internal part of the tube where water flows axially. The flow in each xylem segment is described as a function of the water potential gradient along the xylem and the exchange between the root and the soil as a function of the potential difference between soil-root interface and the water in the root xylem tissue. The root system is assumed not to occupy a volume in the soil domain and the water flow between the soil and root domains is represented by a source/sink term in the soil domain. The information that needs to be exchanged between the two domains are the water potentials and water fluxes at the soil-root interfaces.

Schnepf et al. (2023, 2020) recently benchmarked such functional-structural root architecture models for simulating the root water uptake (RWU) from drying soils. A central part is the coupling between the two domains. In the 3D soil model, the water potentials are calculated at the nodes or the centres of the grid cells that are used to discretize the 3D soil domain. The 3D soil model, in which RWU is represented as a source or sink term, does not resolve the fluxes and water potential gradients around the root segments within a grid cell. In order to obtain water potentials at the soil root interfaces which are used by the root model we employ a perirhizal model around the root segments that incorporates nonlinear soil conductance based on Schröder et al. (2008). This is crucial, since in dry soil a mere increase in macroscopic resolution fails to accurately characterize the sharp gradients in soil potential (Khare et al., 2022). Following Vanderborght et al. (2023) the perirhizal zone is approximated

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by a cylindrical domain. Typically, the domain volume is approximated in proportion to the segment's root length, surface or volume in a given macroscopic soil element volume (e.g. De Bauw et al., 2020; Mai et al., 2019). It is well known that the inter-root distance influences the uptake potential (de Willigen, 1987) and Graefe et al. (2019) underlines the importance of the outer perirhizal cylinder radii distribution. Kohl et al. (2007) used Voronoi diagrams to determine the outer radii in 2D, and Schlüter et al. (2018) used distance functions in 3D to quantify the perirhizal zone. In this work we present a novel approach using Voronoi diagrams in 3D to obtain more realistic perirhizal volumes than the approaches based root densities.

Moving to larger scale models the first obvious step is to reduce the dimensions of the macroscopic soil model. de Willigen et al. (2012) simulated RWU at different complexities, 1D, 2D and 3D soils. They found that acknowledging the lateral water potential gradients resulted in a reduction of simulated actual transpiration. However, they considered a soil with the same lateral (x and y) dimension, with the root system in the middle, which is not consistent with the inter-plant and inter-row distances of most agricultural crops. Couvreur et al. (2014) demonstrated that failing to account for lateral variations in root density and bulk soil water potentials results in an overestimation of simulated collar water potentials for row crops but worked sufficiently well for crops with rather uniform lateral root distributions.

The representation of the root architecture in an upscaled, e.g. 1D, soil water flow model can be of different complexity. When the 3D root architecture model is coupled with a 1D soil model, a first assumption that could be made is that the water potentials at the soil-root interface are uniform at a given depth or in a certain layer of the discretized 1D soil profile. When the hydraulic root system model is assumed to be linear, i.e., it is assumed that the conductance of the different segments does not depend on the water potential, then an exact upscaled root hydraulic model can be derived (Vanderborght et al., 2021). This exact upscaled model can be approximated by a so-called parallel root model that assumes that the water that is taken up by root segments in a certain soil layer is directly transferred to the root collar through an effective laterally impermeable root pipe that does not exchange water with other soil layers so that RWU from different soil layers occurs in parallel (Couvreur et al., 2014; Vanderborght et al., 2021). Vanderborght et al. (2021) showed that it reproduced the uptake by 3D root architectures quite well. When the root architecture model is coupled with a 1D soil model, the 1D soil model simulates the bulk soil water potential and assumes that they are uniform at a certain depth. When the soil is sufficiently wet and the hydraulic conductivity of the soil sufficiently large, the soil water potential at the soil root interface can be assumed to be equal to the bulk soil water potential. But when soils dry out, the water potentials at the soil root interfaces differ from the bulk soil water potentials and depend on the flow to a specific root segment. In order to couple the 3-D root architecture model with an upscaled 1D soil model, Vanderborght et al. (2023) used cylindrical perirhizal models around the single root segments and assumed that the bulk soil water potentials and outer radii of the perirhizal cylinders were the same for all root segments. The radii were derived assuming that all roots in a soil layer were parallel and equidistant. To simplify the model further, they used parallel root model assuming that the xylem water potential in and the water flow to each root segment in a certain soil layer were the same. Despite the fact that the flow rate and water potentials in the xylem and at the soil-root interfaces of root segments of the 3D architecture that was coupled to the 1D model varied a lot between the root segments, the parallel root model could describe the total RWU

https://doi.org/10.5194/egusphere-2024-1319
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from a soil layer quite well and with a strongly reduced computational cost.

However, the consequences of assuming uniform bulk soil water potentials were not considered in Vanderborght et al. (2023, 2021). In this study we systematically test these new upscaling methods for the first time for scenarios that realistically represent the distribution of plants in an agricultural field. We use spring barley as a representative non-row crop and maize as a representative row crop. We simulate plant transpiration over two weeks in three soil types loam, clay and sandy loam an observe soil water depletion and the occurrence of plant water stress. We perform the simulations with the full hydraulic 3D model and compare the accuracy of the approximations in each upscaling step.

The full hydraulic architecture combined with a 3D soil model enables us to study the processes in detail. However, the computational costs make it inefficient for large-scale applications. Also, the full hydraulic architecture is not easily included in large-scale models, and it is preferable to use a RWU sink term that is only based on the soil states explicitly. Vanderborght et al. (2023) showed how such sink terms can be derived from more mechanistic models using 3D root hydraulics. We divide the different upscaling steps in three categories (see Figure 1) and analyse the steps regarding accuracy and speed:

1. The way the root hydraulic system is represented: By individual potentials for root segment at the soil root interface (Figure 1, column 1, A), same potentials within a soil element for all segments (column 1, B), or approximated by a parallel root system with similar macroscopic hydraulic properties (column 1, C).
2. Representation of the perirhizal radius: Either using 3D Voronoi diagrams to obtain the volume of the perirhizal zone (Figure 1, column 2, A), or assumeing homogeneously distributed roots within each soil cell (column 2, B).
3. The macroscopic soil is described in 3D (see Figure 1, column 3, A). To obtain a speed up in computation we consider soil models with lower dimensionality, where we assume soil water potential does not change in specific directions (see Figure 1, column 3, B).

We use the three columns of Figure 1 for a precise categorization of the upscaling steps involved, AAA being the most accurate model, and CBB the fastest and coarsest model.

2 Materials and Methods

We describe water flow in the plant-rhizosphere-soil system by considering each subdomain as mathematical sub-problems that are solved sequentially (see Koch et al. 2021 for alternative monolithic schemes). We sequentially compute the macroscopic soil model (Section 2.1), the root architecture development (Section 2.2), and using a fixed point iteration, where we solve the root hydraulic model and perirhizal model (Section 2.3). From the resulting root xylem potentials $\mathbf{H}_x$ and the total potentials at the root-soil interface $\mathbf{H}_{sr}$ the RWU is determined, which then acts as a sink for the macroscopic soil model, see Figure 2.

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The models were implemented in CPlantBox (Zhou et al., 2020; Schnepf et al., 2018) and dumux-rosi (Giraud et al., 2023) which are available on GitHub and are open source which facilitates reproducibility and further advancements (Barba, 2022). The use of upscaled models fundamentally increases performance. Depending on the root architecture and soil type we could achieve speed ups up to 15000%. We discuss the trade off between model accuracy and computational speed which guides users how to pick the appropriate modelling approach for specific applications.

In the following we describe each part of Figure 2 in detail, first the macroscopic soil model (Section 2.1), the root architecture development model (Section 2.2), and the fixpoint iteration, where we iterate the full root hydraulic model and the perirhizal model (Section 2.3). These models are of type Axx (see Figure 1). We present two upscaled models, first the upscaled aggregated model (Section 2.5) corresponding to the models Bxx, and the parallel root model (Section 2.6) corresponding to the models Cxx. Next, we describe the two approaches to obtain the outer perirhizal radii (Section 2.4) corresponding to the models xAx and xBx. Finally, in Section 2.7 we define test scenarios to benchmark the efficiency of the simplifications of the larger scale models against the reference full hydraulic model.

2.1 Macroscopic soil model

Water movement is described by the Richards equation

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (K(\theta)\, \nabla H_s) + S, \tag{1}$$

where θ [1] is the water content, K [cm^2/day] is the soil hydraulic conductivity, H_s [cm] is the soil total potential, and S is a sink term that describes RWU [1/day].

We can solve the Richard equation 3D (these models are named xxA) or assume no change in water potential in specific directions using a 1D or 2D soil grid (xxB). We use the finite volume solver DuMu^x (Koch et al., 2021) to numerically solve Eqn 1. The sink our source S is calculated for each finite volume cell as a function of the root xylem total potentials H_x and the total potentials at the root surface interface H_{sr}. Generally, H_{sr} is derived as a function of H_x and H_s using a perirhizal model, as described in Section 2.3. For each finite volume cell i the sink or source S_i [cm^3/day] is calculated as

$$S_i = \sum_{j \in cell_i} 2 a_j \pi k_{r,j} dl_j (H_{sr,j} - H_{x,j}), \tag{2}$$

where j is the root segment index of a segment located within the finite volume cell i, a_j [cm] root radius, $k_{r,j}$ [1/day] root radial conductivity, dl_j [cm] segment length, $H_{sr,j}$ [cm] total potential at the soil-root interface, and segment xylem total potential $H_{x,j}$ [cm].

The relation between θ and the soil matric potential h_s by is given by the water retention curve, which we describe by the Van Genuchten model (Van Genuchten, 1980). The conversion between total and matric potentials can readily be done as

$$h_s = H_s - z, \tag{3}$$

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where z is the elevation.

2.2 Root architecture development model

We use the model CPlantBox to describe the root architecture (Zhou et al., 2020; Schnepf et al., 2018), which is able to represent the development of different root architecture geometries. CPlantBox is an open source software, the code is available at GitHub. The root architecture is represented as straight 1D segments in 3D space (1D/3D), where the segment length is less or equal the axial resolution dx.

Parameters are defined per root type. Typical parameters are length of the basal zone (l_b), the inter-lateral distance (l_n), the maximal root length (the number of laterals is deduced from maximal length) (l_{max}), the length of apical zone (l_a), or apical delay time (l_{delay}), root radius (a), initial growth rate (r), as well as type and probability of successor roots. We chose root architecture parameter sets for spring barley according to Eloundou (2021) based on Postma et al. (2017) and for maize according to (Landl et al., 2018) which are available within the CPlantBox repository.

2.3 Root hydraulic and perirhizal model (Axx)

We use the model of Doussan et al. (1998) and in the following describe it using methods from graph theory. The root system can be interpreted as a directed graph of n nodes and $n-1$ edges representing the root segments. The connections between the nodes of the root system is given by its incidence matrix $\mathbf{C} \in \mathbb{R}^{n \times n-1}$ in such a way that its ij^{th} entry is equal to -1 when edge j is leaving node i, and 1 when edge i arrives in node j. We can use the Laplace matrix $\mathbf{L}$ to describe Kirchhoff's law as

$$\mathbf{L} \begin{bmatrix} H_{collar} \\ \mathbf{H}_x \end{bmatrix} = \begin{bmatrix} t_{act} \\ \mathbf{q}_{root} \end{bmatrix}, \tag{4}$$

where the symmetric Laplacian matrix $\mathbf{L} \in \mathbb{R}^{n \times n}$ is given by

$$\mathbf{L} = \mathbf{C}\, diag(\mathbf{K}_x)\, \mathbf{C}^T, \tag{5}$$

and H_{collar} is the total root collar potential [cm], $\mathbf{H}_x$ the $(n-1) \times 1$ vector of the total root water potentials [cm] of the other root nodes, and $\mathbf{K}_x$ is the $(n-1) \times 1$ vector of root axial conductances [cm^2/day], where

$$(\mathbf{K}_x)_i = K_{x,i} = k_{x,i}/l_{root,i}, \tag{6}$$

$k_{x,i}$ being the intrinsic root axial conductance [cm^3/day] and $l_{root,i}$ the segment length [cm] of root segment i. The right hand side $\mathbf{q}_{root}$ [cm^3/day] describes the sources (positive sign) and sinks (negative sign) which represents water uptake or loss by the roots.

To solve specific root hydraulic scenarios, we need to define the RWU and adjust Eqn (4) to include root collar boundary conditions.

