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## Call for participation: Collaborative benchmarking of functional-structural root architecture models. The case of root water uptake

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1 Call for participation: Collaborative benchmarking of  
2 functional-structural root architecture models.  
3 The case of root water uptake.

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35 **Abstract**

36 Three-dimensional models of root growth, architecture and function are becoming im-  
37 portant tools that aid the design of agricultural management schemes and the selection of  
38 beneficial root traits. However, while benchmarking is common in many disciplines that use  
39 numerical models such as natural and engineering sciences, functional-structural root archi-  
40 tecture models have never been systematically compared. The following reasons might induce  
41 disagreement between the simulation results of different models: different representation of  
42 root growth, sink term of root water and solute uptake and representation of the rhizosphere.  
43 Presently, the extent of discrepancies is unknown, and a framework for quantitatively compar-  
44 ing functional-structural root architecture models is required. We propose, in a first step,

45 to define benchmarking scenarios that test individual components of complex models: root  
46 architecture, water flow in soil and water flow in roots. While the latter two will focus mainly  
47 on comparing numerical aspects, the root architectural models have to be compared at a conceptual  
48 level as they generally differ in process representation. Therefore defining common  
49 inputs that allow recreating reference root systems in all models will be a key challenge. In  
50 a second step, benchmarking scenarios for the coupled problems are defined. We expect that  
51 the results of step 1 will enable us to better interpret differences found in step 2. This benchmarking  
52 will result in a better understanding of the different models and contribute towards  
53 improving them. Improved models will allow us to simulate various scenarios with greater  
54 confidence and avoid bugs, numerical errors or conceptual misunderstandings. This work will  
55 set a standard for future model development.

## 56 1 Introduction

57 A growing number of different modelling techniques and software libraries are now available to  
58 build functional-structural root architecture models. Different available models of root architecture  
59 and functions have been discussed and qualitatively compared in Dunbabin et al. (2013).  
60 The available models differ in the way they represent different processes such as root growth, water  
61 flow, solute transport are captured and translated into mathematical equations (process-level  
62 differences); in how they solve mathematical problems by their choice of analytical or numerical  
63 approach, numerical scheme, programming technique (solution-level differences); and in how they  
64 couple the different processes to the full model (coupling-level differences). However, the extent of  
65 discrepancies is currently unknown. Thus, a framework for quantitatively comparing functional-  
66 structural root architecture models is required. In addition to the explanatory or predictive power  
67 of a model, it is also important to understand the performance of these models, e.g. in terms of  
68 accuracy or computational cost. The most commonly used type of functional-structural root architecture  
69 models represent the structure of the root system as a 1-dimensional branched network  
70 of discrete segments which is geometrically embedded in a 3-dimensional soil domain (Koch et al.,  
71 2018b). The root architecture may either be known from measurements, such as 2D or 3D images,  
72 or from root architectural models. Suitable models are then used to simulate the "functions",  
73 such as carbon flow and use in root systems (Bidel et al., 2000, e.g.), rhizodeposition (Nygren and  
74 Perttunen, 2010), competition between species (Dun), plant anchorage (Dupuy et al., 2007), water  
75 and nutrient uptake (Dunbabin et al., 2006; Javaux et al., 2008). Exchange between soil and root  
76 is typically modelled via source/sink terms. From the point of view of the soil domain, roots are  
77 often considered as line sources, i.e. it is assumed that their diameter is small compared to the  
78 relevant spatial scale of the soil. The advantage of this approach is that it does allow to consider  
79 root system architecture (position of each segment in time and 3D space) explicitly while being  
80 computationally less expensive than an explicit representation of root volumes in the soil domain.  
81 By direct comparison with explicit 3D simulations, Daly et al. (2017) showed that the error made  
82 by neglecting root volumes physically present in the soil domain is negligibly small in case of root  
83 water uptake. Thus, models of this type are sufficiently accurate and computationally cheaper than  
84 explicit 3D. The challenge is now to develop a commonly accepted framework for benchmarking  
85 functional-structural root architecture models. This includes defining a set of benchmark problems  
86 to test model accuracy and performance. We propose that models should be evaluated against two  
87 different kinds of references: First, we will develop simple benchmark scenarios, if possible with  
88 analytical solutions, that serve as a reference for model verification. Secondly, we define data  
89 sets that can be used as references for the evaluation of more complex models without analytical  
90 solution. These data sets should as good as possible describe the system we want to model and  
91 contain as little uncertainty as possible (Luo et al., 2012). This benchmark activity focuses on two  
92 processes, root architecture development and root water uptake. We propose this benchmarking  
93 framework to be used by the community of modellers and other participants to compare their  
94 model outputs against those of the reference solutions of benchmarks defined in this paper. The  
95 use of this framework thus aims to be a collaborative effort. We will refer to any numerical model  
96 that implemented some or all of the benchmark problems as "participating model" or "simulator".

## 97 2 Benchmark problems for models of root architecture and 98 function

99 In order to benchmark models of root architecture and function, we propose a multi-step approach  
100 with growing level of complexity. The individual benchmarks refer as much as possible to published  
101 work, however, we streamlined the different problems and made the notation consistent throughout  
102 this paper. A list of symbols is provided in Table 1. The intrinsic nature of functional-structural  
103 root architecture models involves multiple coupled domains and processes. A single process in a  
104 single domain (e.g. water flow in soil) is referred to as “module” here. The first set of benchmarks  
105 (M1-M3) is about individual modules (M) only, i.e. they either deal with only root growth,  
106 water flow in soil or water flow inside roots. The scenarios are simple, possibly have analytical  
107 solutions, and the goal is to build trust in the accuracy of the individual participating models and  
108 to help interpret potentially diverging results of the coupled benchmark problems. Benchmark  
109 problems M1 are about root architecture development. It is known that the representation of  
110 growth processes can be very different between different simulators. Thus, the goal is to calibrate  
111 each simulator individually to given root image data (reference data). M2 is about modelling water  
112 flow in soil. Here all participating models solve the same equation, namely the Richards equation,  
113 and differences may occur due to differences in numerical implementation. M3 deals with water  
114 flow inside the root system for static soil water conditions. As for M2, differences between models  
115 are expected to be mainly due to the numerical implementation of this well defined process. The  
116 second set of benchmarks (C1 and C2) is about coupled root-soil models. Benchmark problems C1  
117 consider a static (non-growing) root system and focus on comparison of numerical representation of  
118 agreed-upon equations and process representations as well as on the coupling approach to compute  
119 the sink term for root water uptake. For this benchmark, we provide a reference solution that is  
120 based on a computational mesh that was generated with consideration of the physical presence of  
121 the roots in the soil domain. Thus, root water uptake was simulated not by a sink term but as a  
122 boundary condition at the root surface in soil. Our approach is similar to Daly et al. (2017) but  
123 in addition couples the soil domain to the root domain so that pressure gradients along the roots  
124 are simulated. Benchmark problem C2 compares the water uptake of fully coupled models with  
125 growing root systems.

126 Each benchmark problem is described in a Jupyter Notebook that is publicly available on a  
127 github repository. We will provide codes for automatic analyses and comparison of different model  
128 results with the reference solutions or reference data. This makes the analysis transparent and  
129 easily modifiable and facilitates including even future participating models’ outputs at any later  
130 time.

131  
132 **Levels of contribution** Any group using or developing functional-structural root architecture  
133 models is invited to participate in this collaborative model comparison. Not every model might be  
134 suited for all of the provided benchmark problems. Thus, every participant may decide in which  
135 individual benchmark problem they would like to participate. However, to reach a certain level of  
136 complexity, the “module” benchmarks should be simulated first before the “coupled” benchmarks.  
137 Table 2 gives an overview of the key features of these problems and their implementations. One  
138 important aim of this activity is a joint publication that shows and discusses the results of the  
139 different participating models in comparison to the reference solutions and reference data provided  
140 as well as to gain an overview of the extent of deviations between the different simulators.

141 **How to participate** The participation includes three steps:

142  
143 **(1) Registration** Any interested researcher is welcome to contact the corresponding author of  
144 this paper, Andrea Schnepf, with the following information: Name, affiliation, name or reference  
145 to the participating simulator. Upon signing a letter of agreement confirming that results of other  
146 participants will not be published without consent, researchers will be accepted as participants and  
147 enabled to include their individual simulation results to the github repository of this benchmark  
148 initiative, <https://github.com/RSA-benchmarks/collaborative-comparison>.

149 **(2) Simulation** Each participant implements all or a selected number of benchmark problems in  
150 their respective simulator and makes the results in the prescribed formats available to the github  
151 repository through pull requests. Requested formats include RSML (Lobet et al., 2015) for root  
152 architectures and VTK (Schroeder et al., 2006) for 3D and 1D simulation outputs. Python scripts

153 to read and write RSML files will be provided on the github repository. Packages to read and write  
154 VTK files are for example available at <https://pypi.org/project/vtk/>.  
155 **(3) Analysis and publication** The analysis of results and computation of relevant metrics, such  
156 as root mean square error, coefficient of determination or Nash–Sutcliffe efficiency, will be done by  
157 the code implemented in the Jupyter Notebooks for each benchmark problem. The final goal is to  
158 jointly publish the results.

Table 1: List of notations

Symbol	Units	Description
$d$	cm	depth
$D_w$	$\text{cm}^2\text{d}^{-1}$	water diffusivity
$\mathbf{e}_3$	(0,0,1)	standard unit vector
$J$	$\text{cm}^3\text{cm}^{-2}\text{d}^{-1}$	water flux per unit soil surface area
$k_r$	$\text{cm}^3\text{cm}^{-2}\text{cm}^{-1}\text{d}^{-1}$	root radial conductivity (defined as volume of water per unit root surface area, pressure head gradient and time)
$k_x$	$\text{cm}^4\text{cm}^{-1}\text{d}^{-1}$	specific root axial conductance
$K(\theta)$	$\text{cm}^3\text{cm}^{-2}\text{d}^{-1}$	soil hydraulic conductivity
$K_{sat}$	$\text{cm}^3\text{cm}^{-2}\text{d}^{-1}$	saturated soil hydraulic conductivity
$l$	cm	length
$n$	-	van Genuchten shape parameter
$q$	$\text{cm}^3\text{cm}^{-2}\text{d}^{-1}$	water flux per unit root surface area
$Q$	$\text{cm}^3\text{d}^{-1}$	volumetric water flow rate
$\bar{Q}$	$\text{cm}^3\text{d}^{-1}$	daily average volumetric water flow rate
$Q_r$	$\text{cm}^3\text{d}^{-1}$	radial root water flow rate
$Q_x$	$\text{cm}^3\text{d}^{-1}$	axial root water flow rate
$r_{root}$	cm	root radius
$S_w$	$\text{cm d}^{-0.5}$	sorptivity (infiltration) or desorptivity (evaporation)
$t$	d	time
$\mathbf{v}$	$(v_1, v_2, v_3)$	normalised direction of the xylem, pointing towards the root tip
$w$	cm	width
$x, y, z$		spatial coordinates, z-axis pointing upward, soil surface is at $z=0$
$Y$	-	cumulative root fraction from surface to depth $d$
$\alpha$	$\text{cm}^{-1}$	van Genuchten shape parameter
$\beta$	-	root distribution index
$\eta$	cm	position of the infiltration front (eqn. (4))
$\lambda$	-	van Genuchten-Mualem parameter
$\Lambda$	-	root domain (network of root center-lines)
$\Omega$	-	soil domain
$\Phi$	$\text{cm}^2\text{d}^{-1}$	matric flux potential
$\theta$	$\text{cm}^3\text{cm}^{-3}$	volumetric water content
$\theta_a$	$\text{cm}^3\text{cm}^{-3}$	reference water content
$\theta_{res}$	$\text{cm}^3\text{cm}^{-3}$	residual water content
$\theta_{sat}$	$\text{cm}^3\text{cm}^{-3}$	saturated water content
$\psi$	cm	water pressure head, described as potential energy per unit weight of water (i.e. units are cm of water column), given as relative to air pressure of 1020 cm and excluding the gravitational potential
$\zeta$		local coordinate along root axis
<b>sub indices</b>		
collar	root collar (upper boundary of root system domain)	
i	initial	
pot	potential	
r	radial	
res	residual	
s	soil	
sat	saturation	
seg	root segment	
sim	simulation	
sur	soil surface	
tip(s)	root tip(s) (boundaries of root system domain)	
top	top, position of the soil surface	
out	outer radius of soil cylinder around a single root	
x	xylem	

Table 2: Description of benchmark scenarios to be implemented in 3D functional-structural root architecture models.<sup>1</sup>

	Benchmark problem	Domain	Initial conditions	Boundary conditions	Evaluation	Remarks
RSA	M1.1: RSA calibration	$t_{sim}=11$ (8) for lupine (maize)	seed position (0,0,-3)	n.a.	Comparison against the measured root systems provided - traits and persistent homology (PH)	Model parameters are determined from calibration against traced images provided in the github repository in RSML format in the folder in M1.1 RSA calibration/M1.1 Reference data; 100 realisations for each model setup
	M1.2: RSA simulation	$t_{sim}=60$	seed position (0,0,-3)	n.a.	No reference solution, comparison amongst models - traits, PH, RLD	RSA model parameters from M1.1; 10 realisations for each model setup
Soil	M2.1: Infiltration	$1 \times w \times d = 10 \times 10 \times 200$ , $t_{sim}=1$	$\psi_{s,i} = -400$	at $z = 0$ $\begin{cases} J_s = 100 \text{ if } \psi_s < 0 \\ \psi_s = 0 \text{ else} \end{cases}$ , $\frac{\partial \psi_s}{\partial z}  _{z=200} = 1$ , no-flux at the sides	Analytical solution, eqn. (3)	sand, loam, clay (Table 3)
	M2.2: Evaporation	$1 \times w \times d = 10 \times 10 \times 100$ , $t_{sim}=10$	$\psi_{s,i} = -40$ for sand and $-200$ for all other scenarios	at $z = 0$ $\begin{cases} J_s = J_{s,ref} \text{ if } \psi_s > -10,000 \\ \psi_s = -10,000 \text{ else} \end{cases}$ , no-flux at all other boundaries	Analytical solution, eqn. (4)	scenario 1: sand, $J_{s,ref} = -0.1$ , scenario 2: loam, $J_{s,ref} = -0.1$ , scenario 3: loam, $J_{s,ref} = -0.3$ , scenario 4: clay, $J_{s,ref} = -0.3$
Xylem	M3.1: Single root	1 vertical root, $L=50$	n.a.	$\psi_x _{collar} = -1000$ , $Q_r _{tip} = 0$	Analytical solution, Eq. (11)	$k_x=0.0432$ , $k_r=1.73 \times 10^{-4}$ , $\psi_s = -200$
	M3.2: Root system	14-day old root system	n.a.	$\psi_x _{collar} = -500$ , $Q_r _{tips} = 0$	Hybrid analytical solution (Meunier et al., 2017)	root hydraulic properties in scenario (a): Table 4, (b): Fig. 7, $\psi_s = -200$ , static RSA given in the <code>root_grid</code> folder of this benchmark
Coupled 1	C1.1: Single RWU	1D radially symmetric, $r_{root} = 0.02$ , $r_{out} = 0.6$ , $t_{sim}=20$	$\psi_{s,i} = -100$	at $r = r_{root}$ $\begin{cases} q_r = q_{root}, \text{ if } \psi_s > -15,000 \\ \psi_s = -15,000 \text{ else} \end{cases}$ , $q_r _{r=r_{out}} = 0$	Analytical solution, Eqs. (16) and (17)	sand, loam, clay (Table 3), scenarios 1-3: $q_{root}=0.1$ , scenarios 4-6: $q_{root}=0.05$
	C1.2: RWU, static RSA	static 8-day old root system, soil: $1 \times w \times d = 8 \times 8 \times 15$ , $t_{sim}=3$	$\psi_{s,i} = -659.8 - z$	$Q_r _{collar} = \begin{cases} Q_r = 6.4 \text{ if } \psi_s > -15,290 \\ \psi_s = -15,290 \text{ else} \end{cases}$ , $Q_r _{tips} = 0$ , no-flux at all soil faces	Reference solution: explicit 3D simulation	loam (Table 3), static RSA given in the <code>root_grid</code> folder of this benchmark, root hydraulic properties in scenario (a): Table 4, (b): Fig. 7
Coupled 2	C2.1: RWU, dynamic RSA	growing root system, soil: $1 \times w \times d = 25 \times 25 \times 100$ , $t_{sim}=60$	$\psi_{s,i} = -200$	$Q_r _{collar} = \begin{cases} Q_r = 0.5 \cdot rel_{LAI} \text{ if } \psi_x > -15,000 \\ \psi_x = -15,000 \text{ else} \end{cases}$ , $Q_r _{tips} = 0$ , no-flux at all soil faces	No reference solution, comparison amongst models	loam (Table 3), $k_x=0.0432$ , $k_r=1.73 \times 10^{-4}$ , RSA parameters from M1.1, $rel_{LAI}$ scales the potential transpiration

<sup>1</sup> All paths are relative to the github repository <https://github.com/RSA-benchmarks/collaborative-comparison.git>. For other abbreviations and units see Table 1.

## 160 2.1 Benchmarks for individual modules

### 161 2.1.1 Module M1: Root system architecture models

162 Root system architecture models (RSA models) are that module within a complex functional-  
163 structural plant model that simulates the structure, topology, and 3D placement of the roots. They  
164 simulate the growth of root systems as (upside down) tree-like structures based on rules regarding  
165 elongation, branching and death. Mostly, they are discrete models and represent the root system  
166 by a mathematical graph (i.e., nodes and edges/root segments). Each node or segment may be  
167 additionally associated with attributes such as radius, age or hydraulic properties.

168 The aim of this first benchmarking exercise is to determine if root architecture models currently  
169 available are able to reproduce realistic root architectures when being parameterised on the basis  
170 of a common experimental data set (Fig. 2a). The particular challenge to benchmark RSA models  
171 is to include the stochastic nature of these models. We propose to perform the benchmarking of  
172 those models in four steps: (1) Parameterising the root architecture models based on the provided  
173 experimental data, (2) Simulating a set of root systems for a dicotyledonous (*Lupinus albus*) and a  
174 monocotyledonous (*Zea mays*) plant species following two benchmark scenarios (M1.1 and M1.2),  
175 (3) Export and store the simulated root systems as Root System Markup Language (RSML) files  
176 (Lobet et al., 2015), and (4) Compare the simulation results using the data analysis pipelines  
177 available in the associated Jupyter Notebooks. The analysis pipelines are explained below and  
178 illustrated in Fig. 1. In particular, we include persistent homology as an approach that augments  
179 purely trait-based comparisons, i.e., two root systems with the same total root length could be  
180 very different based on the persistent homology approach.

181 **M1.1 Root system architecture model calibration** The different available root architecture  
182 models (see e.g. Dunbabin et al., 2013) are partly different in the way they represent the growth  
183 processes, i.e. we are looking at process-level differences between the different models. Thus, each  
184 participating RSA model will have a different set of parameters that drive root growth. This is the  
185 reason why, in this benchmark, we do not prescribe a parameter set as in e.g. M2 or M3, but we  
186 let each participating model derive its respective model parameters based on a reference dataset.  
187 In this first benchmark (M1.1), modellers simulate root systems for the same duration as the age  
188 of the root systems in the reference dataset.

189 **Reference data set** Although the parameterisation of 3D models using a set of parameters  
190 derived from 2D images has some limitations, it has been shown to be a simple and efficient strategy  
191 allowing the simulation of realistic 3D root systems (Landl et al., 2018). Our reference dataset  
192 contains two distinct sets of images: (1) images of lupin roots grown for 11 days in an aeroponic  
193 setup (Lobet et al., 2011), and (2) images of maize roots grown for 8 days on filter papers (Hund  
194 et al., 2009). All images were analysed using the semi-automated root image analysis software  
195 SmartRoot (Lobet et al., 2011) and root tracings were saved as RSML files for further analysis  
196 (Fig. 1). These RSML files were then processed using functions of the R package archiDART  
197 developed to compute root system- and single root-level metrics (Delory et al., 2016, 2018). These  
198 metrics have been made open-access ([https://github.com/RSA-benchmarks/collaborative-  
199 comparison/tree/master/root\\_architecture/data](https://github.com/RSA-benchmarks/collaborative-comparison/tree/master/root_architecture/data)) and should help modellers to parameterise  
200 their respective RSA model.

201 **Required output** The following results are to be uploaded via pull requests to this path  
202 on the github repository: M1 Root architecture development/M1.1 RSA calibration/M1.1  
203 Numerical results.

- 204 1. A text file including the outcome of the calibration step, i.e., the set of model input parameters  
205 required for the specific simulator.
- 206 2. Simulation output from running the root architecture model using this parameter set in  
207 RSML format. Due to the stochastic nature of root architecture models, 100 realisations of  
208 each model setup are requested. The file format should be RSML and the file name should  
209 be of the form "modelname\_replicate", e.g. "CRootBox\_1.rsm1".



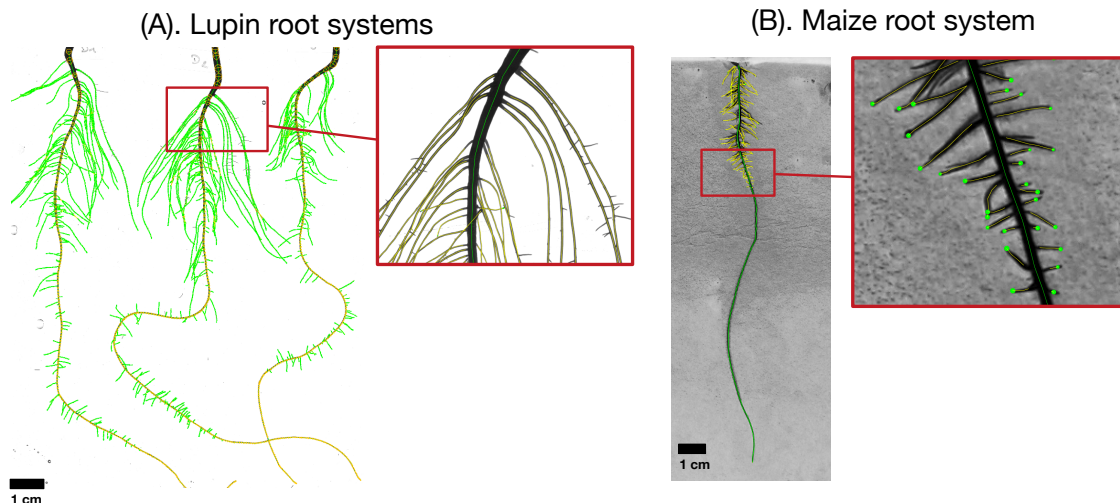


Figure 1: Example of root images used for the benchmarking dataset. Panel (A) shows an image of lupin root systems, 11 days old, growing in an aeroponic setup. Panel (B) shows an image of a maize root system growing on filter paper (5 days old). All images were analysed using the semi-automated root image analysis software SmartRoot (Lobet et al., 2011), colours distinguish different root orders. The RSML files containing the full information about the root systems are provided on the github repository in the folder "M1.1 RSA calibration\M1.1 Reference data".