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The volumetric RWU $\mathbf{q}_{root}$ [cm^3/day] is given for a total xylem potential $\mathbf{H}_x$ [cm] and a total water potential at the soil root interface $\mathbf{H}_{sr}$ [cm] as

$$\mathbf{q}_{root} = diag(\mathbf{K}_r)(\mathbf{H}_{sr} - \mathbf{H}_x), \tag{7}$$

where $\mathbf{H}_{sr}$ is the $(n-1)\times 1$ vector of the total soil water potentials at the soil root interface, and $\mathbf{K}_r$ is the $(n-1)\times 1$ vector of the root radial conductances [cm^2/day], where

$$(\mathbf{K}_r)_i = K_{r,i} = 2\, a_{root,i}\, \pi\, l_{root,i}\, k_{r,i} \tag{8}$$

$k_{r,i}$ being the intrinsic root radial conductance [1/day], and $a_{root,i}$ is the root segment radius [cm] of root segment i.

Including a Dirichlet boundary condition at the root collar, which is assumed to be located at the first node, Eqn (4) can be rewritten as

$$\mathbf{L}_d \begin{bmatrix} H_{collar} \\ \mathbf{H}_x \end{bmatrix} = \begin{bmatrix} H_{prescribed} \\ diag(\mathbf{K}_r)(\mathbf{H}_{sr} - \mathbf{H}_x) \end{bmatrix}, \tag{9}$$

where $\mathbf{L}_d$ is the Laplacian Matrix adjusted for the Dirichlet boundary condition such that the first entry of the first row is equal to 1 and all other entries are zeros. If we want to solve for $\mathbf{H}_x$ we can re-write above equation as

$$-K_{x,1}\mathbf{e}_1\, H_{collar} + \mathbf{L}_{n-1}\, \mathbf{H}_x = diag(\mathbf{K}_r)\, \mathbf{H}_{sr} - diag(\mathbf{K}_r)\, \mathbf{H}_x, \tag{10}$$

where $\mathbf{L}_{n-1}$ is the $(n-1)\times(n-1)$ submatrix of $\mathbf{L}$ with removed first row and column, and $\mathbf{e}_1$ is the $(n-1)\times 1$ unit vector (see also Vanderborght et al. (2021), Eqn A5). Then, for any known $\mathbf{H}_{sr}$, we can solve for $\mathbf{H}_x$ as

$$\underbrace{(\mathbf{L}_{n-1} + diag(\mathbf{K}_r))}_{=:\mathbf{A}}\, \mathbf{H}_x = \underbrace{diag(\mathbf{K}_r)\, \mathbf{H}_{sr} + K_{x,1}\mathbf{e}_1\, H_{collar}}_{=:\mathbf{b}_d}, \tag{11}$$

where $\mathbf{A}$ is symmetric and diagonal dominant for $(K_r)_i > 0$, and therefore positive definite, the right hand side $\mathbf{b}$ depends on the matric potential of the soil root interface H_{sr} and the total root collar potential H_{collar}.

When developing larger scale soil models we generally do not want to consider individual root water potentials since it is not feasible to explicitly describe the root architecture in such models. Thus, the effective sink term for RWU should be formulated in a way such that the values $\mathbf{H}_x$ are not explicitly needed. For Dirichlet boundary conditions we calculate $\mathbf{H}_x$ from Eqn (11) and insert it into the Eqn (7) which describes RWU as

$$\mathbf{q}_{root} = diag(\mathbf{K}_r)(\mathbf{H}_{sr} - (\mathbf{A}^{-1}\, diag(\mathbf{K}_r)\, \mathbf{H}_{sr} + \mathbf{A}^{-1}\, K_{x,1}\mathbf{e}_1\, H_{collar})) \tag{12}$$

$$\mathbf{q}_{root} = diag(\mathbf{K}_r)(\mathbf{I} - \mathbf{A}^{-1}\, diag(\mathbf{K}_r))\mathbf{H}_{sr} - diag(\mathbf{K}_r)\mathbf{A}^{-1}\, K_{x,1}\mathbf{e}_1\, H_{collar}, \tag{13}$$

corresponding to Vanderborght et al. (2021), Eqn A16. For big sparse matrices $\mathbf{A}$ it is not efficient to compute $\mathbf{A}^{-1}$ since this matrix is dense, so we express above equation as

$$\underbrace{\mathbf{A}\, diag(\mathbf{K}_r)^{-1}}_{=:\mathbf{A}_q}\mathbf{q}_{root} = \underbrace{(\mathbf{A} - diag(\mathbf{K}_r))\mathbf{H}_{sr} - K_{x,1}\mathbf{e}_1\, H_{collar}}_{=:\mathbf{b}_q}. \tag{14}$$

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and we can solve this sparse linear system for $\mathbf{q}_{root}$ for given $\mathbf{H}_{sr}$ and H_{collar} (note that $diag(\mathbf{K}_r)^{-1}$ is sparse).

We can easily switch between Dirichlet boundary conditions, where we set the total potential H_{collar} [cm] at the root collar, and Neumann boundary conditions, where we predetermine a volumetric transpiration t_{act} [cm^3/day]. In the simulation the boundary condition will be automatically switched between Neumann and Dirichlet assuring that the root collar potential cannot be below a critical potential where we assume the plants wilting point. The relationship between $t_{act} = \sum_i q_{root,i}$ and H_{collar} is given by

$$t_{act} = K_{rs}(H_{eff} - H_{collar}), \tag{15}$$

$$H_{collar} = (K_{rs}H_{eff} - t_{act})/K_{rs}, \tag{16}$$

where K_{rs} [cm^2/day] is the root system conductivity, $H_{eff} = \mathbf{SUF}^T \cdot \mathbf{H}_{sr}$ [cm] is the effective water potential at the soil root interface, and $\mathbf{SUF}$ [1] as defined by Couvreur et al. (2012), which corresponds with the $\mathbf{q}_{root}/t_{act}$ calculated for a uniform H_{sr}. Eqn (15) is derived by summing up the rows of Eqn (13). For a detailed derivation we refer to Vanderborght et al. (2021), Appendix A.

In dry soils, RWU is often limited by low soil hydraulic conductivity near the root surface, i.e., in the perirhizal zone that is influenced by the radial water flow towards the root. Therefore, we consider an additional perirhizal resistance for each root segment as described by Vanderborght et al. (2023) which is based on Schröder et al. (2008) to determine the total potential at the soil root interface H_{sr}. We assume a steady rate in the perirhizal zone, i.e. $d\theta/dt$ does not vary with radial distance from the root axis r. The steady rate is dependent on the bulk soil total potential H_s and the root xylem potential H_x. Note that in with respect to the model application the steady rate approach can also be replaced by more complex dynamic rhizosphere models to determine H_{sr} (e.g. Khare et al., 2022; De Bauw et al., 2020; Mai et al., 2019).

The RWU of a single segment is given by

$$q_r = 2a_{root}\pi l_{root}k_r(H_{sr} - H_x) = \frac{H_{sr} - H_x}{r_1}, \tag{17}$$

where q_r [cm^3/day] is the volumetric flow rate, see Eqns (7) and (8), and $r_1 = (2a_{root}\pi l_{root}k_r)^{-1}$ [day/cm^2] is the radial resistance to water flow trough the root.

The volumetric flow rate q_{sr} [cm^3/day] towards the soil-root interface through the perirhizal zone is equal to

$$q_{sr} = 2\pi l_{root}K_{prhiz}B\,(H_s - H_{sr}) = \frac{H_s - H_{sr}}{r_2}, \tag{18}$$

where H_s [cm] is the mean total soil potential of the segments perirhizal zone, K_{prhiz} [cm/day] is the average hydraulic conductance in the perirhizal zone and defined by

$$K_{prhiz} = \frac{\Phi(h_s) - \Phi(h_{sr})}{H_s - H_{sr}}, \tag{19}$$

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Preprint. Discussion started: 28 June 2024
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where Φ is the soil matric flux potential [cm^2/day], and $h_s := H_s - z$ is the soil matric potential in the perirhizal cylinder corresponding to the average volumetric water content in that cylinder and to the soil matric potential of the macroscopic soil model. Furthermore, $h_{sr} := H_{sr} - z$ is the matric potential at the soil root interface, B [1] is a geometry factor, and $r_2 = (2a_{root}\pi l_{root} K_{prhiz} B)^{-1}$ [day/cm^2] is the resistance to water flow trough the perirhizal zone. The geometry factor B [1] is dependent on ρ [1] which is the ratio of the outer radius of the perirhizal zone a_{prhiz} [cm] and the root radius a_{root} [cm]. The geometry factor is given by

$$B = \frac{2(\rho^2 - 1)}{(1 - 0.53\rho)^2 + 2\rho^2 \ln(0.53\rho)}, \tag{20}$$

$$\rho = \frac{a_{prhiz}}{a_{root}}. \tag{21}$$

A derivation of the geometry factor can be found in Schröder et al. (2008); Van Lier et al. (2006). The factor 0.53 represents the ratio between the radial distance from the root surface at which the water content is equal to the average perirhizal water content and the perirhizal radius.

For the steady rate assumptions the flux into the root q_r equals the flux through the perirhizal zone q_{sr}, i.e. $q_r = q_{sr} := q$. Since root and perirhizal zone resistances are serial we can compute the overall resistance as

$$q = \frac{H_s - H_x}{r_1 + r_2} = \frac{2\pi a_{root} l_{root} B k_r K_{prhiz}}{a_{root} k_r + B K_{prhiz}} (H_s - H_x) \tag{22}$$

where $r_1 + r_2$ is the resistance to water flow trough the root and perirhizal zone.

From $q_r = q_{sr}$ we can compute H_{sr} as

$$H_{sr} = \frac{a_{root} k_r H_x + B K_{prhiz} H_s}{a_{root} k_r + B K_{prhiz}}. \tag{23}$$

Note that K_{prhiz} is a function of H_{sr}, see Eqn (19), and we need to solve this implicit nonlinear equation for H_{sr} for given H_s and H_x. Note that for a simulation with a Neumann boundary condition, H_x is variable and depends also on H_{sr}. Thus, for any given value of H_s, two consistent values of H_x and H_{sr} need to be found.

To speed up computation time we pre-compute the solutions of Eqn (23) for a specific soil and create a four dimensional look up table depending on H_x, H_s, (a_{root} k_r), and ρ. We use a fixed point iteration to find consistent values H_x and H_{sr}, see Algorithm 1. Initialization of H_{sr} is done with H_{sr}^{prev} the soil-root interface potential of the previous time step, or H_s for the first time step.

2.4 Perirhizal geometry (xAx) versus uniform root length density (xBx)

The geometry of the perirhizal zone is cylindrical and determined by the root radius a_{root} [cm] and the outer perirhizal radius a_{prhiz} [cm]. The ratio ρ [1] between these two values enter the geometry factor B, see Eqn (20), and therefore affects the potential at soil root interface H_{sr}, see Eqn (23). We use use either 3D Voronoi mesh to obtain the outer perirhizal radii (models

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Algorithm 1 Fixed point iteration to find consistent values H_x and H_{sr}

Initialize: $k := 0$, $\mathbf{H}_x^0 := f_{root}(\mathbf{H}_{sr}^{prev})$, see Eqn (11)

(1) $\mathbf{H}_{sr}^{k+1} := f_{prhiz}(\mathbf{H}_x^k,\ \mathbf{H}_s)$, see Eqn (23)

(2) $\mathbf{H}_x^{k+1} := f_{root}(\mathbf{H}_{sr}^k)$, see Eqn (11)

(3) $k := k + 1$, and proceed with Step (1). until $\mathbf{H}_x^{k+1} \approx \mathbf{H}_x^k$ and $\mathbf{H}_{sr}^{k+1} \approx \mathbf{H}_{sr}^k$

of type xAx) or root length, surface or volume densities (models of type xBx).