210 **Reference data analysis and automated model comparison** Statistical evaluation of a  
211 root architecture model has for example been done by Schnepf et al. (2018); Delory et al. (2018).  
212 This motivated the creation of two data analysis pipelines for the first benchmark (M1.1) that  
213 will be used to compare simulation outputs with reference experimental data (reference root sys-  
214 tems) (Fig. 2a). These two data analysis pipelines are implemented in the Jupyter Notebook  
215 `RSA calibration.ipynb` that can be found on the github repository that contains code that will  
216 automatically include every model output in the analysis that is available in the prescribed folder.  
217 The analysis relies on the functions available in the **R** package `archiDART` (Delory et al., 2016,  
218 2018). In the first pipeline, traits computed at the root system level (e.g., total root system  
219 length, number of roots per branching order) are compared between all simulated and reference  
220 root systems. This comparison takes place in three steps: (1) identifying the key morphological,  
221 architectural, and topological (Fitter indices, Fitter 1987; Fitter and Stickland 1991) traits ex-  
222 plaining differences between simulated and reference root systems using multivariate data analysis  
223 techniques (e.g., discriminant analysis and principal component analysis), (2) looking at the point  
224 in time, beyond the time period for which there are measurements, when simulated and reference  
225 root systems start to diverge/converge with regard to the key root system traits identified in the  
226 previous step and how large these differences are, and (3) assess the degree of dissimilarity between  
227 simulated and reference root systems using dissimilarity metrics based on the raw data (Janssen  
228 and Heuberger, 1995).

229 In the second pipeline, dissimilarities in architecture between reference and simulated root sys-  
230 tems are compared using persistent homology. Persistent homology is a topological framework  
231 that has proven to be a very powerful tool for capturing variations in plant morphology at dif-  
232 ferent spatial scales (Li et al., 2017, 2018). The main output of a persistent homology analysis  
233 is a persistence barcode recording the appearance and disappearance of each root branch when  
234 a distance function traverses the branching structure (see Fig. 1 in Delory et al., 2018). The  
235 degree of similarity between different root system topologies can be assessed by computing a pair-  
236 wise distance matrix to compare persistence barcodes. In addition, Delory et al. (2018) showed  
237 that both trait-based and persistent homology approaches nicely complement each other and allow  
238 root researchers to more accurately describe differences in root system architecture (Delory et al.,  
239 2018). In our data analysis pipeline, a persistent homology analysis comprises the following steps:  
240 (1) computing a persistence barcode for each simulated and reference root system using a geodesic  
241 distance function, (2) computing dissimilarities between persistence barcodes using a bottleneck  
242 distance, (3) visualize dissimilarities between root systems using multidimensional scaling, and

243 (4) test specific hypotheses using permutational multivariate analysis of variance (PERMANOVA)  
244 (Anderson, 2001).

245 **M1.2 Long model simulations** In this benchmark, modellers use the same input parameter  
246 set as in M1.1, but simulate root system growth and development for a longer time period (60  
247 days). The aim of this second benchmarking exercise is to assess if the different models diverge (or  
248 converge) if simulations are run for a longer time period and extrapolate beyond the provided data  
249 set (Fig. 2b). This is of great importance, as parameterisation of RSA models is often based on  
250 relatively young plants, whereas knowledge of RSA of older root systems is scarce. Therefore, for  
251 this M1.2 scenario, experimental data are not used as the basis of comparison anymore. It has to  
252 be noted that these two benchmark problems focus on root architecture dynamics modelling only,  
253 thus effect of soil properties on root growth is not explicitly modelled.

254 **Required output** The following results are to be uploaded via pull requests to this path on  
255 the github repository: M1 Root architecture development/M1.2 RSA simulation/M1.2 Numerical  
256 results.

- 257 1. A text file including the model input parameters used for the specific simulator.
- 258 2. Simulation output from running the root architecture model using this paramter set in RSML  
259 format. Due to the stochastic nature of root architecture models, 100 realisations of each  
260 model setup are requested. The file file format should be RSML and the file name should be  
261 of the form "modelname\_replicate", e.g. "CRootBox\_1.rsml".

262 **Analysis pipeline for M1.2** For the second benchmark (M1.2), three data analysis pipelines  
263 are used to compare simulation outputs given by different root architecture models. For this  
264 benchmark, the reference experimental data cannot be used as a reference as data of 60 day old  
265 plants is not available. The first two data analysis pipelines for M1.2 are very similar to the ones  
266 described earlier for the M1.1 benchmark. First, model outputs are compared using morphological,  
267 architectural, and topological traits computed at the root system level. Second, differences in root  
268 system morphology are analysed using persistent homology. In addition to these two analysis  
269 pipelines, we included a third one to analyse differences in vertical root distribution between root  
270 systems simulated with different root architecture models. To do so, we use the modelling approach  
271 described in Oram et al. (2018). Briefly, relative cumulative root length density ( $Y(d)$ ) is computed  
272 using Eq. (1)

$$Y(d) = \frac{\sum_{i=0}^{i=d} RLD(i)}{\sum_{i=0}^{\infty} RLD(i)} \quad (1)$$

273 Eq. (2) is fitted to the computed  $Y(d)$  using a non-linear least square means fitting procedure.  
274 The fitting constant  $\beta$  is used to compare modeled rooting depth, with high  $\beta$  corresponding to  
275 deep rooting.

$$Y(d) = 1 - \beta^d, \quad (2)$$

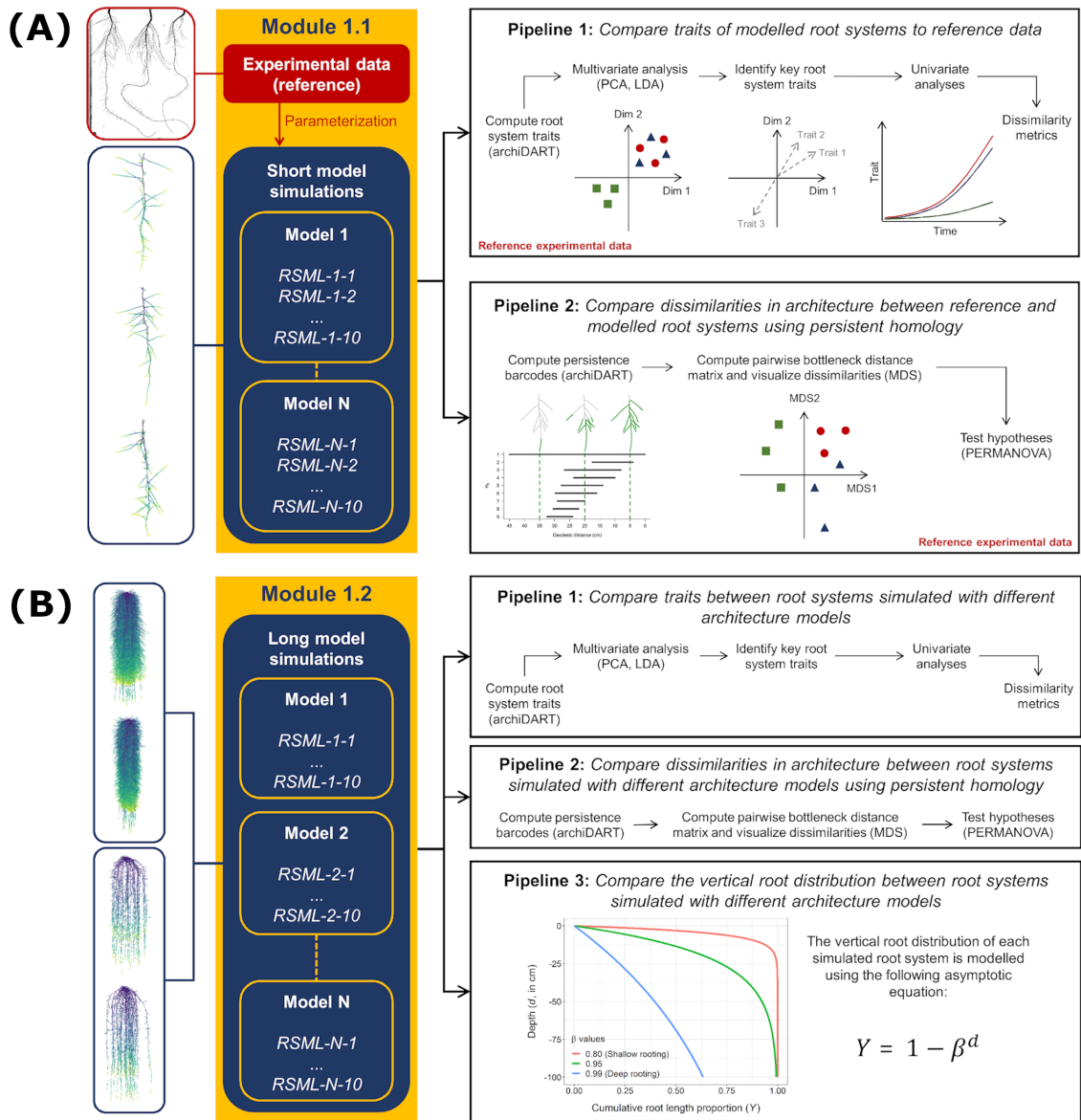


Figure 2: Presentation of the data analysis pipelines used for the benchmarking of root architecture models. Panels a and b show the first (M1.1) and second (M1.2) benchmark scenarios, respectively.

## 276 2.1.2 Module 2: Water flow in soil only

277 In this module, we describe benchmark problems that only relate to water flow in soil. Water flow  
278 in soil is most commonly described by the Richards equation in three dimensions:

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (K(\theta) (\nabla \psi_s + \mathbf{e}_3)), \quad (3)$$

279 where  $\theta$  is the volumetric soil water content ( $\text{cm}^3 \text{cm}^{-3}$ ),  $K$  is the hydraulic conductivity ( $\text{cm}$   
280  $\text{day}^{-1}$ ),  $\psi_s$  is the soil water pressure head (cm), and  $\mathbf{e}_3 = (0, 0, 1)$  is the downward unit vector.

281 The relationship between soil water pressure head and water content is generally described by  
282 the water retention curve. In the following we will use the van Genuchten equation (Van Genuchten,  
283 1980) to describe this curve specifying the soil moisture characteristic of specific soils.

284 We expect differences between the outputs of different simulators to be mainly numerical  
285 solution-level differences, i.e., due to numerical scheme and implementation. Different numer-  
286 ical solutions of the Richards equation have been analysed before, and for some settings analytic  
287 solutions exist. We will use the benchmarks presented by Vanderborcht et al. (2005) to benchmark  
288 the part of the participating functional structural root architecture models where water movement

289 in soil is described. The analytical solutions provided in that paper are related to vertical changes  
 290 in the soil profile only. As most functional-structural root architecture models have a 3D soil mod-  
 291 292 and width for the numerical implementation of those problems.

293 In the following we will describe the benchmarks for water movement in soil. Table 3 gives an  
 294 overview of the soil hydraulic properties that will be used throughout all the benchmarks involving  
 water flow in soil.

Table 3: Soil hydraulic taken from Vanderborght et al. (2005).  $\theta_{res}$  is the residual water content,  $\theta_{sat}$  is the saturated water content,  $\alpha$  and  $n$  are the van Genuchten parameters,  $K_{sat}$  is the saturated soil hydraulic conductivity and  $\lambda$  is the van Genuchten-Mualem parameter

Soil type	$\theta_{res}$ (-)	$\theta_{sat}$ (-)	$\alpha$ ( $\text{cm}^{-1}$ )	$n$ (-)	$K_s$ ( $\text{cm d}^{-1}$ )	$\lambda$ (-)
sand	0.045	0.43	0.15	3.0	1000	0.5
loam	0.08	0.43	0.04	1.6	50	0.5
clay	0.1	0.40	0.01	1.1	10	0.5

295

296 **M2.1: Infiltration** This benchmark scenario is taken from Vanderborght et al. (2005). All  
 297 parameters, initial and boundary conditions are given in Table 2 and are described below. For  
 298 each of the soil types, sand, loam and clay, we consider the rate of infiltration into a soil with an  
 299 initial homogeneous soil water pressure head of  $\psi_s = -400$  cm. All profiles are 200 cm deep, at the  
 300 top boundary we prescribe a constant influx of  $100 \text{ cm d}^{-1}$  as long as the soil is still unsaturated,  
 301 and a Dirichlet boundary condition of  $\psi_s = 0$  cm as soon as the soil is fully saturated. At the  
 302 bottom boundary, we prescribe free drainage. Since this problem only produces gradients in the  
 303 vertical direction, we compare numerical model results with the 1D analytical solution described  
 304 in Vanderborght et al. (2005).