In the first approach we use a 3D Voronoi mesh around the nodes of the root system. In this way the soil volume is partitioned into cells, where each node has a corresponding Voronoi cell, see Figure 3. The Voronoi cell faces are located at mid-distance between the neighbouring nodes. Therefore, the volume of the Voronoi cells are a good approximation of the node perirhizal volume, and we define the root segment's perirhizal volume vol_j [cm^3] as the the volume of the Voronoi cell of the segment's apical node. We approximate this volume by a cylindrical geometry of the same volume, i.e.,

$$vol_j = \pi l_{root,j}(a_{prhiz,j}^2 - a_{root,j}^2), \tag{24}$$

and we can calculate the outer perirhizal radius $a_{prhiz,j}$ for each root segment j as

$$a_{prhiz,j} = \sqrt{\frac{vol_j}{\pi l_{root,j}} + a_{root,j}^2}. \tag{25}$$

The more commonly used approach so far is to approximate the perirhizal geometry using root length density [cm/cm^3], surface density [cm^2/cm^3], or volume density [cm^3/cm^3] in a finite soil volume vol_{soil} [cm^3] (e.g. De Bauw et al., 2020; Mai et al., 2019). Assuming that the roots are evenly distributed, the perirhizal volume is given by

$$vol_j = t_j\ vol_{soil} \tag{26}$$

where t_j [1] is the ratio between segment length (surface, or volume) and total root length (surface, or volume) within the finite soil volume. The outer radius $a_{prhiz,j}$ for each root segment j is again given by Eqn (25).

If we couple the perirhizal models with a macroscopic soil model the Voronoi mesh or the density based method must be aligned with the macroscopic finite volume cells for mass conservation. For both methods this will affect the distribution of perirhizal radii, see Section 3.2. This density based approach is suitable for soils where the soil grid cells are 3D with edge length in the order of centimeters. For 1D layered soil grids, the Voronoi mesh-based is preferable allowing more realistic distributions of the true perirhizal zones within each soil layer. Note that both approaches are approximations since we assume a cylindrical perirhizal zone which is generally not the case. The Voronoi method computes more realistic perirhizal volumes but is computational expensive and less feasible for dynamic root growth.

https://doi.org/10.5194/egusphere-2024-1319
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2.5 Upscaling by aggregating RWU from root segment to soil element level (Bxx)

For developing larger scale models we want to describe the effect of the root system without keeping track of the exact root system geometry. Generally, the number of root segments is much higher, than the number of finite soil volumes for 1D, 2D or 3D soil models. Therefore, we aim for models that are described on the soil element level. These models are of category Bxx.

The linear system in Eqn (14) describes one equation per root node excluding the root collar, i.e $n-1$ equations. The number of soil cells m is generally much lower $m << n-1$, and we will rewrite the linear system in variables given per soil cell. We can sum up Eqn (13) regarding the soil cells by multiplying with the matrix $\mathbf{M}$, i.e.

$$\mathbf{M}\,\mathbf{q}_{root} = \mathbf{M}\,diag(\mathbf{K}_r)(\mathbf{I} - \mathbf{A}^{-1}\,diag(\mathbf{K}_r))\mathbf{H}_{sr} - \mathbf{M}\,diag(\mathbf{K}_r)\,\mathbf{A}^{-1}\,k_{x,1}\mathbf{e}_1\,H_{collar}, \tag{27}$$

where $\mathbf{M}$ is a $m \times (n-1)$ matrix mapping each root node index to a soil cell index. For each column (i.e. node index-1) the matrix contains exactly a 1 in the row of the soil cell index where the node is located and zero otherwise. Therefore, the RWU from a soil volume $\mathbf{q}_{soil}$ [cm^3/day] is given by

$$\mathbf{q}_{soil} = \mathbf{M}\,\mathbf{q}_{root}, \tag{28}$$

and right hand side of Eqn (27) exactly computes the soil fluxes. Now, we can simplify the system by assuming that the soil-root matric potential is the same in each soil cell.

We define $\mathbf{H}_{sr}^{soil} \in \mathbb{R}^m$ to be the mean value of the $\mathbf{H}_{sr}$ in each soil volume. Note that $(\mathbf{M}\,\mathbf{M}^T)$ is a $m \times m$ diagonal matrix containing the number of root nodes within each soil cell, therefore the mean value is given by

$$\mathbf{H}_{sr}^{soil} \;:=\; (\mathbf{M}\,\mathbf{M}^T)^{-1}\,\mathbf{M}\,\mathbf{H}_{sr} = (\mathbf{M}^T)^{+}\,\mathbf{H}_{sr}, \tag{29}$$

where $\mathbf{M}^{T+}$ is the Moore Penrose pseudo inverse of $\mathbf{M}^T$. We can approximately solve above equation for $\mathbf{H}_{sr}$ yielding

$$\mathbf{M}^T\,\mathbf{H}_{sr}^{soil} \;\approx\; \mathbf{H}_{sr}, \tag{30}$$

where $\mathbf{M}^T$ is an $n \times m$ matrix, $\mathbf{H}_{sr}^{soil}$ is a m dimensional vector at soil element level, and $\mathbf{H}_{sr}$ is a n dimensional vector at root segment level. Note that in this case, all entries of $\mathbf{H}_{sr}$ will be the same within every soil element and this assumption causes loss of information.

Inserting the approximation of Eqn (30) into Eqn (27) yields

$$\mathbf{q}_{soil} = \underbrace{\mathbf{M}\,diag(\mathbf{K}_r)(\mathbf{I} - \mathbf{A}^{-1}\,diag(\mathbf{K}_r))\mathbf{M}^T}_{\mathbf{A}_{up} \in \mathbb{R}^{m \times m}}\,\mathbf{H}_{sr}^{soil} - \underbrace{\mathbf{M}\,diag(\mathbf{K}_r)\,\mathbf{A}^{-1}\,k_{x,1}\mathbf{e}_1\,H_{collar}}_{\mathbf{b}_{up} \in \mathbb{R}^m}. \tag{31}$$

This much smaller linear system can be solved very quickly after calculating $\mathbf{A}_{up}$ once. However, the number of root nodes might be limiting since it is necessary to explicitly calculate $\mathbf{A}^{-1}$.

https://doi.org/10.5194/egusphere-2024-1319
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For including the perirhizal model in the aggregated approach (Eqn 31) the total potential $\mathbf{H}_x^{soil}$ can be calculated from $\mathbf{q}_{soil}$ summing up Eqn (7) over the soil cells:

$$\mathbf{M}\mathbf{q}_{root} = \mathbf{M}\, diag(\mathbf{K}_r)(\mathbf{H}_{sr} - \mathbf{H}_x) \tag{32}$$

$$\mathbf{M}\mathbf{q}_{root} = \mathbf{M}\, (diag(\mathbf{K}_r)^{-1} + diag(\mathbf{K}_{prhiz})^{-1})^{-1}(\mathbf{H}_s - \mathbf{H}_x) \tag{33}$$

$$\mathbf{q}_{soil} = \mathbf{M}\, diag(\mathbf{K}_r)(\mathbf{M}^T\, \mathbf{H}_{sr}^{soil} - \mathbf{M}^T\, \mathbf{H}_x^{soil}), \text{yielding} \tag{34}$$

$$\mathbf{H}_x^{soil} = \mathbf{H}_{sr}^{soil} - (\underbrace{\mathbf{M}\, diag(\mathbf{K}_r)\, \mathbf{M}^T}_{\mathbf{K}_{r,up} \in \mathbb{R}^{m \times m}})^{-1}\, \mathbf{q}_{soil}. \tag{35}$$

A suitable pair $\mathbf{H}_x^{soil}$ and $\mathbf{H}_{sr}^{soil}$ (both on soil element level) is found using a fixed point iteration as before for values per segment:

Algorithm 2 Fixed point iteration to find consistent values $\mathbf{H}_x^{soil}$ and $\mathbf{H}_{sr}^{soil}$

Initialize: $k := 0$, $\mathbf{H}_x^{soil,0} := h_{soil}(q_{soil}(\mathbf{H}_{sr}^{soil,prev}))$, applying Eqn (31) first, and then Eqn (35)

(1) $\mathbf{H}_{sr}^{soil,k+1} := f_{prhiz}(\mathbf{H}_x^{soil,k}, \mathbf{H}_s)$, Eqn (23), with averaged root and perirhizal radii per soil volume (3D) or soil layer (1D).

(2) $\mathbf{H}_x^{soil,k+1} := h_{soil}(q_{soil}(\mathbf{H}_{sr}^{soil,k}))$, , applying Eqn (31) first, and then Eqn (35)

(3) $k := k + 1$, proceed with Step (1), until $\mathbf{H}_x^{soil,k+1} \approx \mathbf{H}_x^{soil,k}$ and $\mathbf{H}_{sr}^{soil,k+1} \approx \mathbf{H}_{sr}^{soil,k}$

2.6 Upscaling by root architecture simplification - The parallel root system approach (Cxx)

In a further simplification step we replace the exact root system by a parallel root system, where we assume exactly one single root segment per soil element (Vanderborght et al., 2021). Each of these segments is is connected directly to the root collar by an artificial root segment, see Figure 4. The RWU of such a system is described by

$$\mathbf{q}_{soil} = K_{rs}\, diag(\mathbf{SUF}^{ups})\, (\mathbf{H}_{sr} - \mathbf{H}_{collar}), \tag{36}$$

where $\mathbf{H}_{sr}^{ups}$ is the total potential at the soil root interface and $\mathbf{H}_x^{ups}$ the total xylem potential of the parallel root system model. Root hydraulic parameters are chosen in a way that the macroscopic hydraulic properties of the exact root system are preserved. These properties are the root system conductance K_{rs}, the standard uptake fraction $\mathbf{SUF}^{ups}$, the total root length $\mathbf{l}^{ups}$, surface $\mathbf{surf}^{ups}$ and root radial conductance $\mathbf{K}_r^{ups}$ per each soil element. These models are of category Cxx. This model is simpler than Bxx, as the general incidence matrix representing the hydraulic root architecture and mapped to the soil elements is replaced by a simple diagonal matrix. This results in a computationally less expensive simulation at the cost of loss of accuracy, particularly noticeable for highly heterogeneous soil water potentials, as hydraulic lift can only occur via a 'detour' via the root collar.

https://doi.org/10.5194/egusphere-2024-1319
Preprint. Discussion started: 28 June 2024
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First, we obtain SUF, length, surface and root radial conductance per soil element by summing the corresponding values given per each root segment over each soil layer or soil volume,

$$\mathbf{SUF}^{ups} := \mathbf{M}\,\mathbf{SUF} \tag{37}$$

$$\mathbf{l}^{ups} := \mathbf{M}\,\mathbf{l} \tag{38}$$

$$\mathbf{surf}^{ups} := \mathbf{M}\,\mathbf{surf} \tag{39}$$

$$\mathbf{K}_r^{ups} := \mathbf{M}\,\mathbf{K}_r, \tag{40}$$

where $\mathbf{M}$ is a $m \times (n-1)$ matrix mapping each root node index to a soil cell index as described in the previous section. Therefore, $\mathbf{SUF}^{ups}$, $\mathbf{l}^{ups}$, $\mathbf{a}^{ups}$, and $\mathbf{K}_r^{ups}$ are $m \times 1$ vectors where m is the number of soil layers.

Next, we choose the axial conductance $\mathbf{K}_x^{ups}$ of the artificial segments, that connect the single root segments to the collar, in such a way, that the macroscopic root system hydraulic properties $\mathbf{SUF}$ and K_{rs} are the same as in the exact hydraulic model. For each soil layer the RWU can be described as

$$(\mathbf{q}^{soil})_i = K_{rs} SUF_i^{ups}((\mathbf{H}_{sr}^{ups})_i - H_{collar}) \tag{41}$$

$$= K_{r,i}^{ups}((\mathbf{H}_{sr}^{ups})_i - (\mathbf{H}_x^{ups})_i) \tag{42}$$

$$= K_{x,i}^{ups}((\mathbf{H}_x^{ups})_i - H_{collar}). \tag{43}$$

From these equations, we can we calculate $\mathbf{K}_x^{ups}$ as

$$(\mathbf{K}_x^{ups})_i = \frac{K_{rs} SUF_i^{ups}}{1 - K_{rs} SUF_i^{ups}/K_{r,i}^{ups}}, \tag{44}$$

using $K_{rs}SUF_i/K_{r,i}^{ups} = (H_{sr,i}^{ups} - H_{x,i}^{ups})/(H_{sr,i}^{ups} - H_{collar})$ from Eqns (41) and (42).

We use the same iteration as in Algorithm 1 but the exact root architecture is replaced by the parallel root model. We iterate to find a suitable pair of $\mathbf{H}_{sr}^{ups}$ and $\mathbf{H}_x^{ups}$.

Algorithm 3 Fixed point iteration to find consistent values $\mathbf{H}_{sr}^{ups}$ and $\mathbf{H}_x^{ups}$

Initialize: $k := 0$, $\mathbf{H}_x^{ups,0} := f_{root}(\mathbf{H}_{sr}^{ups,prev})$, see Eqn (11)

0: $\mathbf{H}_{sr}^{ups,k+1} := f_{prhiz}(\mathbf{H}_x^{ups,k}, \mathbf{H}_s^{ups})$, see Eqn (23)

0: $\mathbf{H}_x^{ups,k+1} := f_{root}(\mathbf{H}_{sr}^{ups,k})$, see Eqn (11)

0: $k := k+1$, and proceed with Step (1). until $\mathbf{H}_x^{ups,k+1} \approx \mathbf{H}_x^{ups,k}$ and $\mathbf{H}_{sr}^{ups,k+1} \approx \mathbf{H}_{sr}^{ups,k}$

With the parallel root system approach the exact root architecture and hydraulic properties can be neglected, while K_{rs} and $\mathbf{SUF}^{ups}$ are still preserved. The simplified model is typically much faster to solve having less than 1% of the degrees of freedom of the original root system. Furthermore, root hydraulics is solely depend on the parameters K_{rs}, $\mathbf{l}^{ups}$, $\mathbf{a}^{ups}$, and $\mathbf{K}_r^{ups}$, which are much easier to handle compared to the full hydraulic model. At a constant total soil potential the approximation will be exact, but we expect differences in dynamic settings where strong variations in soil potentials can appear.

https://doi.org/10.5194/egusphere-2024-1319
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2.7 Root soil hydraulic scenarios

Root hydraulic properties are given by the root radial conductivities and root axial conductances. These values were taken from literature (Knipfer and Fricke, 2010) for spring barley using linear regression, and (Couvreur et al., 2012) for maize. The hydraulic properties depend on the age of the root segments, see Figure 5. For both measurements axial conductances increase with root age, while radial conductances decrease. Soil hydraulic properties were described by the van Genuchten model (Van Genuchten, 1980). We obtained typical parameters for loam, clay, and sandy loam using the Hydrus 1D soil catalog (Simunek et al., 2005), see Table 1.

In order to simulate field conditions, we consider the root architectures of spring barley and maize in a periodic domain. In this way we have to contrasting set-ups: For spring barley, we choose an inter-row distance of 13 cm and plant spacing of 3 cm. For maize, we choose a larger inter-row distance of 76 cm and plant spacing of 16 cm. We consider both plants at the end of their vegetative stage, resulting in a growth period of 7 weeks for spring barley and 8 weeks for maize.

All the following scenarios include nonlinear conductivities from the perirhizal model. The simulations describe depletion from an initially wet soil of -200 cm total potential using a transpiration rate of 0.5 [cm/day] with a sinusoidal shape from 6 am to 6 pm with maximal transpiration at noon, and no uptake during night. Actual RWU and corresponding cumulative uptake is calculated over two weeks.

3 Results

In the following we first present the simulation results of root architecture, and the corresponding precomputed perirhizal outer radii. Then we show simulation results of the root hydraulic models using the dynamic scenarios presented in Section 2.7. The implementation of the new up-scaled models was performed in the framework of CPlantBox and dumux-rosi, and the following results can be found in the branch 'upscaling'.

3.1 Root architectures for spring barley and maize

Figure 6 shows the root architecture development after 7 weeks for spring barley and after 8 weeks for maize, and illustrates the concept of using periodicity to mimic field conditions. The roots axial resolution is set to a maximum of 0.5 cm yielding a final amount of 6.92×10^3 nodes for the spring barley and 4.82×10^4 segments for the maize root system.

From root topology and root hydraulic parameters at segment level (see Section 2.7) we calculated the macroscopic root system hydraulic parameters K_{rs}, and SUF, see left lower subplots in Figure 6. Spring barley has a K_{rs} of 0.0064 [cm^2/day] and maize of 0.1345 [cm^2/day].

https://doi.org/10.5194/egusphere-2024-1319
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3.2 Perirhizal outer radii

Perirhizal outer radii are precomputed for both root systems. The first approach (xAx, see Section 2.4) is using a Voronoi mesh that is aligned to the soil grids, i.e., the maximum Voronoi cell volume is equal to soil cell volume. Figure 7 shows the distribution of perirhizal outer radii top soil 0-30 cm depth and subsoil 30-150 cm depth. Note that the perirhizal radius can be larger than $\sqrt{vol_{soil}/\pi}$ if the root segment length is small, see Eqn(25). In both root architectures root density in the top soil is higher leading to a smaller mean outer perirhizal radius in the top soil. For spring barley mean outer radius is 0.51 cm (3D) and 0.71 cm (1D) in topsoil, and 0.53 cm (3D) and 0.92 (1D) in subsoil; for maize 0.47 (3D), 0.65 (2D), 0.75 (1D) cm in topsoil, and 0.55 (3D), 0.92 (2D), 1.14 (1D) cm in subsoil. A reduction in dimensions of the soil grid generally leads to higher mean outer perirhizal radii.

The second approach (xBx, see Section 2.4) uses root length, surface or volume densities to compute the perirhizal outer radii. Figure 8 shows the distribution of perirhizal outer radii in top and subsoil based on length densities for the soil grid types used in the simulations. As for the Voronoi method top soil mean outer radii are smaller due to higher root density: 0.43 (3D), 0.72 (1D) cm for spring barley and 0.42 (3D), 0.65 (2D), 1.05 (1D) cm for maize. For sub soil mean radii are 0.51 (3D), 1.02 (1D) cm for spring barley, and 0.49 (3D), 0.93 (2D), 1.5 (1D) cm for maize. For the 1D soil layers the histogram is strongly divided into radii classes because the limited number of soil layers, where most smaller outer radii are located in the upper layers. For 1D soil grids we expect the largest deviation in model results compared to using the Voronoi method.

3.3 Root soil hydraulic simulation results

3.3.1 Full hydraulic model where using a 3D grid (AAA) compared to a lower dimensional grid (AAB)

The full hydraulic 3D model is solved as described in Section 2.3 and perirhizal radii were determined using the Voronoi method (see Section 2.4) for the scenarios presented in Section 2.7. We compare using a 3D macroscopic soil with a resolution of 1 cm^3 (reference scenario AAA) to using a 1D macroscopic soil with layers of 1 cm thickness (AAB), where only the vertical water movement is considered. Figure 9 shows the resulting soil matric potential for maize in loam soil after 2 weeks of simulation time, and highlights the difference between the 3D grid and the 1D grid where horizontal water movement is neglected. Using a 3D grid (left subplot) shows the development of local water depletion around areas with high RLD, while using a 1D grid (right subplot) relies on averaged values per layer.

The actual and cumulative transpiration is presented in Figure 10 for the three soil types. The solid curve represents the reference scenario (AAA), the dashed line the scenario using a 1D macroscopic soil grid (AAB). Additionally, for maize the dotted line shows the solution using a 2D macroscopic grid, where water movement along the plant rows is neglected. Generally, for maize water stress occurred earlier compared to spring barley for loam and clay. For sandy loam both root systems were immediately in stress. The differences in cumulative root uptake are much higher for maize, since there is more variation

https://doi.org/10.5194/egusphere-2024-1319
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in RLD due to the distance between the planting rows. Using a 2D macroscopic grid, where water movement in this direction is enabled, yields an improved accuracy. For spring barley RLD is much more uniform due to smaller planting distances, and therefore the error by neglecting lateral water movement is small. Additionally, the differences are smaller in finer textured soils since they redistribute the water over larger distances so that the soil water potential is more uniform.

A lower dimensional soil grid leads to an overestimation of RWU. For spring barley after one week cumulative root uptake differed 1% for loam, 0.7% for clay, and 12.5% for sandy loam, after two weeks the error increases to 1.6% for loam, 1.7% for clay and 13.9% for sandy loam. For maize cumulative transpiration is largely overestimated using a 1D soil grid. After one week simulation time it differed 43.5% for loam, 28.1% for clay, and 115.1% for sandy loam, after two weeks 62.4% for loam, 42.5% for clay, and 110.8% for sandy loam. Using a 2D soil grid errors for maize reduced to 13.3% for loam, 8% for clay, and 45.5% for sandy loam after one week, and 13.4%, 8.4%, and 34.9% after two weeks.

Figures 11 and 12 show the RWU of spring barley and maize from soil at noon (top row) and redistribution during night (bottom row) for the three soil types. Solid lines represent the results using a 3D soil grid (AAA), while dashed lines use a 1D grid (AAB). The different root architectures result in different RWU patterns. In the beginning (blue line) the RWU is proportional to the SUF since the initial soil total potential is constant. First, water is taken up from the upper layers, later when the upper layer becomes drier, more water is taken up from the lower layers, qualitatively changing the shape of the RWU profile. During night water is redistributed from the lower layers into the upper layers. Redistribution is strongest for clay for both, spring barley and maize, and negligible for sandy loam.

Using a 1D soil grid leads to differences in RWU patterns: For spring barley the differences are small in all soil types over the whole period of two weeks. Differences in maize are strong due to the overestimated cumulative transpiration (see right column Figure 10), which also impacts the local uptake. For loam and clay soil uptake from the upper layer is largely overestimated at the beginning leading to a delayed dynamic in water uptake and redistribution. For loam and clay the RWU is proportional to the SUF for the first two days until the profile changes due to soil water depletion in the upper layers.

While introducing errors, computational time decreases. For spring barley the model runs 5 times faster for loam and clay, and 3 times for sandy loam. For maize the speed up compared to the 3D soil grid is higher, since the 3D domain is larger, yielding a speed up of 15 times for loam, 18 times for clay, an 11 times for sandy loam for the 1D grid, and 8 times for loam and clay, and 10 times for sandy loam for the 2D grid.

https://doi.org/10.5194/egusphere-2024-1319
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3.3.2 The impact of using density based outer perirhizal radii instead of the Voronoi method (AAA vs. ABA, and AAB vs. ABB)

We compare the full hydraulic model using the 3D macroscopic soil and Voronoi method for the outer perirhizal radii (AAA) to the same model, where the outer radii were based on root length, surface or volume (ABA). Actual transpiration and the shape and dynamics of the resulting RWU were similar, and errors of cumulative transpiration were under 1% after two weeks.

The approximation has a a stronger impact on the results in 1D, because the soil layers are much larger than the soil volumes in 3D, and root length, surface or volume densities are constant in each of these soil volumes. Figure 13 shows a comparison between the full hydraulic 3D model in a 1D soil grid using Voronoi method (AAB) and an approximation based on densities (ABB). The choice to calculate outer radii based on root length, surface or volume showed negligible differences on the overall cumulative root uptake, with exception of maize in loam soil: Radii based on length densities overestimate the cumulative flux for 1%, while it is underestimated for 6% based on surface or volume. For spring barley the difference between Voronoi and density based methods is small. After two weeks cumulative flux is underestimated less than 1% for loam and clay, and 3.1% for sandy loam. For maize the differences are stronger leading to an error of approximately 6% for loam using surface or volume densities (1.2% for length), 5% for clay, and 16% for sandy loam.

Figures 14 and 15 show the RWU from soil at noon (top row) and redistribution during night (bottom row) for spring barley and maize using a 1D grid for the three soil types comparing the two different methods of determination of perirhizal radii, using Voronoi method, or based on RLD. Solid lines represent the results using Voronoi method (AAB), and dashed lines use outer radii based on RLD (ABB). Figure 14 shows that for spring barley the shape and dynamics of RWU are similar. For maize (Figure 15) small deviations can be observed around day 6 for loam and clay. For clay soil the error increases leading to less water redistribution using the approximation. For sandy loam RWU is strongly underestimated in the beginning of the simulation but RWU profiles become more similar for later simulation times (day 6 and day 13).

The Voronoi method is computational expensive, but the outer radii can be precomputed. Therefore, there is no speed up in simulation time using the density based methods. The approximation using density based outer radii is very accurate regarding RWU but needs review for more complex rhizosphere models, e.g. including root solute uptake.

3.3.3 Full hydraulic model (ABB) compared to the upscaled root hydraulic model (BBB)

In the next step we replace the full 3D hydraulic model with a 1D grid (ABB) by the aggregated model (BBB) (see Section 2.5), and compare plant actual and cumulative transpiration, see Figure 16. The approximation works very well for loam and clay: for spring barley the error is less than 0.8%, for maize less 1.9% for loam and 5.7% for clay after two weeks. For sandy loam the cumulative transpiration is underestimated for around 20% for spring barley and 9.5% for maize. This indicates that in the case of sandy loam the variation in root xylem potentials across one soil layer is high, and therefore, we introduce a

https://doi.org/10.5194/egusphere-2024-1319
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larger error by using the same total potential at the root-soil interface and the xylems for each layer, see approximation Eqn (30).