305 **Reference solution** The analytical solution is given by the travelling wave equation

$$\Delta\eta(\theta) = \eta(\theta) - \eta(\theta_a) = (\theta_{sur} - \theta_i) \int_{\theta}^{\theta_a} \frac{D_w(\theta)d\theta}{[K(\theta_{sur}) - K(\theta_i)](\theta - \theta_i) - [K(\theta) - K(\theta_i)](\theta_{sur} - \theta_i)}, \quad (4)$$

306 where  $D_w$  is the water diffusivity (defined as  $D_w = K(\theta) \frac{\partial \psi_s}{\partial \theta}$ ),  $\theta_{sur}$  is the water content at the  
 307 soil surface,  $\theta_i$  is the initial water content,  $\theta_a$  is a reference water content (taken to be  $\theta_a =$   
 308  $(\theta_{sur} + \theta_i)/2$ ),  $\eta = |z| - \frac{[K(\theta_{sur}) - K(\theta_i)]t}{\theta_{sur} - \theta_i}$  and  $\Delta\eta(\theta)$  is the distance of the front to the the position  
 309 of the reference water content. The implementation of this analytical solution, implemented in the  
 310 Jupyter Notebook **M2.1 Benchmark problem.ipynb**, reproduces Figure 4abc from Vanderborght  
 311 et al. (2005), where the water content is plotted after 0.1, 0.2, and 0.3 days for the sand scenario;  
 312 0.2, 0.5, and 1 days for the loam scenario; and 0.1, 0.2, and 0.5 days for the clay scenario (see Fig.  
 313 (3)).

314 **Required output** The following simulation results of participating models are to be up-  
 315 loaded via pull requests to this path on the github repository: **M2 Water flow in soil/M2.1**  
 316 **Infiltration/M2.1 Numerical results**.

- 317 1. A text file consisting of two rows containing comma separated depth values (cm) in the first,  
 318 and water content ( $\text{cm}^3\text{cm}^{-3}$ ) in the second for each time point and infiltration scenario (i.e.  
 319 3 (time points)  $\times$  3 (scenarios) results = 18 rows). The file name should be of the form  
 320 "simulatorname.txt", e.g. "DuMux.txt".

321 Note that we do not prescribe spatial or temporal resolution of the outputs, as that may depend  
 322 on the individual numerical schemes.

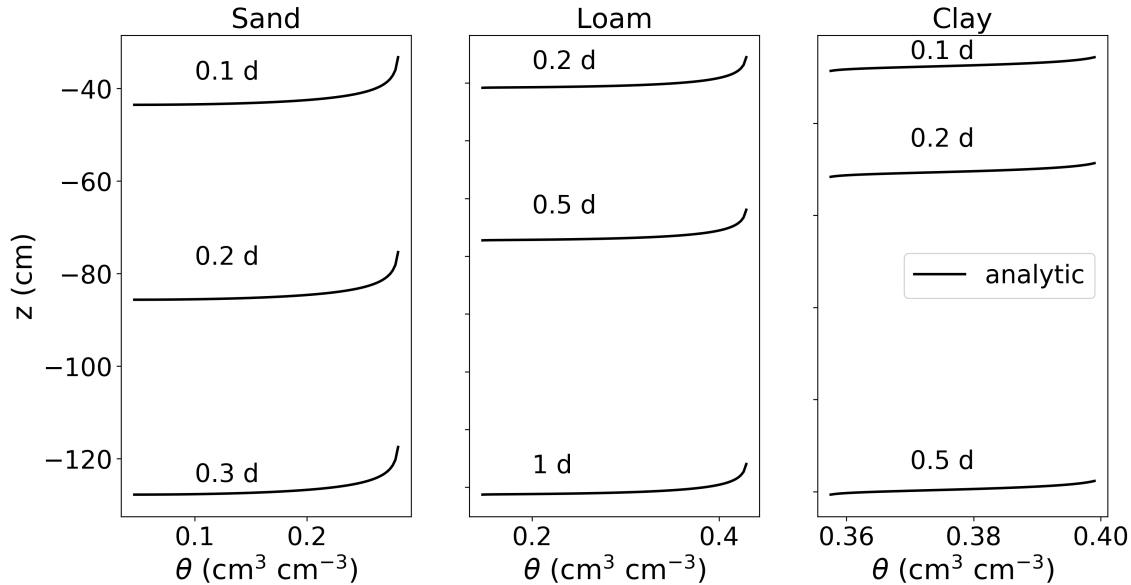


Figure 3: Results of M2.1: Infiltration into three initially dry soils: sand, loam and clay.

323 **M2.2: Evaporation** This benchmark reproduces Fig. (5) of Vanderborght et al. (2005). We  
 324 consider four scenarios (sand, loam 1, loam 2, clay) in which we are interested in the actual  
 325 evaporation over time from an initially moist soil ( $\psi_i = -40\text{cm}$  for the sand scenario and  $\psi_i$   
 326  $= -200\text{cm}$  for all other scenarios). The domain is 100 cm deep with a width and length of 10 cm.  
 327 At the top boundary, we prescribe a constant efflux of  $J_{s,pot}=0.1 \text{ cm d}^{-1}$  for the sand and loam 1  
 328 scenario, and 0.3 cm/day for the loam 2 and clay scenarios, at the bottom we prescribe zero-flux.  
 329 When the soil reaches a critical soil water pressure head of -10.000 cm at the surface, we switch to  
 330 a Dirichlet boundary condition with  $\psi_s = -10.000 \text{ cm}$ .

331 **Reference solution** The analytical solution to this problem is given by

$$J_s(z=0, t) = \begin{cases} J_{s,pot} & \text{for } t < t_{pot} \\ \frac{S_w(\theta_{sur}, \theta_i)}{2\sqrt{t' + t - t_{pot}}} & \text{for } t \geq t_{pot} \end{cases} \quad (5)$$

332 where  $t' = \frac{S_w^2(\theta_{sur}, \theta_i)}{4J_{s,pot}^2}$ ,  $t_{pot} = \frac{S_w^2(\theta_{sur}, \theta_i)}{2J_{s,pot}^2}$ ,  $S_w(\theta_i, \theta_{sur}) = (\theta_i - \theta_{sur}) \sqrt{\frac{4}{\mu} \int_0^1 D_w(\Theta) d\Theta}$ ,  $\Theta = \left| \frac{\theta - \theta_{sur}}{\theta_i - \theta_{sur}} \right|$ ,  
 333  $\mu = \frac{3\beta \left( 1 + \left\{ 1 - \frac{14}{9} \left[ 1 - \frac{\alpha}{(1-\beta)^2} \right] \right\}^{0.5} \right)}{2(1-\beta) \left[ \frac{\alpha}{(1-\beta)^2} - 1 \right]}$ ,  $\alpha = \frac{\int_0^1 (1-\beta\Theta)^2 D_w(\Theta) d\Theta}{\int_0^1 D_w(\Theta) d\Theta}$ , and  $\beta = \left[ \frac{\int_0^1 \Theta D_w(\Theta) d\Theta}{\int_0^1 D_w(\Theta) d\Theta} \right]^2$ . Fig. (4) shows  
 334 the rate of evaporation over time for the four scenarios soil, loam 1, loam 2, clay.

335 **Required output** The following simulation results of participating models are to be up-  
 336 loaded via pull requests to this path on the github repository: M2 Water flow in soil/M2.2  
 337 Evaporation/M2.2 Numerical results.

338 1. A text file consisting of two rows containing comma separated depth values (cm) in the first,  
 339 and root pressure head (cm) in the second for each scenario (i.e. 4 (scenarios)  $\times$  2 (rows) =  
 340 8 rows). The file name should be of the form "simulatorname.txt", e.g. "DuMux.txt".

341 Note that we do not prescribe spatial or temporal resolution of the outputs, as that may depend  
 342 on the individual numerical schemes. It is the responsibility of each participant, to upload the best  
 343 possible solution.

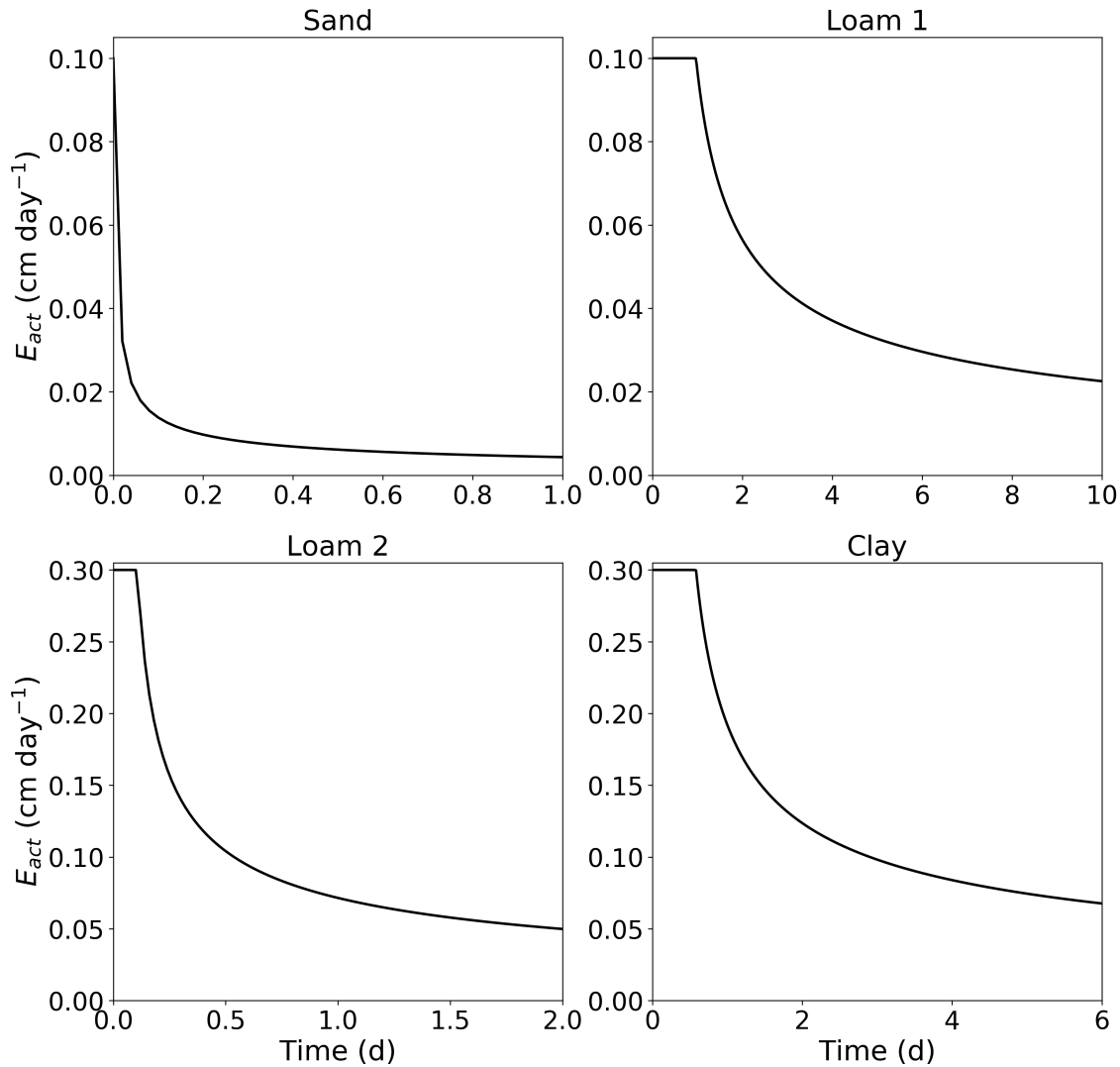


Figure 4: Results of M2.2: Rate of evaporation with respect to time from sand with  $J_{s,pot}=0$  1cm/d, loam with  $J_{s,pot}=0$  1cm/d, loam with  $J_{s,pot}=0$  3cm/d and clay with  $J_{s,pot}=0$  3cm/d

### 344 2.1.3 Module 3: Water flow in roots

345 In this benchmark, we consider water flow in xylem with constant and homogeneous soil water  
 346 pressure head. This problem is well described, e.g., in Roose and Fowler (2004) and Doussan et al.  
 347 (1998). Its analytical solution for a single root was already derived by Landsberg and Fowkes  
 348 (1978). In Appendix A, we present a derivation that is equivalent to the solution of Landsberg and  
 349 Fowkes (1978) but uses exponential instead of hyperbolic functions. Briefly, conservation of mass  
 350 in a branched root network with both axial and radial water flow, neglecting plant water storage  
 351 and osmotic potential, yields Eq. (6),

$$2r_{root}\pi k_r(\psi_s - \psi_x) = -k_x \frac{\partial^2 \psi_x}{\partial \zeta^2}, \quad (6)$$

352 where  $r_{root}$  is the root radius (cm),  $k_r$  is the radial conductivity ( $d^{-1}$ ),  $\psi_s$  is the soil water pressure  
 353 head of the surrounding soil (cm),  $\psi_x$  is the root water pressure head inside the xylem (cm),  $k_x$  is  
 354 the axial conductance ( $cm^3 d^{-1}$ ), and  $\zeta$  is the axial coordinate (cm).