Figure 17 Figure 18 presents the RWU profiles for spring barley and maize. It reveals that aggregation works well for loam and clay. However, for sandy soil the profiles show qualitative differences, strongly underestimating RWU in the lower soil layers for both plants and in the case of maize initially overestimating RWU in the upper layers.

Compared to the full 3D root hydraulic model using a 1D soil grid (ABB), computation time was 6-8 times faster for spring barley, and 75-100 times faster for the maize using the aggregated model. Generally, the speed up of the method is mainly dependent on the number root of segments, which is reduced to the number of soil elements. The total speed up of aggregated model in a 1D soil (BBB) compared to the full hydraulic model using a 3D soil grid (ABA) is around 25 times for spring barley and 1000 times for maize.

3.3.4 Full hydraulic model (ABB) compared to the parallel root system (CBB)

As a further simplification, we replace the 3D full hydraulic root model using a 1D grid (ABB) by the parallel root model (CBB) (see Section 2.6). Figure 19 shows the actual and cumulative transpiration of spring barley and maize. For spring barley the parallel root system underestimates the actual transpiration. After two weeks the error of the cumulative transpiration is 11.9% for loam, 12.3% for clay, and 20.2% for sandy loam. For the maize root system the actual transpiration is overestimated with errors of 1.7%, 6.4% and 30.4% for loam, clay, and sandy loam.

Figure 20 and Figure 21 show the RWU profiles for the parallel root system model for spring barley and maize. For loam and clay the profiles look very similar, for spring barley redistribution is shifted upwards after day 6. As in the case of the aggregated model, sandy loam has the largest error.

The computational speed up of the parallel root system model (CBB) compared to the full hydraulic model (ABB) is similar of the speed up of the aggregated model. The reason for this is that in both models the degrees of freedom are proportional to the number of soil layers. Compared to the full root hydraulic model, computation time was 7-8 times faster for spring barley and 96-126 times faster. The total speed up of the parallel model in a 1D soil (CBB) compared to the full hydraulic model using a 3D grid (ABA) is around 30 times for spring barley and 1180 times for maize.

The advantage of the parallel root system is that the number of parameters are small compared to the full hydraulic model or the aggregated model. The root system hydraulic properties are solely described by SUF, length l, root surface $surf$, and radial conductivity K_r per soil layer, see Section 2.6, which can be easily managed by larger scale models.

https://doi.org/10.5194/egusphere-2024-1319
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4 Discussion

The right spatial and temporal scale of a mathematical model is often a balance between accuracy and efficiency. Equally important, small scale mechanistic models are often hard to parameterize and not feasible for larger scale applications (Roose and Schnepf, 2008). In this study we showed step by step how to develop larger scale models, from fully parameterized mechanistic hydraulic root-soil interaction models, such as presented by Schnepf et al. (2023, 2020). We analyse the increase of efficiency by each upcaling step, the error that is introduced, and the number of model parameters that are needed. Tables 2, and 3 show the errors and the corresponding speed ups introduced by the upscaled models for spring barley, and maize using a 1D grid or 2D grid. Results suggest that the error introduced by the upscaling steps depend on the root architecture as well as the root and soil hydraulic properties.

Reducing the dimensionality of the macroscopic soil model from 3D to 1D (AAA vs. AAB) works well if lateral water movement can indeed be neglected. This is the case if roots are evenly distributed with similar root hydraulic properties (Couvreur et al., 2014). Furthermore, even if the roots are evenly distributed, they also need to be sufficiently dense, depending on the soil hydraulic conductivity. Otherwise, isolated depletion zones can develop which would lead to horizontal fluxes in the 3D soil domain that are not represented in the 1D soil layer. For spring barley this worked well for loam and clay, but for sandy loam we observed a larger error due to low soil conductivity. For maize errors were larger due to its non-uniform root distribution. Generally, the accuracy of 1D soil models is dependent on the inter-row and planting distance. In the maize scenario root density strongly varies in the direction between two plant rows. Therefore, to maintain a more precise model it is recommendable to neglect only one dimension, keeping the direction orthogonal to the the planting row, and averaging along the direction of the planting row, where changes of root density are expected to be smaller. In case of maize using a 2D macroscopic soil model reduced the error, with a speed up between five to ten times dependent on the soil type (see Table 3).

We used a new method to determine the outer radii of the perirhizal zones based on Voronoi diagrams in 3D similar as Kohl et al. (2007) did for 2D root observations in trenches. We compared these more exact results to the common approach calculating the radii based on length, surface or volume densities (AAB vs. ABB), e.g. (Schröder et al., 2008; Van Lier et al., 2006). Generally, the approximation using densities works very well with negligible impact for 3D soil grids, and stronger impact using 1D soil layers. In the 1D case, using the Voronoi approach leads to higher radii at the root tips, since the Voronoi cell volumes are statistically larger at the root tip nodes where a small root segment has access to a large soil volume. Thus, those parts of the root system with a higher root radial conductance have access to a larger soil volume compared to the uniformly distributed roots, leading to an increased actual transpiration. Since restricting the model to vertical movement leads to an overestimation of actual transpiration, the underestimation of actual transpiration of the more classical approaches seems beneficial. Overall, we showed that perirhizal radii based on length, surface, and volume densities introduced only a small error compared to the other upscaling steps. For both plants the sandy loam scenario lead to the highest discrepancies in cumulative plant uptake because low soil conductivity leads to steeper gradients in the rhizosphere, and generally increases the importance

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of the perirhizal zones.

Upscaling by aggregating RWU from root segment to soil element level was introduced by Couvreur et al. (2012) not considering any perirhizal conductance's. In this case the total potential at the soil root interface is the same for all root segments in each soil layer in the full hydraulic model and the aggregated one. Vanderborght et al. (2023) included perirhizal conductance's which leads to individual total potentials at the soil root interface for the full hydraulic model, and aggregation leads to the additional assumption that these total potentials at the soil root interface are equal in each soil layer. In this study we tested this assumption for the first time in dynamic settings. The approximation performs well in loam and clay soil because of the higher soil conductivity with relatives errors less than 1% for spring barley (0.04 mm and 0.05 mm absolute error) and maize (+-0.5 mm absolute error for 1D, and -1.7 mm and -0.6 mm 2D) compared to reference scenario AAB. For sandy loam cumulative transpiration was underestimated around 23% for both plants (5.9 mm for spring barley, and -3.9 mm for maize 1D and -2.5 maize 2D), see Tables 2 and 3. The speed up of the method is dependent on the number of segments within the root system. Depending on soil type the aggregated model is at least 26 times faster for spring barley and 1111 times faster for maize using a 1D grid and 28 times faster using a 2D grid.

In a further step we replaced the root architecture model with a parallel root model to obtain a more efficient model with less parameters, which is easier to parameterise and can be used in an easier way by larger scale models (Vanderborght et al., 2024). It relies only on the root system conductivity K_{rs} and values given per soil layer (SUF, length l, root surface $surf$, and radial conductivity K_r) and needs no additional information on root system topology. Results are exact when the soil-root interface potentials are uniform. For non-uniform soil-root interface potentials, the uptake compensation is not exact anymore. Under the dynamic depletion scenarios this approach lead to an underestimation of cumulative uptake for spring barley and an overestimation for maize, owing to different root hydraulic properties. The parallel model (CBB) is an efficient approximation with the largest speed ups where the lumped parameters are derived from the mechanistic parameters of the detailed model (AAA).

5 Conclusion

RWU is crucial for soil water balance and plant development. We describe soil-root hydraulics and dynamic root architecture in a mechanistic way and analyse upscaling methods to develop efficient sink terms for land surface or crop models.

In this study, we explored the mathematical fundamentals of the different upscaling approaches and the the impact of each simplifications step. Reducing the dimensionality of the macroscopic soil model from 3D to 1D (AAA vs. AAB) worked well if lateral water movement can indeed be neglected. This depended on root distribution, as well as root and soil hydraulic properties. Assuming homogeneously distributed roots to calculate the outer perirhizal radii provided accurate results regarding RWU (AAB vs. ABB), but needs review for more complex rhizosphere models. Generally, the approximation had a stronger

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impact using coarse 1D soil layers, which leads to an underestimation of actual transpiration of the actual transpiration. The exactly upscaled model (BBB) with uniform soil root interface water potentials offered a large speed up in computation time introducing only small errors compared to the error introduced by dimensionality reduction. The parallel root model (CBB) introduced slightly larger errors but can be implemented more easily in larger scale models due to lower number of model parameters.

This study highlights the importance of carefully considering the trade-offs between model complexity and accuracy. By pinpointing the sources of errors and understanding where they accumulate or cancel out, we provide guidance for choosing appropriate models based on the required performance and accuracy. This knowledge facilitates the development of new sink terms and enhances the reliability of RWU modeling in diverse agricultural and environmental contexts.

Code availability. The implementation of the up-scaled models was performed in the framework of CPlantBox and dumux-rosi and results can be found in the branch dumux-rosi branch 'upscaling'.

Author contributions. JV initiated this study on quantifying accuracy and computational speed of efficient macroscopic sink terms including perirhizal resistance. Model implementation was done by DL and codes were revised by AS. All authors contributed to the conceptualization of the paper. DL mainly wrote the paper, which was critically reviewed by all co-authors.

Competing interests. The authors declare that they have no conflict of interest.

Acknowledgements. This project was partially funded by the BMBF in the frame of Rhizo4Bio (Phase 1): RhizoWheat - Rhizosphere processes and yield decline in wheat crop rotations, grant no. 031B091OB.

https://doi.org/10.5194/egusphere-2024-1319
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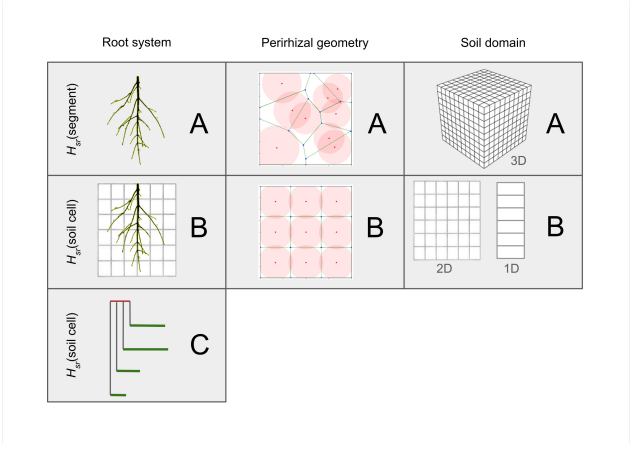


Figure 1. The first column shows the simplification of RWU regarding the root architecture: full (A), exactly upscaled with uniform soil root interface water potentials (B), parallel root model with uniform soil root interface water potentials (C). The second column shows a 2D representation of the perirhizal radii computation using Voronoi diagrams (A) or uniform perirhizal radii for all root segments in a soil element (B). The third column describes the macroscopic soil domain as 3D (A), or the cases where we assume that the soil water potential does not change in specific directions (B).

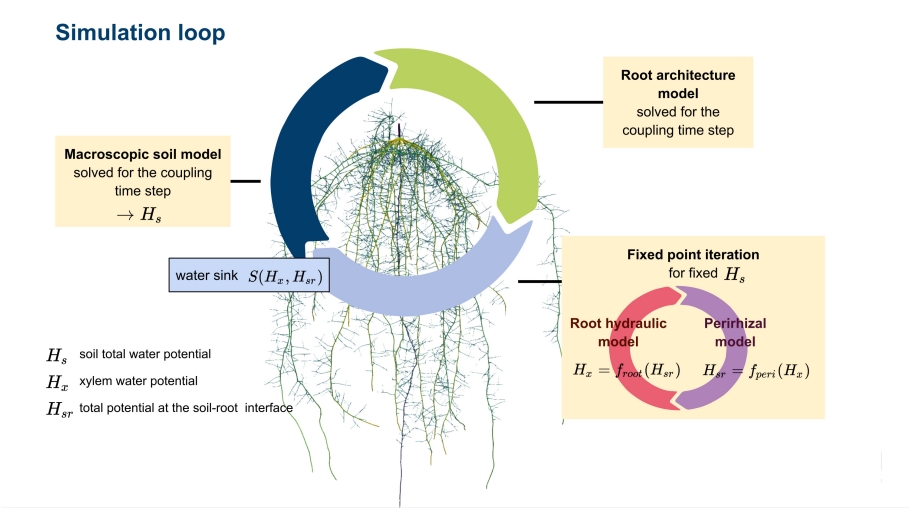


Figure 2. The main simulation loop first solves the macroscopic soil model yielding the total soil potential H_s, next optionally, root architectural development, and finally, finds consistent values for the total xylem water potential H_x and soil-root interface potentials H_{sr} using a fixed-point iteration. Sink terms are calculated from the potentials H_x and H_{sr}.