355 **M3.1: A single root in static soil with constant root hydraulic properties** In this  
 356 benchmark problem, we assume a vertical single straight root segment surrounded by a soil with a  
 357 constant and uniform soil water pressure head (i.e. the soil is not in hydrostatic equilibrium). We

358 prescribe the root water pressure head at the root collar as  $\psi_x|_{\text{collar}} = \psi_0$ , and no axial flow at the  
 359 root tips.

360 **Reference solution** For constant  $k_r$  and  $k_x$  we can solve Eq. (6) yielding

$$\psi_x(\zeta) = \psi_s + d_1 e^{\sqrt{c}\zeta} + d_2 e^{-\sqrt{c}\zeta}, \quad (7)$$

with  $c = 2r_{\text{root}}\pi k_r/k_x$ . The integration constants  $d_1$  and  $d_2$  for above boundary conditions are given by

$$d_1 = d^{-1} \left( e^{-\sqrt{c}l_{\text{seg}}} (\psi_0 - \psi_s) + 1 \right) \quad (8)$$

$$d_2 = -d^{-1} \left( e^{\sqrt{c}l_{\text{seg}}} (\psi_0 - \psi_s) + 1 \right), \quad (9)$$

$$(10)$$

where  $l_{\text{seg}}$  is the segment length, and  $d$  is the determinant of above matrix

$$d = e^{-\sqrt{c}l_{\text{seg}}} - e^{\sqrt{c}l_{\text{seg}}}, \quad (11)$$

361 see Appendix A. Fig. 5 shows the analytical solution to this benchmark using the parameters given  
 362 in Table 4.

Table 4: Parameters of scenario M3.1.

l	50	length of a single straight root (cm)
$r_{\text{root}}$	0.02	radius (cm)
$k_z$	$4.32 \times 10^{-2}$	axial conductivity ( $\text{cm}^3 \text{d}^{-1}$ )
$k_r$	$1.73 \times 10^{-4}$	radial conductivity ( $\text{d}^{-1}$ )
$\psi_s$	-200	static soil water pressure head (cm)
$\psi_0$	-1,000	Dirichlet boundary conditions at the root collar (cm)

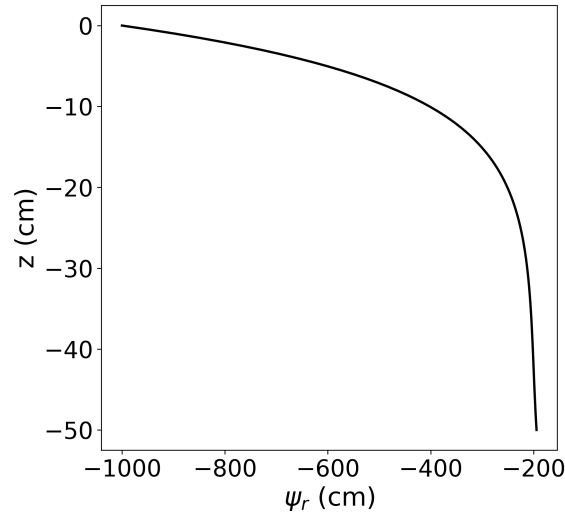


Figure 5: Results of M3.1: Root water pressure head distribution within a single vertical root

363 **Required output** The following simulation results of participating models are to be uploaded  
 364 via pull requests to this path on the github repository: M3 Water flow in roots/M3.1 Single  
 365 root/M31 Numerical results/.

366 1. A text file consisting of two rows containing comma separated depth values (cm) in the  
 367 first, and root pressure head (cm) in the second. The file name should be of the form  
 368 "simulatorname.txt", e.g. "DuMux.txt".

369 Note that we do not prescribe spatial resolution of the outputs, as that may depend on the indi-  
 370 vidual numerical schemes.

371 **Benchmark M3.2: A small root system in a static soil** In the following benchmark, we  
372 extend benchmark M3.1 from a single root to a root system. We consider water flow inside a small  
373 static root system of a lupine plant which was grown for 14 days in a soil-filled column of 20 cm  
374 depth and 7 cm diameter. The root system was imaged by MRI at Forschungszentrum Jülich; the  
375 segmented root structure is provided in RSML, DGF (Dune grid format) (Bastian et al., 2008)  
376 and RSWMS (Javaux et al., 2008) formats in the folder M3 Water flow in roots/M3.2 Root  
377 system/root\_grid on the github repository. It is visualised in Fig. 6(a,b) with colours denoting  
378 root order and root segment age.

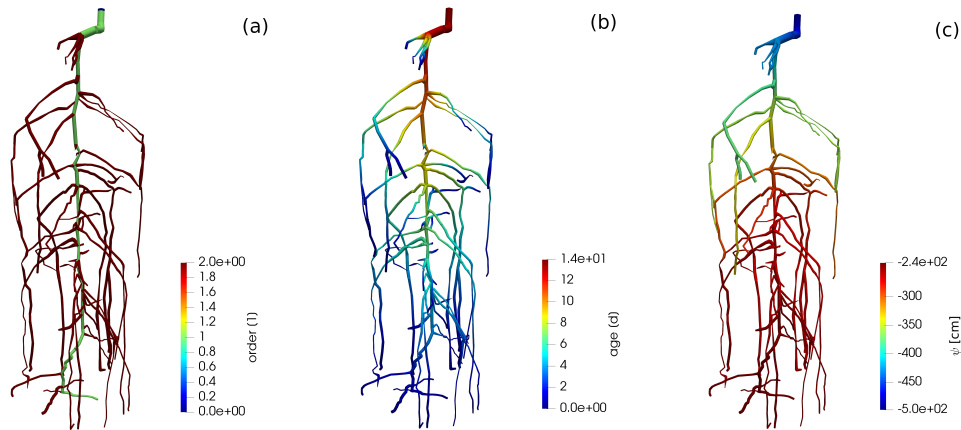


Figure 6: Visualisation of the root system of M3.2 with colours denoting (a) root order, (b) root segment age, (c) root water pressure head.

379 **Reference solution** The reference solution for this problem is given by the hybrid analytical-  
380 numerical solution of water flow in the root hydraulic architecture proposed by Meunier et al.  
381 (2017). The advantage of this solution is that it is independent of the spatial resolution of the root  
382 system (i.e. root segment length).

383 We consider two scenarios. The first one uses the same constant root hydraulic properties  
384 as given in Table 4, i.e. considering the same root hydraulic properties for each root segment.  
385 In the second scenario, we consider age-dependent root hydraulic properties for tap root and  
386 laterals of lupine as obtained by Zarebanadkouki et al. (2016, exponential function scenario) and  
387 converting distance from root tip to root age by assuming a root growth rate of  $1 \text{ cm d}^{-1}$ . This  
388 parameterisation takes into account that roots get a higher axial conductivity and lower radial  
389 conductivity as they are becoming older (see Fig. 7, a table with the actual values is provided on the  
390 github repository, in: M3 Water flow in roots/M3.2 Root system/M3.2 Benchmark problem.  
391 ipynb).

392 A sample 3-D visualisation of the model output is shown in Fig. 6(c) for the constant root  
393 hydraulic properties scenario. Fig. 8 shows the effect of constant and age-dependent root hydraulic  
394 properties under otherwise same (soil and boundary) conditions.

395 **Required output** The following simulation results of participating models are to be uploaded  
396 via pull requests to this path on the github repository: M3 Water flow in roots/M3.2 Root  
397 system/M32a Numerical results and M3 Water flow in roots/M3.2 Root system/M32b Numerical  
398 results for the constant and age-dependent root hydraulic properties cases.

- 399 1. A text file consisting of two rows containing comma separated depth values (cm) in the  
400 first, and root pressure head (cm) in the second. The file name should be of the form  
401 "simulatorname.txt", e.g. "DuMux.txt".

402 Note that we do not prescribe spatial resolution of the outputs, as that may depend on the indi-  
403 vidual numerical schemes.



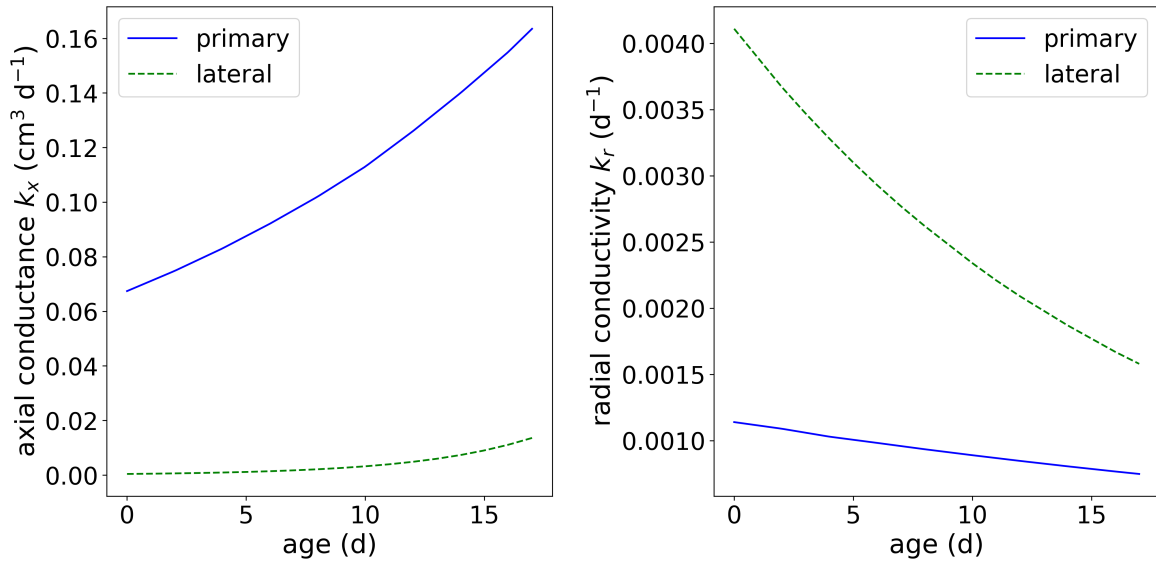


Figure 7: Root hydraulic properties dependency on root type and root segment age.