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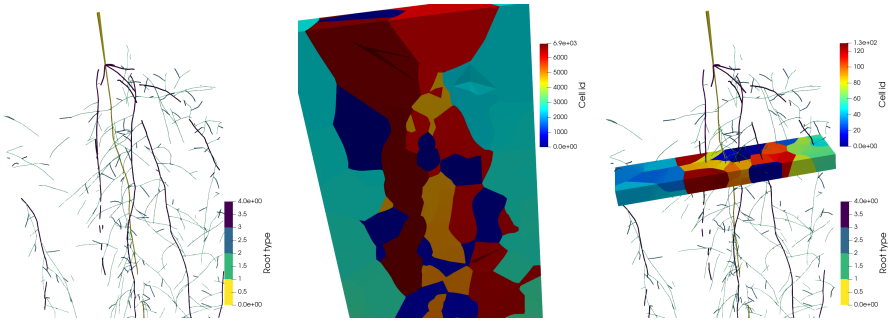


Figure 3. The left plot shows the spring barley root system mapped to a periodic domain. The mid plot shows the Voronoi diagram bounded by the periodic domain, where each Voronoi cell is located around a node. The right plot shows the Voronoi diagram of single layer with 1 cm height.

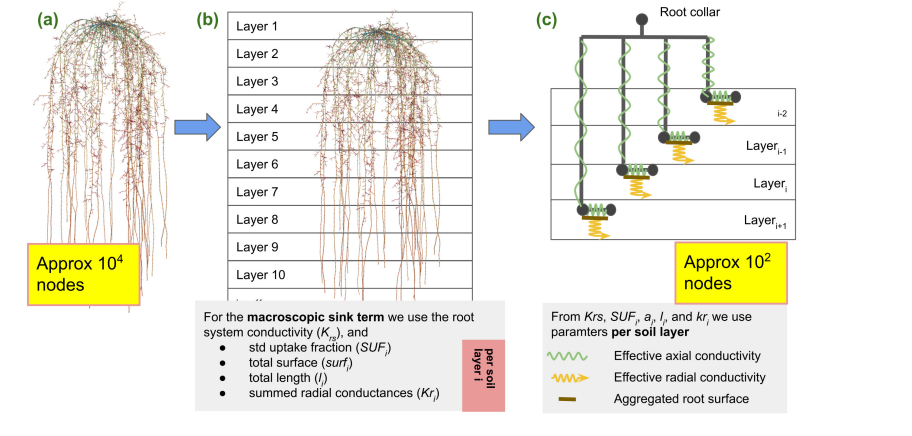


Figure 4. Starting from the full hydraulic model, subplot (a), we first derive the root system conductance K_{rs} and layer aggregated root hydraulic root properties, subplot (b). These are given for each soil layer or soil volume i as SUF_i^{ups}, total root surface $surf_i^{ups}$, total summed length l_i^{ups} and mean radial conductivity $K_{r,i}^{ups}$. In a final step, subplot (c) we neglect the actual root architecture and replace it by a parallel root system with hydraulic parameters preserving the macroscopic hydraulic properties.

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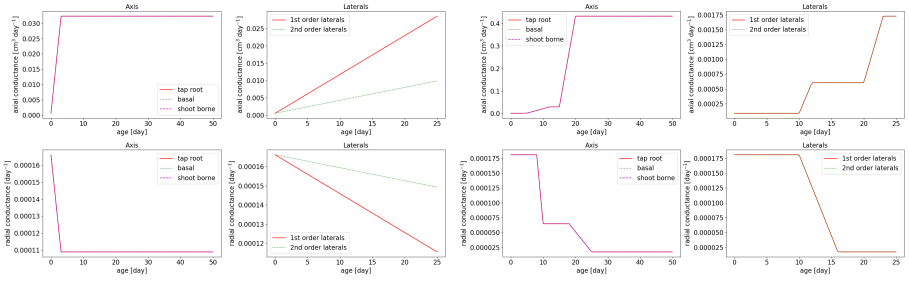


Figure 5. The age dependent root axial conductances and radial conductivities for spring barley (left sub-plot) and maize (right sub-plot).

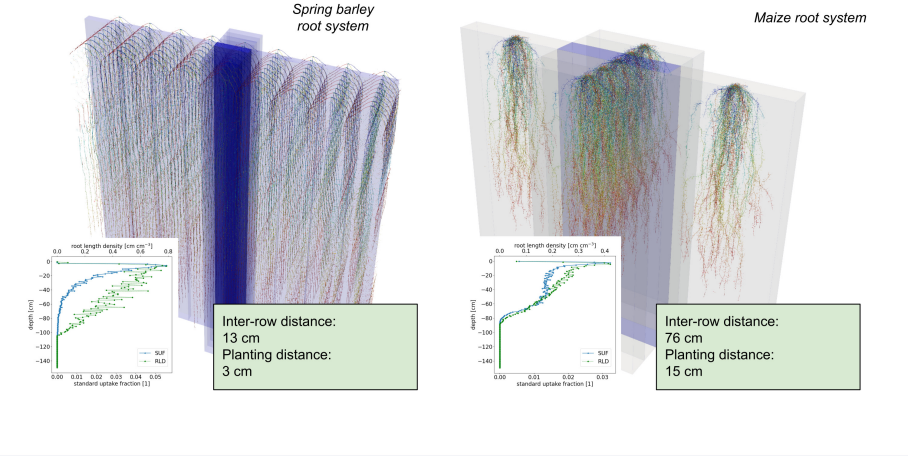


Figure 6. Spring barley (left-subplot) and maize (right-subplot) root architecture under field conditions, both at the end of their vegetative stage (after 7 weeks for spring barley, 8 weeks for maize). In the lower left subplots we show the corresponding SUF and root length density RLD.

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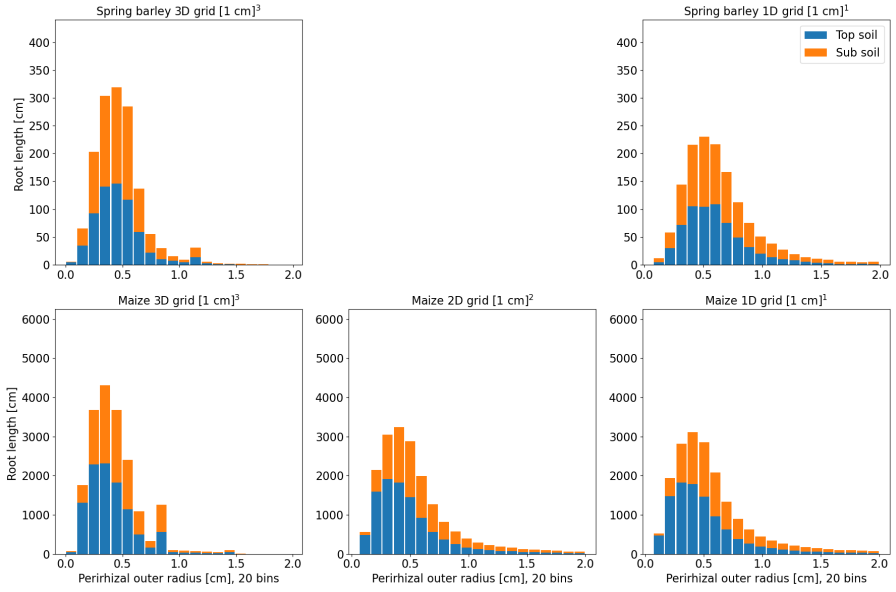


Figure 7. Histogram of perirhizal zone outer radii using a 3D Voronoi diagram for spring barley (top) and maize (right) for the soil grids used in the following sections. Colours denote typical soil horizons: top soil 0-30 cm depth, and subsoil 30-150 cm depth.

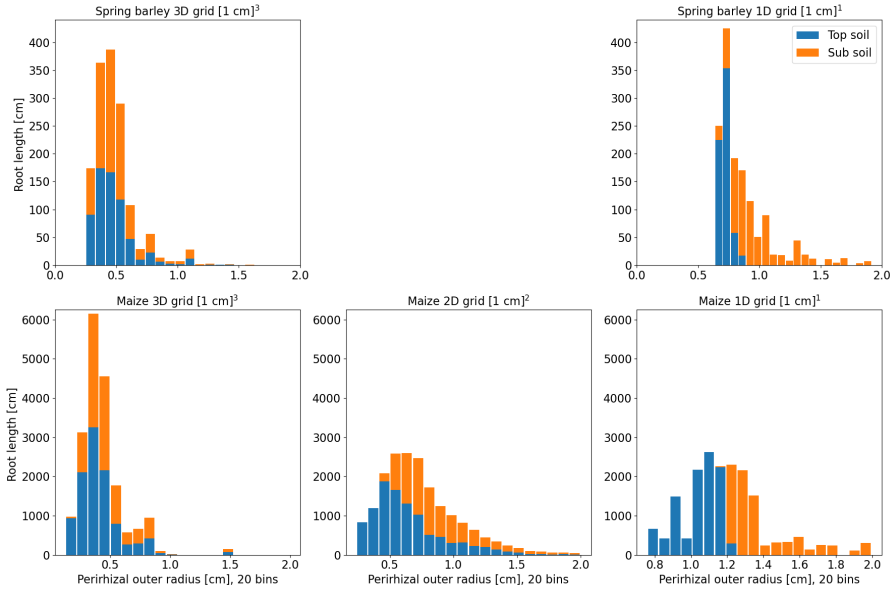


Figure 8. Histogram of perirhizal zone outer radii using root length densities to obtain perirhizal outer radii for spring barley (top) and maize (right) for the soil grids used in the following sections. Colours denote typical soil horizons: top soil 0-30 cm depth, and subsoil 30-150 cm depth.

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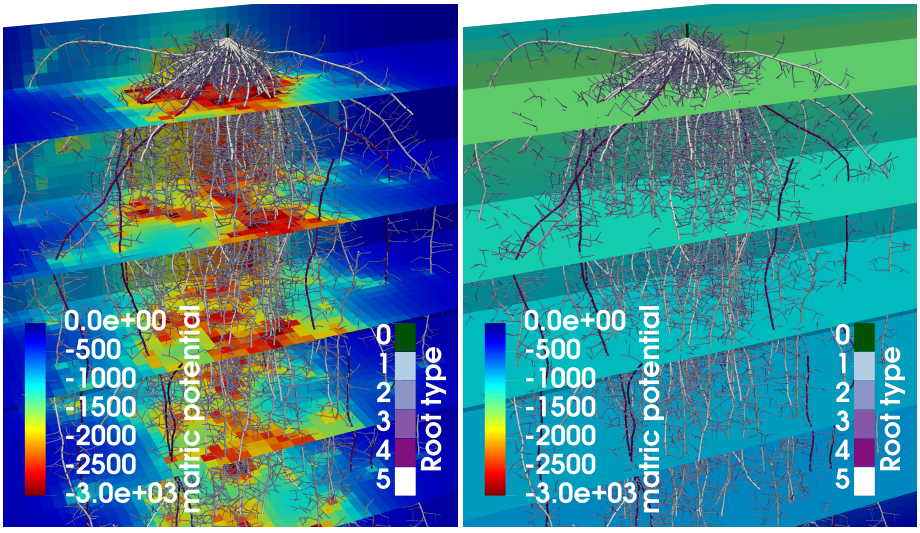


Figure 9. Soil matric potential for maize in loam soil after 2 weeks of simulation time in a 3D grid (left subplot) and a 1D grid (right subplot). In the left subplot local depletion develops around areas with high RLD, while in the right subplot the water potential is constant per soil layer.

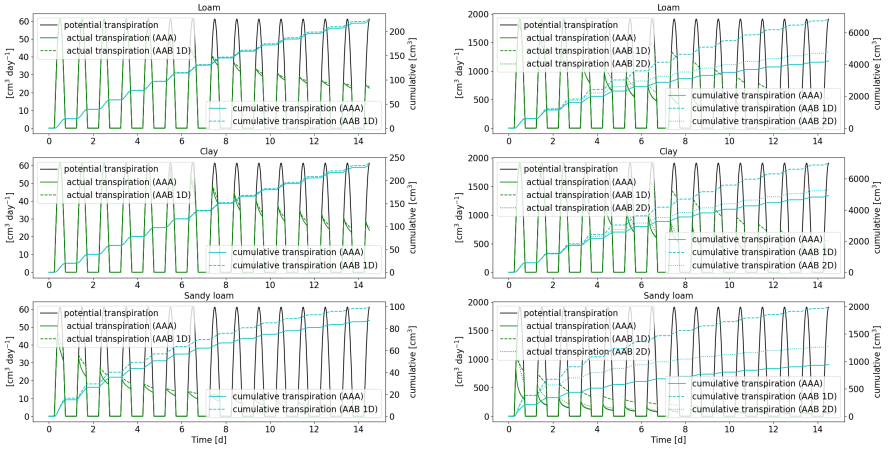


Figure 10. Potential and actual transpiration of the full 3D hydraulic model of spring barley (left) and maize (right) for the soil types loam (top), clay (mid) and sandy loam (bottom). The blue line indicates the cumulative plant water uptake. Solid lines represent the results using a 3D soil grid (AAA), while dashed lines are the results using a 1D grid, and dotted lines a 2D grid (AAB).

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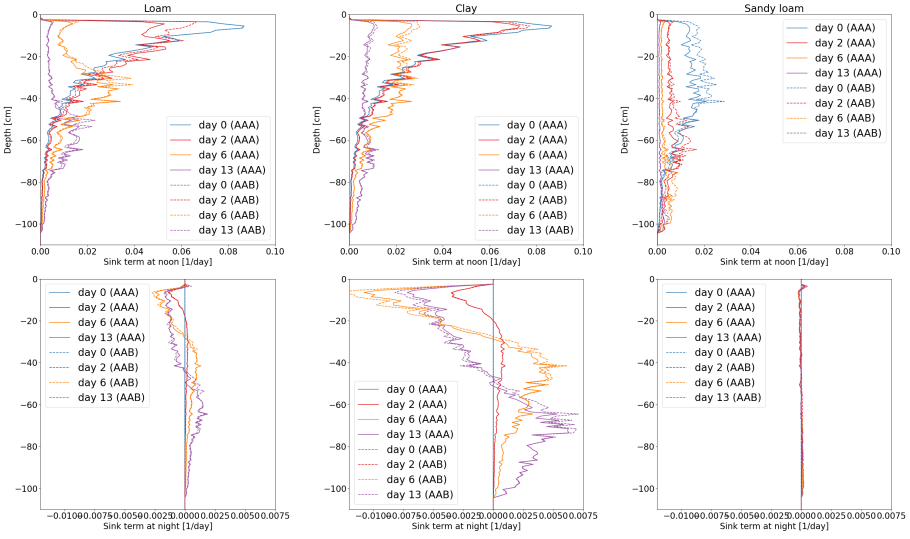


Figure 11. Vertical RWU of the full hydraulic 3D model during noon (top row) and redistribution during night (bottom row) of spring barley for loam (left column), clay (mid column), and sandy loam (right column). Solid lines represent the results using a 3D soil grid (AAA), while dashed lines use a 1D grid (AAB).

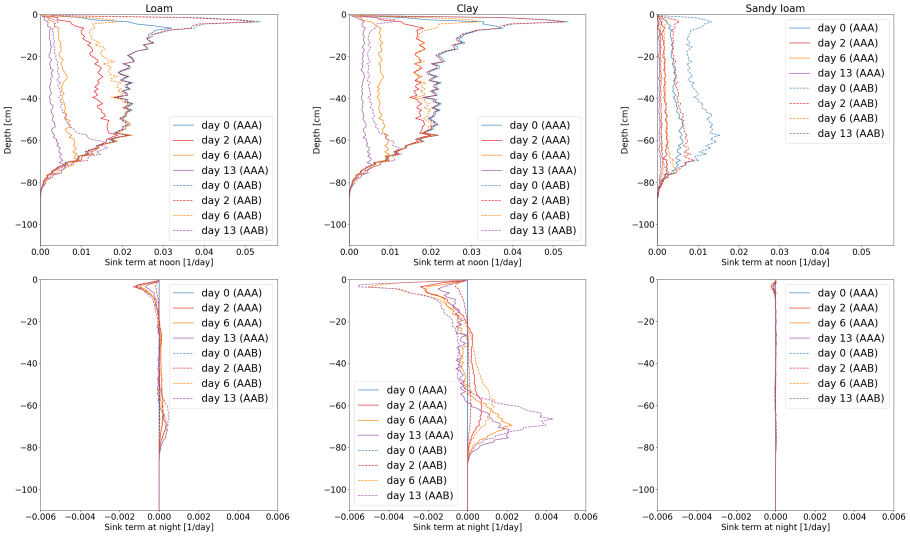


Figure 12. Vertical RWU of the full hydraulic 3D model during noon (top row) and redistribution during night (bottom row) of maize for loam (left column), clay (mid column), and sandy loam (right column). Solid lines represent the results using a 3D soil grid (AAA), while dashed lines use a 1D grid (AAB).

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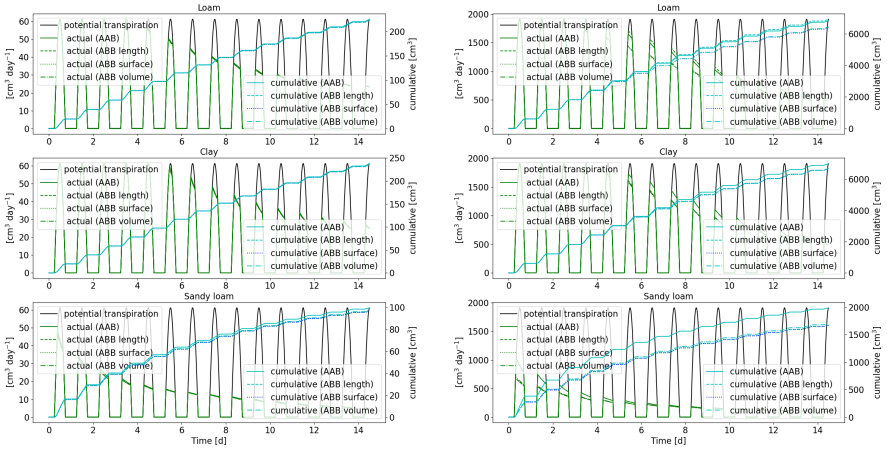


Figure 13. Potential and actual transpiration of the full hydraulic 3D model of spring barley (left) and maize (right) for the soil types loam (top), clay (mid) and sandy loam (bottom) in a 1D soil grid. The blue line indicates the cumulative plant water uptake. Solid lines represent the results using Voronoi method (AAB), while dashed lines use outer radii based on root length, surface or volume densities (ABB).

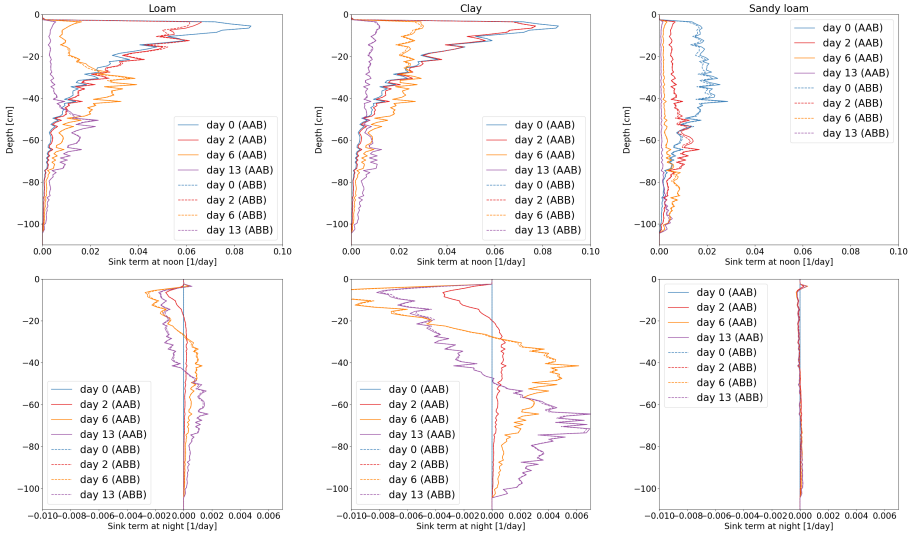


Figure 14. Vertical RWU of spring barley using the full hydraulic 3D model during noon (top row) and redistribution during night (bottom row) of spring barley for loam (left column), clay (mid column), and sandy loam (right column) in a 1D soil grid. Solid lines represent the results using Voronoi method (AAB), while dashed lines use RLD based outer radii (ABB).

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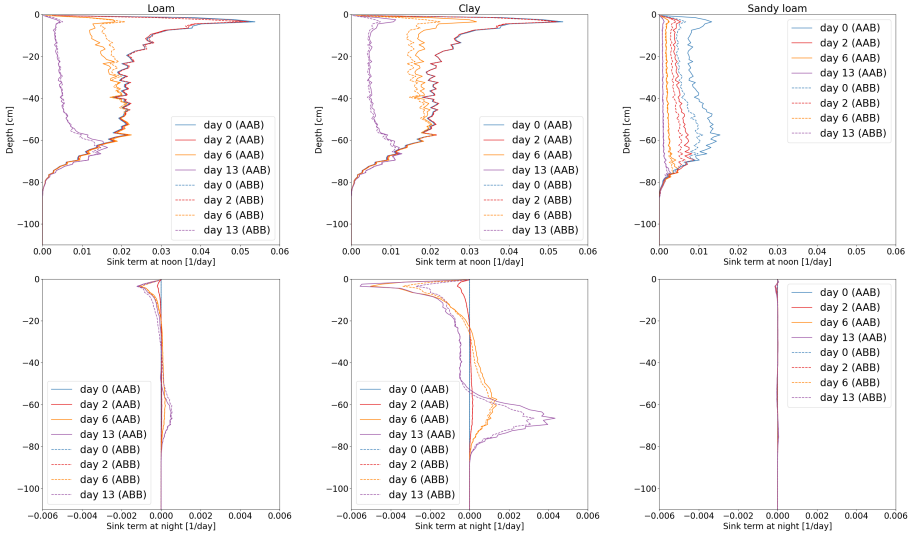


Figure 15. Vertical RWU of the full hydraulic 3D model during noon (top row) and redistribution during night (bottom row) of maize for loam (left column), clay (mid column), and sandy loam (right column) in a 1D soil grid. Solid lines represent the results using Voronoi method (AAB), while dashed lines use RLD based outer radii (ABB).