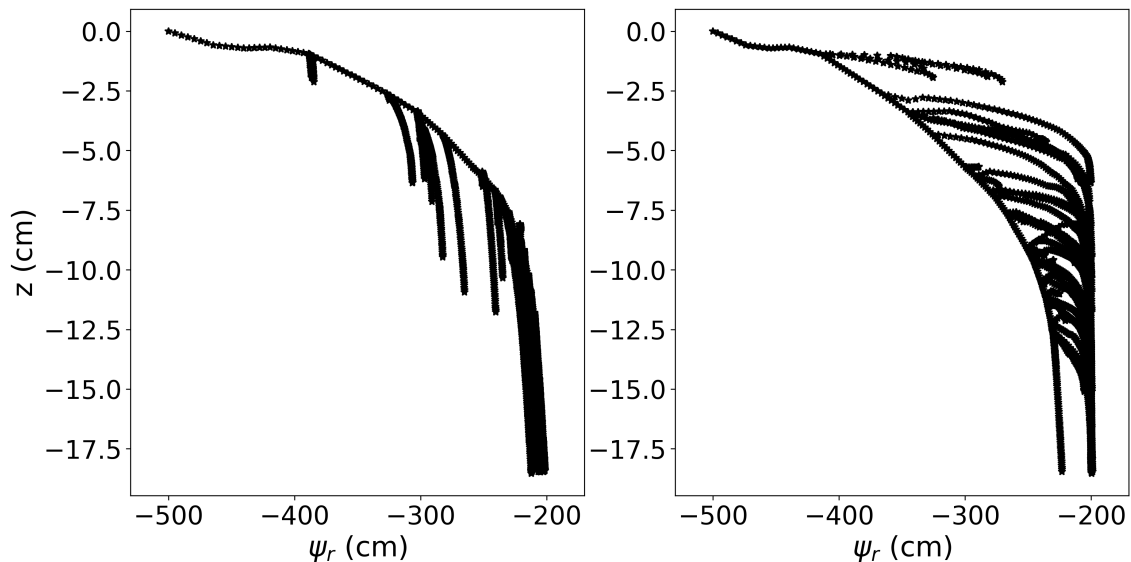


Figure 8: Results of M3.2. Left panel: Xylem pressure in each root segment of a root system with constant hydraulic properties. Right panel: Xylem pressure in each root segment of a root system with age-dependent hydraulic properties.

#### 404 2.1.4 Coupled benchmark scenarios C1: Root water uptake by a static root system

405 The way of coupling can easily introduce differences in simulated results because of numerical  
 406 errors (especially when there is two way coupling) or because different assumption are made when  
 407 implementing the coupling. No analytical solutions exists for the coupled problems presented here,  
 408 but the coupling (C) benchmarks are intended to quantify differences between model outputs of  
 409 coupled models. We may see differences observed in the non-coupled benchmarks to be amplified,  
 410 or to be irrelevant for the coupled problem.

411 **C1.1: Water uptake by a single root** This benchmark follows the paper of Schröder et al.  
 412 (2008). Here we aim to see to what extent the different participating models can reproduce the  
 413 hydraulic conductivity drop near the root surface under different soil conditions and transpiration  
 414 demands. Thus, it requires the participating line-source based models to strongly increase the  
 415 spatial resolution of the 3D soil domain. From this benchmark, we will learn, whether the spatial

416 resolution required to reproduce radial soil water pressure head gradients would be in a feasible  
 417 order of magnitude for larger soil-root systems or not. If not, there are approaches to estimate  
 418 soil water pressure head drop at the root-soil interface from bulk soil values as e.g. in Mai et al.  
 419 (2019); Beudez et al. (2013), see also benchmark C1.2.

420 **Reference solution** The analytical solution is based on the analytical solutions of the 1D radially  
 421 symmetric problem of water uptake by a single root, in which root water uptake is described as  
 422 a boundary condition at the root-soil interface. We consider here two water uptake regimes, a  
 423 non-stressed condition with maximum root uptake ( $q_{root}$ ), and a stressed condition with a limiting  
 424 plant root water potential constraining uptake. Based on the steady-rate assumption and using  
 425 the matric flux potential  $\Phi(h_c) = \int_{-\infty}^{h_c} K(h)dh$  that linearises the Richards equation, the radial soil  
 426 water pressure head profiles for non-stressed and stressed conditions (stress conditions are given  
 427 when the soil water pressure head at the root surface reaches  $-15\,000\text{cm}$ ) are given by

$$\Phi_{nostress}(r) = \Phi_{r_{out}} + (q_{root}r_{root} - q_{out}r_{out}) \left[ \frac{r^2/r_{root}^2}{2(1-\rho^2)} + \frac{\rho^2}{1-\rho^2} \left( \ln \frac{r_{out}}{r} - \frac{1}{2} \right) \right] + q_{out}r_{out} \ln \frac{r}{r_{out}} \quad (12)$$

428 and

$$\Phi_{stress}(r) = \left( \Phi_{r_{out}} - \Phi_{r_{root}} + q_{out}r_{out} \ln \frac{1}{\rho} \right) \frac{r^2/r_{root}^2 - 1 + 2\rho^2 \ln r_{root}/r}{\rho^2 - 1 + 2\rho^2 \ln 1/\rho} + q_{out}r_{out} \ln \frac{r}{r_{root}} + \Phi_{r_{root}}, \quad (13)$$

429 where  $\rho = \frac{r_{out}}{r_{root}}$ .

Given the soil water pressure head at the outer boundary, the solution computes the soil water pressure head profile towards the root. Due to the steady-rate assumption, the problem has become a stationary boundary value problem. However, under non-stressed conditions, we can calculate the time that corresponds to a given radial soil water pressure head profile by dividing the volume of water removed from the soil domain by the known water flow rate. The water remaining in a 1 cm long hollow cylinder around the root is given by

$$V = \int_0^{2\pi} \int_{r_{root}}^{r_{out}} r \theta dr d\phi = 2\pi \int_{r_{root}}^{r_{out}} r \theta dr$$

,  $\theta$  being the water content. The initially available water volume in the soil domain is given by

$$V_i = (r_{out}^2 - r_{root}^2) \pi \theta_i.$$

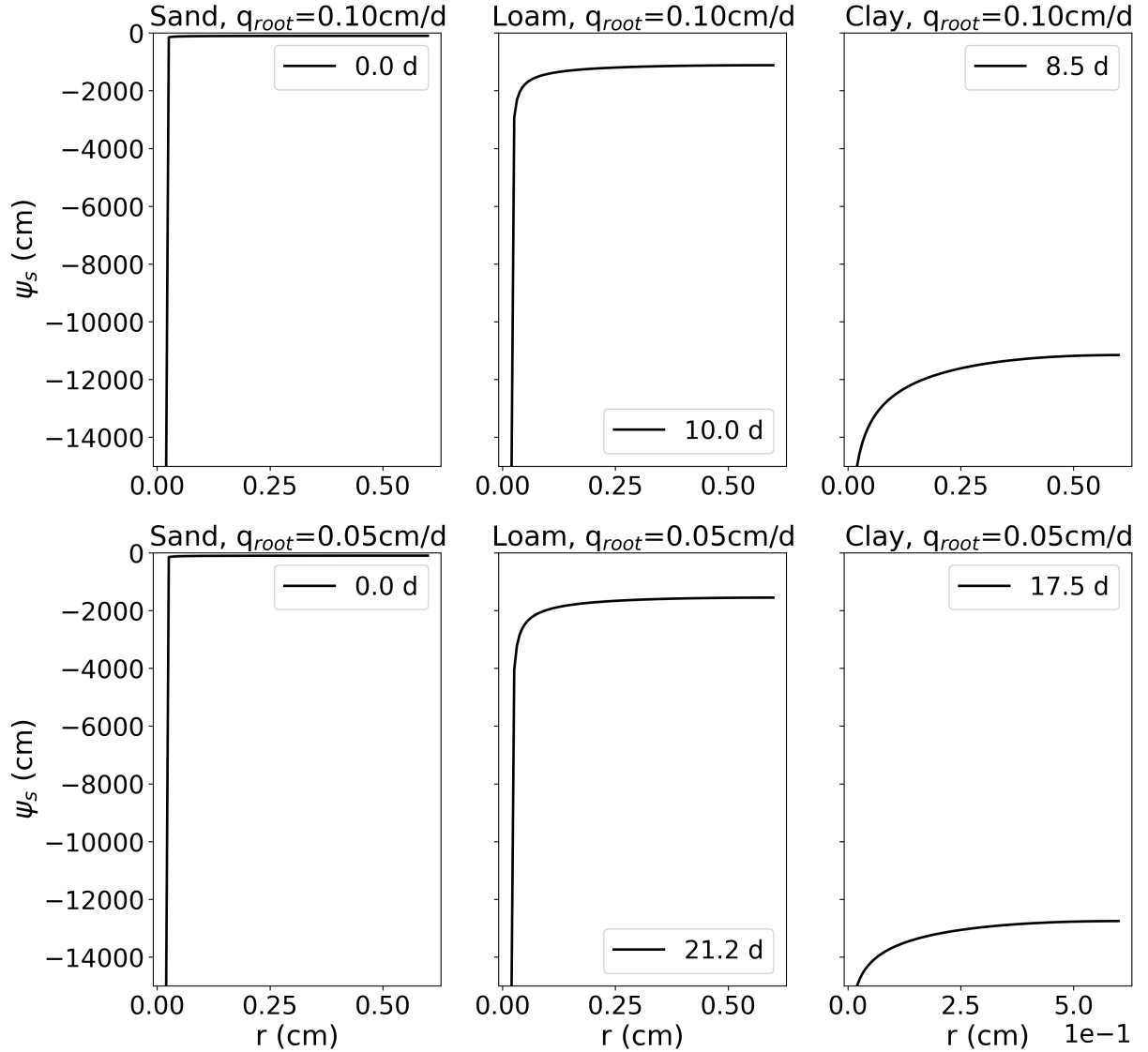
Thus, until the onset of stress, the corresponding time at which a given radial profile is reached is given by

$$t = \frac{(V_i - V)}{2r_{root}\pi q_{root}}.$$

430 For the three soils sand, loam, and clay (Table 3), we compute the analytical solution with the  
 431 following parameters:  $r_{root} = 0.02\text{cm}$ ,  $r_{out} = 1\text{cm}$ ,  $q_{root} = 0.5\text{cm/d}$ ,  $\psi_{s,lim} = -15000\text{cm}$ ,  $q_{out} =$   
 432  $0\text{cm/d}$  and for different soil water pressure heads at the outer end of the cylinder. Fig. 9 shows the  
 433 soil water pressure head gradients at the onset of stress (i.e., when the soil water pressure head at  
 434 the root surface reached  $-15\,000\text{cm}$ ) and the time of its occurrence. The value of the initial water  
 435 content is taken to be  $\theta_i = -100\text{cm}$ . This analytical solution is for radial water flow in soil towards  
 436 the root only, i.e., not considering gravity or water flow inside the roots. Ideally, in their numerical  
 437 implementation of this benchmark, the different participating models will turn off gravity effects.  
 438 The soil domain for this numerical implementation has a size of  $l \times w \times d = 1 \times 1 \times 1\text{ cm}$ . The  
 439 horizontal spatial resolution is high enough such that hydraulic conductivity drop near root surface  
 440 can be resolved. The axial and radial conductances are high, such that the pressure inside the root  
 441 is everywhere the same and the uptake flux is uniform.

442 **Required output** The following simulation results of participating models are to be uploaded  
 443 via pull requests to this path on the github repository: M3 Water flow in roots/M3.2 Root  
 444 system/M32a Numerical results and M3 Water flow in roots/M3.2 Root system/M32b Numerical  
 445 results for the constant and age-dependent root hydraulic properties cases.

Figure 9: Results of C1.1: Soil water pressure head gradients around a single, transpiring, root at the onset of stress and the time of its occurrence



446 1. A text file consisting of two rows containing comma separated radial distances from the  
 447 root surface (cm) in the first, and soil pressure head (cm) in the second for each soil and  
 448 transpiration rate scenario (i.e., 3 (soils)  $\times$  2 (transpiration rates)  $\times$  2 = 12 rows. The file  
 449 name should be of the form "simulatorname.txt", e.g. "DuMux.txt".