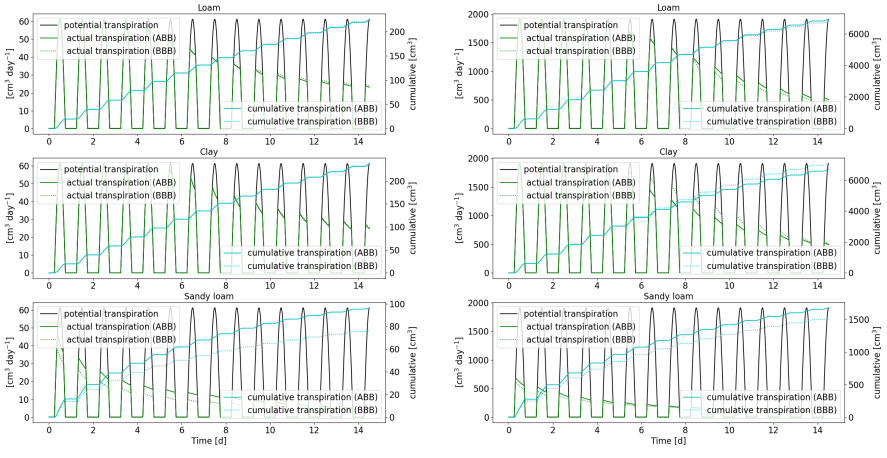


Figure 16. Comparison of the the full hydraulic model (ABB) to the aggregated model (BBB) using a 1D soil grid. Potential and actual transpiration of spring barley (left) and maize (right) for the soil types loam (top), clay (mid) and sandy loam (bottom). The blue line indicates the cumulative plant water uptake.

https://doi.org/10.5194/egusphere-2024-1319
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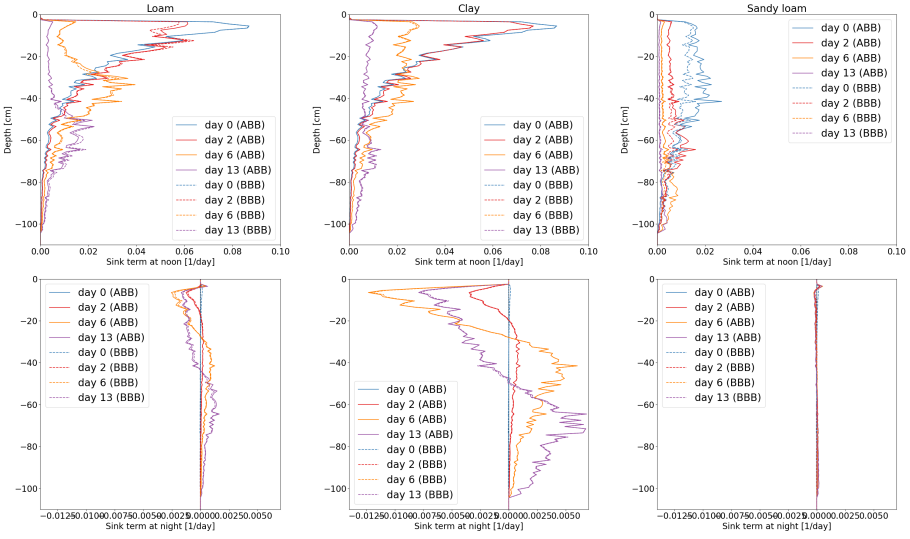


Figure 17. Comparison of the full hydraulic model (ABB) with the aggregated model (BBB) for spring barley using a 1D soil grid. Vertical RWU during noon (top row) and redistribution during night (bottom row) of spring barley for loam (left column), clay (mid column), and sandy loam (right column).

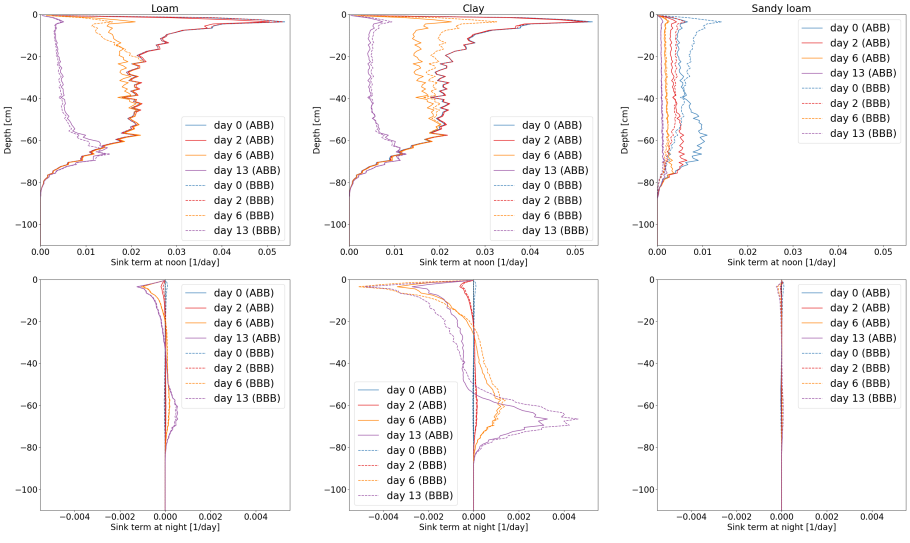


Figure 18. Comparison of the full hydraulic model (ABB) with the aggregated model (BBB) for maize using a 1D soil grid. Vertical RWU during noon (top row) and redistribution during night (bottom row) of maize for loam (left column), clay (mid column), and sandy loam (right column).

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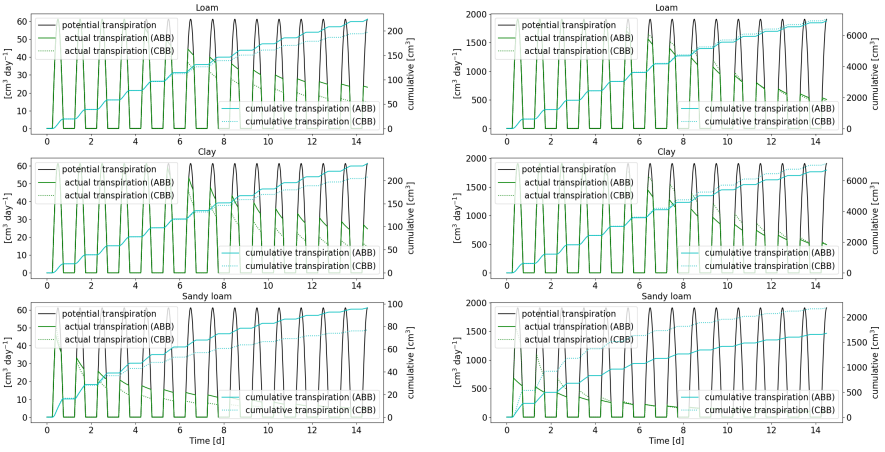


Figure 19. Comparison of the full hydraulic model (ABB) and the parallel root model (CBB) using a 1D soil grid. Potential and actual transpiration of spring barley is shown in the left sub-plot, maize in the right sub-plot. The blue line indicates the cumulative plant water uptake.

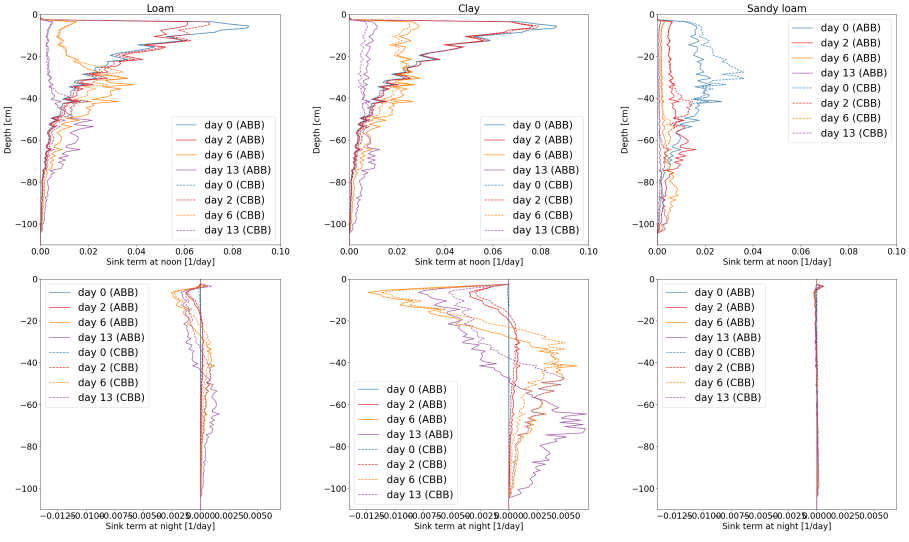


Figure 20. Comparison of the full hydraulic model (ABB) and the parallel root model (CBB) for spring barley using a 1D soil grid. Vertical RWU during noon (top row) and redistribution during night (bottom row) of spring barley for loam (left column), clay (mid column), and sandy loam (right column).

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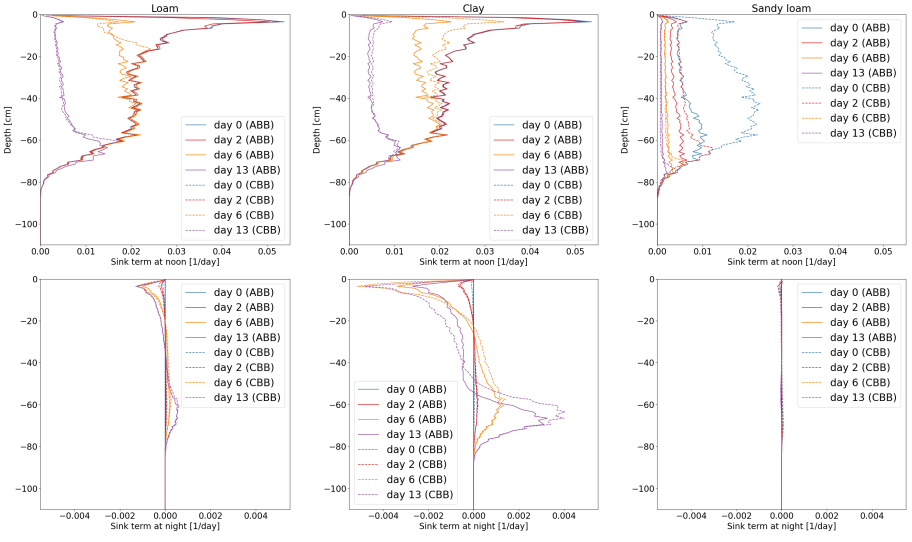


Figure 21. Comparison of the full hydraulic model (ABB) and the parallel root model (CBB) for maize using a 1D soil grid. Vertical RWU during noon (top row) and redistribution during night (bottom row) of maize for loam (left column), clay (mid column), and sandy loam (right column).

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Table 1. Van Genuchten parameters for loam, clay, and sandy loam from Hydrus 1D soil catalog (Simunek et al., 2005).

Soil type	θ_{res} (-)	θ_{sat} (-)	α (cm^{-1})	n (-)	K_s ($cm\ d^{-1}$)
Loam	0.078	0.43	0.036	1.56	24.96
Clay	0.068	0.38	0.008	1.09	4.8
Sandy loam	0.065	0.41	0.075	1.89	106.1

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Table 2. Error and speed up for spring barley after two weeks: red cells denote the absolute error in cumulative plant uptake [mm]. The corresponding speed up is given by the green cells in multiplicity.

Spring barley	AAA			AAB			ABB			BBB			CBB		
	loam	clay	sandy loam	loam	clay	sandy loam	loam	clay	sandy loam	loam	clay	sandy loam	loam	clay	sandy loam
AAA				5	5	3	5	5	3	26	28	27	35	34	24
AAB	0.9	1.0	3.1				1	1	1	5	5	10	7	7	8
ABB	0.5	0.7	2.3	-0.4	-0.3	-0.8				5	6	8	7	7	7
BBB	0.9	1.0	-2.8	0.0	-0.0	-5.9	0.4	0.3	-5.1				1	1	1
CBB	-6.3	-6.8	-2.7	-7.2	-7.8	-5.8	-6.8	-7.5	-5.0	-7.2	-7.8	0.1			

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Table 3. Error and speed up for maize after two weeks: red cells denote the absolute error in cumulative plant uptake [mm]. The corresponding speed up is given by the green cells in multiplicity.

Maize	AAA			AAB			ABB			BBB			CBB		
	loam	clay	sandy loam	loam	clay	sandy loam	loam	clay	sandy loam	loam	clay	sandy loam	loam	clay	sandy loam
AAA				15	18	11	15	12	11	1,148	1,172	1,111	1,555	1,499	1,072
AAB	21.7	17.2	8.6				1	1	1	77	65	103	104	83	99
ABB	22.3	14.6	6.0	0.7	-2.6	-2.6				75	98	100	101	126	96
BBB	21.2	17.8	4.7	-0.5	0.5	-3.9	-1.1	3.2	-1.3				1	1	1
CBB	23.3	18.1	10.2	1.6	0.9	1.6	1.0	3.5	4.2	2.1	0.3	5.5			

Maize (2D)	AAA			AAB			ABB			BBB			CBB		
	loam	clay	sandy loam	loam	clay	sandy loam	loam	clay	sandy loam	loam	clay	sandy loam	loam	clay	sandy loam
AAA				6	5	10	6	7	9	33	28	33	51	47	46
AAB	4.6	3.4	2.7				1	1	1	6	6	3	9	9	5
ABB	3.7	2.7	2.0	-1.0	-0.6	-0.7				6	4	4	9	6	5
BBB	2.9	2.8	0.2	-1.7	-0.6	-2.5	-0.7	0.0	-1.8				2	2	1
CBB	8.0	6.5	3.7	3.4	3.1	1.0	4.4	3.7	1.7	5.1	3.7	3.4			