450 Note that we do not prescribe spatial or temporal resolution of the outputs, as that may depend  
 451 on the individual numerical schemes.

### 452 2.1.5 C1.2: Water uptake by a root system from drying soil

This benchmark scenario considers water uptake by a static 8-day-old lupine root system given in the public data set (Koch, 2019) as RSML or DGF. The root is the same as the one in benchmark M3.2, only younger, in order to reduce the computational cost for the reference scenario. The root system has been segmented from MRI measurements. The lupine is embedded in a soil box of  $l \times w \times d = 8 \times 8 \times 15$  cm filled with loam (soil hydraulic properties given in Table 3). The benchmark is to evaluate the accuracy of root water uptake models under conditions of drying soil. To this end, the soil has an initial water content of  $\theta_{top} = 0.129$ , corresponding to a pressure head  $\psi_{s,top} = -659.8$  cm at the soil surface ( $z = 0$ ). The pressure head in the rest of the domain

initially follows a hydrostatic distribution

$$\psi_{s,i} = \psi_{s,\text{top}} - z, \quad (14)$$

where  $z$  (in cm) denotes the vertical position (upward-pointing axis, zero at soil surface). At all soil boundaries, as well as at the root tips, no-flux boundaries are prescribed. A potential transpiration rate is given as the sinusoidal diurnal function

$$Q_{\text{pot}}(t) = \bar{Q} \left[ 1 + \sin \left( 2\pi t - \frac{\pi}{2} \right) \right], \quad (15)$$

453 where the mean transpiration rate is  $\bar{Q} = 6.4 \text{ cm}^3 \text{ d}^{-1}$ , the time  $t$  is given in days, and  $Q_{\text{pot}}(t =$   
 454  $0) = 0$ , that is, the simulation starts at night. The potential transpiration rate  $Q_{\text{pot}}$ , Eq. (15),  
 455 is enforced at the root collar (Neumann boundary condition) as long as the root water pressure  
 456 head at the root collar is above  $\psi_{x,\text{crit}} = -15.290 \text{ cm}$  (corresponding to  $-1.5 \text{ MPa}$ ). If this critical  
 457 root water pressure head at the root collar is reached, the boundary condition is switched to a  
 458 Dirichlet type boundary condition, enforcing a constant pressure head  $\psi_{x,\text{crit}} = -15.290 \text{ cm}$  at  
 459 the root collar. This informal description is intentional, as the actual implementation of such a  
 460 boundary condition may vary from simulator to simulator. We consider two scenarios. In scenario  
 461 C1.2a the root hydraulic properties are constant. The tap root and lateral root conductivities  
 462 are  $k_x = 4.32 \times 10^{-2} \text{ cm}^3 \text{ d}^{-1}$  and  $k_r = 1.73 \times 10^{-4} \text{ d}^{-1}$  (Table 4). For scenario C1.2b the root  
 463 hydraulic properties depend on the root type and root age and are shown in Fig. 7.

Given the soil domain  $\Omega$  and the network of root center-lines  $\Lambda$ , we solve the following coupled system of equations

$$\frac{\partial \theta}{\partial t} - \nabla \cdot (K(\theta)(\nabla \psi_s + e_3)) = q(\psi_x, \psi_s) \quad \text{in } \Omega, \quad (16)$$

$$-\frac{\partial}{\partial \zeta} \left( k_x \frac{\partial \psi_x}{\partial \zeta} + \frac{\partial z}{\partial \zeta} \right) = \hat{q}(\psi_x, \psi_s) \quad \text{on } \Lambda, \quad (17)$$

464 subject to the boundary conditions specified above, where  $\zeta$  is a scalar parametrisation (local axial  
 465 coordinate) of the root segments. The specific radial flux  $\hat{q}$  in units ( $\text{cm}^2 \text{ d}^{-1}$ ) is given by the average  
 466 soil water pressure head on the root surface. The formulation of  $q$  in Eq. (16) may be different  
 467 between different participating models. A discussion on singularity issues when evaluating the soil  
 468 water content at the root center line can be found in Koch et al. (2018b). In many cases, the soil  
 469 discretisation is much larger than the root diameter, and thus the drop in hydraulic conductivity  
 470 near the root surface in dry soils may not be sufficiently resolved in the soil domain. Approaches to  
 471 estimate soil water pressure head drop at the root-soil interface from bulk soil values can be found  
 472 in Mai et al. (e.g. 2019); Beudez et al. (e.g. 2013). Different approaches for the determination of  
 473 the sink term for root water uptake are likely to differ most in dry soil. The reference solution to  
 474 this benchmark is designed to evaluate possible differences between the models in that regard.

**Reference solution** As no analytical solutions exist for this problem of coupled water flow in the soil-root system, we designed a reference solution with a numerical model that explicitly considers the physical presence of roots in the soil domain, i.e., the soil mesh is highly refined around all roots and water uptake is modelled via boundary conditions at all the root surfaces. Thus, this reference solution does not make any assumptions that are inherent in the definition of the sink terms for root water uptake in the line source-based models. An explicit 3D soil grid is also used in Daly et al. (2017). However here, the soil is additionally coupled to the xylem flow in the root. The root is still modeled as a network of one-dimensional segments (center-line representation). Each segment has a specific radius as specified in the RSML grid file to this benchmark. A three-dimensional representation of the root system is implicitly given by the union of all spheres along the root center-lines. Using this implicit representation a soil grid excluding the root system was generated using the C++ geometry library CGAL (The CGAL Project, 2019). In order to reduce the number of vertices in the mesh, the mesh is locally refined around the root-soil interface. The resulting mesh is available in the Gmsh format (Geuzaine and Remacle, 2009) in the data set. For the evaluation of the radial flux, which is a coupling condition on the soil faces  $\sigma$  representing the root-soil interface, we integrate over each face

$$F_r = \int_{\sigma} r_{\text{root}} k_r (\psi_s - \psi_x) dA. \quad (18)$$

475 While the soil water pressure head is defined on the face, the corresponding root xylem water  
476 pressure head has to be found by a mapping. To this end the integration point is first mapped onto  
477 the root surface using its implicit representation. Then the point is mapped onto the corresponding  
478 root center-line (a line segment) by finding the closest point on the line segment. There,  $\psi_x$  is  
479 evaluated. The flux is added as a source term in the corresponding segment in the root. The  
480 model is implemented in the open-source porous media simulator DuMu<sup>x</sup> (Flemisch et al., 2011;  
481 Koch et al., 2019; Koch et al., 2018a). The coupled system is solved with a fully coupled manner,  
482 using Newton's method, and monolithic linear solver (block-preconditioned stabilized bi-conjugate  
483 gradient solver) in each Newton iteration. The equations are discretized in time with an implicit  
484 Euler method, and in space with a locally mass conservative vertex-centered finite volume method  
485 (BOX method (Helmig et al., 1997)). The maximum time step size is  $\Delta t = 1200$  s. The actual time  
486 step size may be sometimes chosen smaller, depending on the convergence speed of the Newton  
487 method. Output files are produced in regular intervals every 1200 s starting with the initial solution.  
488 The simulation time is 3 d.

489 Soil water content and root water pressure head in a three-dimensional plot is shown in Fig.  
490 10 for C1.2b. Fig. 11A shows the potential and actual transpiration rates for both scenarios,  
491 with constant and age-dependent root hydraulic properties. The curves hardly differ since the  
492 water pressure head drop is dominated by the low conductivity of the dry soil. In Fig. 11B, the  
493 differences between scenarios are more clearly visible in terms of the minimal and maximal root  
water pressure head with respect to time.

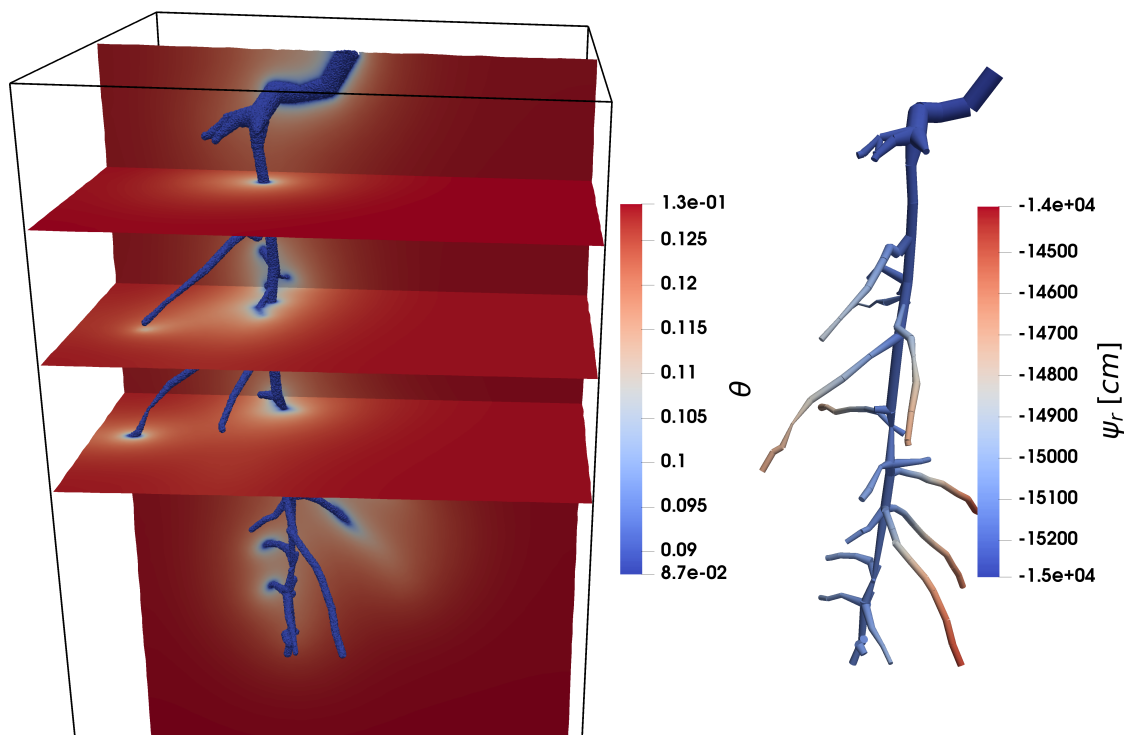


Figure 10: C1.2: Root water uptake by a static root system over time. Soil colours denote volumetric water content, root colours denote root water pressure head.

494

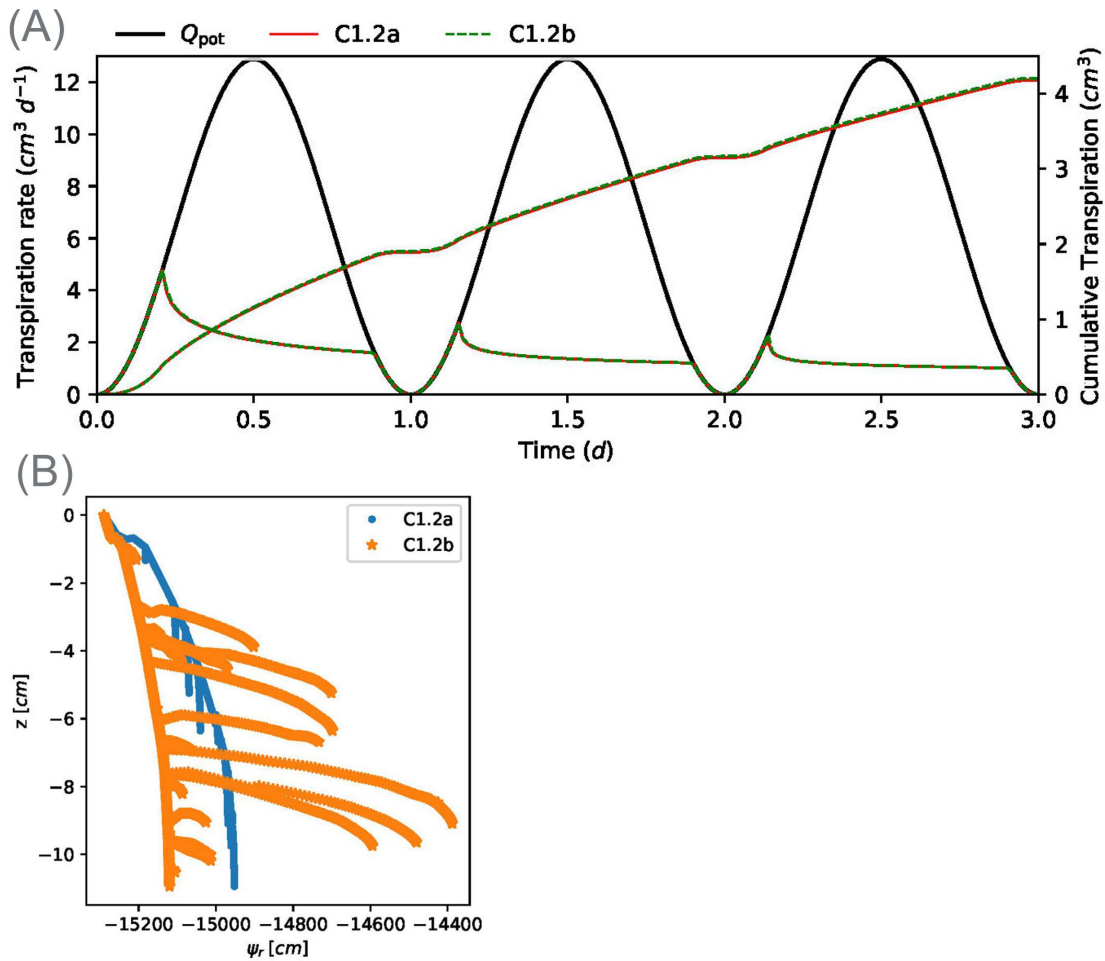


Figure 11: Results of C1.2 for two scenarios, constant and age-dependent root hydraulic properties. A: Actual transpiration of reference solution. B: Root water pressure head distributions inside the root system.

495 **Required outputs** To compare the results between the participating models, the desired  
 496 outputs are

- 497 • VTK files (3D) of soil water pressure head and water content on the first, second and third  
 498 day ( $t = 0.5$  d, 1.5 d, 2.5 d). For output written every 1200s this means the output files with  
 499 the number 36, 108, and 180.
- 500 • VTK files (lines in 3D) of root water pressure head in the first, second and day ( $t =$   
 501 0.5 d, 1.5 d, 2.5 d)
- 502 • CSV file with three data points per time step (each 1200s starting with  $t = 0$ ): time and  
 503 actual transpiration rate
- 504 • CSV file with three data point per time step: time and minimum and maximum root water  
 505 pressure head

506 File names of the VTK files should indicate the simulator name, the state variable, the domain, and  
 507 the output time in days, e.g. "DuMux\_soil\_theta\_1d.vtk". File names of the CSV files should  
 508 indicate the simulator name and output time it days, e.g., "Dumux\_1.csv".

## 509 **2.2 Coupled benchmark scenarios C2: Root water uptake by a dynamic** 510 **root system**

511 In this benchmark, we wish to explore differences caused by the approach of root growth modelling.  
512 We assess how the differences in root architecture parameters resulting from M1.2 propagate (or  
513 not) in the computation of the root water uptake from soil. In this example, we do not consider  
514 the effect of soil properties on root growth, but only the differences that arise from the different  
515 root systems according to M1.2.

### 516 **2.2.1 C2.1: Water uptake by a single root**

517 Before looking at the root system, we look at how the implementation of the growth itself affects  
518 computed root water uptake for a single root. This scenario is analogous to C1.1, but with a single  
519 root growing at an elongation rate of 2 cm/d from 1 to 10 cm length.

520 **Required outputs** The required outputs for model intercomparison are

- 521 • VTK files of 3D soil water pressure head and water content in soil at a temporal resolution  
522 of 1 day up until 60 days (point data)
- 523 • VTK files of xylem water pressure head (point data)
- 524 • Text files with two lines: time and corresponding actual transpiration

### 525 **2.2.2 C2.2: Water uptake by a root system**

526 This scenario is the same as C1.2b, but replacing the static root system with a growing root  
527 system. The root growth parameters are for each model the results of M1.2; simulations start from  
528 a seed and run until a 60 day old root system. The domain size is  $25 \times 25 \times 100$  cm, the potential  
529 transpiration  $Q_{pot} = 0.5 \text{ cm}^3 \text{ d}^{-1}$  is scaled proportional to the root volume divided by the maximal  
530 root volume at maturity.

531 **Required outputs**

- 532 • VTK files of 3D soil water pressure head and water content in soil at a temporal resolution  
533 of 1 day up until 60 days (point data)
- 534 • VTK files of xylem water pressure head (point data)
- 535 • Text files with two lines: time and corresponding actual transpiration

536 File names of the VTK files should indicate the simulator name, the state variable, the domain, and  
537 the output time in days, e.g. "DuMux\_soil\_theta\_1d.vtk". File names of the CSV files should  
538 indicate the simulator name and output time in days, e.g., "Dumux\_1.csv".

## 539 **2.3 Automated comparison within all benchmark problems**

540 Each benchmark folder on the github repository contains a Jupyter Notebook named "Automated  
541 comparison". It provides the analytical solution of the respective benchmark and in addition  
542 includes Python code that automatically loads all the outputs of participating models that are  
543 provided in the "Numerical results" folder of that benchmark. As soon as new outputs are provided,  
544 they are automatically included in the analysis. Currently, different model outputs are already  
545 available. We envision more participating models' outputs to be provided in this way. Future  
546 analysis will include graphical and quantitative approaches.

## 547 **3 Conclusions**

548 Functional-structural root architecture models have been compared qualitatively (Dunbabin et al.,  
549 2013, e.g.), but until now no quantitative benchmarking existed. In other communities, bench-  
550 marking has been done or is ongoing, e.g., AgMIP (Porter et al., 2014) for crop models, CMIP  
551 (Eyring et al., 2016) for climate models, subsurface reactive transport models (Steffel et al., 2015).

552 With this paper, we propose a framework for collaborative benchmarking of functional-structural  
553 root architecture models that allows quantitative comparison of the outputs of different simulators  
554 with reference solutions and with each other. This framework is presented using Jupyter Note-  
555 books. Behind every "module" benchmark, there is a working code that explains and implements  
556 the reference solution or analysis of reference data. For both, "module" and "coupled" benchmarks,  
557 Jupyter Notebooks facilitate the automated comparison of simulator simulation outputs that are  
558 stored in specified folders of a public github repository. In this way, new numerical simulators  
559 that may be developed in the future may still be added to the automated comparison. All the  
560 analysis that is done in the Jupyter Notebooks is freely available so that the comparisons and  
561 analysis of uploaded model outputs will be transparent and repeatable. Future efforts will aim at  
562 extending the benchmarks from water flow in root and soil systems to further processes such as  
563 solute transport, rhizodeposition, etc. We expect that this benchmarking will result in a better  
564 understanding of the different models and contribute towards improved models, with which we can  
565 simulate various scenarios with greater confidence. It will set standards for future model devel-  
566 opments, ensuring that bugs, numerical errors or conceptual misunderstandings do not affect the  
567 value of future work. This is a step towards developing those models into the much-needed aid  
568 in the design of agricultural management schemes and model-guided crop breeding. These models  
569 may also be useful in ecology, e.g. to study species complementarity.



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## 703 A Derivation of the analytical solution of water flow inside 704 the root system

705 The axial water flow rate in the xylem  $Q_x$  ( $\text{cm}^3 \text{ day}^{-1}$ ) is given by

$$706 Q_x = -k_x \left( \frac{\partial \psi_x}{\partial \zeta} + v \cdot \mathbf{e}_3 \right), \quad (19)$$

707 where  $k_x$  is the axial conductance ( $\text{cm}^3 \text{ day}^{-1}$ ),  $\psi_x$  is the pressure inside the xylem (cm),  $\zeta$  is  
708 the local axial coordinate  $\mathbf{e}_3$  the unit vector in  $z$ -direction, and  $v$  the normalised direction of the  
709 xylem.

709 The radial water flow rate is given by

$$Q_r = -2r_{root}\pi l_{seg}k_r(\psi_s - \psi_x) \quad (20)$$

710 with units ( $\text{cm}^3 \text{ day}^{-1}$ ), where  $r_{root}$  is the root radius (cm),  $l_{seg}$  is the length of each root segment  
 711 (cm),  $k_r$  is the radial conductivity ( $\text{day}^{-1}$ ), and  $\psi_s$  is the soil water pressure head of the surround-  
 712 ing soil (cm). The equation is neglecting osmotic potential and is based on Eq. (3.3) of Roose  
 713 and Fowler (2004). Note that around the root a homogeneous soil water pressure head is assumed,  
 714 therefore there is actually no hydrostatic equilibrium.

715

For each segment of length  $l_{seg}$  mass conservation yields

$$0 = Q_x|_{l_{seg}} - Q_x|_0 + Q_r \quad (21)$$

$$-\frac{1}{l_{seg}}Q_r = -\frac{1}{l_{seg}}(Q_x|_0 - Q_x|_{l_{seg}}) \quad \text{and for } l_{seg} \rightarrow 0 \quad (22)$$

$$2r_{root}\pi k_r(\psi_s - \psi_x) = -k_x \frac{\partial^2 \psi_x}{\partial \zeta^2} \quad (23)$$

716 see Eq. (3.4) of Roose and Fowler (2004), where  $v_3$  is the  $z$ -component of the normalised xylem  
 717 direction (cm).

Integrating this ordinary differential equation leads to an explicit equation for  $\psi_x(\zeta)$

$$\psi_x(\zeta) = \psi_s + d_1 e^{\sqrt{c}\zeta} + d_2 e^{-\sqrt{c}\zeta}, \quad (24)$$

718 where  $c := 2a\pi k_r/k_x$ , and  $d_1$ , and  $d_2$  are integration constants that are derived from the boundary  
 719 conditions.

720

721 To exemplify, we calculate  $d_1$ , and  $d_2$  for a Dirichlet boundary condition at the root collar, and  
 722 no-flux boundary conditions at the tip. The Dirichlet boundary conditions at the collar of the root  
 723 system  $\psi_x|_{\text{collar}} = \psi_0$  is inserted into the analytic solution Eq. (24), and yields

$$\psi_s + d_1 + d_2 = \psi_0. \quad (25)$$

724 The Neumann boundary condition  $Q_x|_{l_{seg}} = 0$  (Eq. 20) leads to

$$\frac{\partial \psi_x}{\partial \zeta}|_{l_{seg}} = v_3, \quad (26)$$

725 where  $l_{seg}$  is the length of the root segment. Using the derivation of the analytical solution yields

$$d_1 \sqrt{c} e^{\sqrt{c}l_{seg}} - d_2 \sqrt{c} e^{-\sqrt{c}l_{seg}} = v_3. \quad (27)$$

For a straight downward segment  $v_3 = -1$ , Eqns (25) and (27) can be summarized as

$$\begin{pmatrix} 1 & 1 \\ \sqrt{c}e^{\sqrt{c}l_{seg}} & -\sqrt{c}e^{-\sqrt{c}l_{seg}} \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = \begin{pmatrix} \psi_0 - \psi_s \\ -1 \end{pmatrix} \quad (28)$$

Solving this linear equation for  $d_1$  and  $d_2$  yields

$$d_1 = d^{-1} \left( e^{-\sqrt{c}l_{seg}} (\psi_0 - \psi_s) + 1 \right) \quad (29)$$

$$d_2 = -d^{-1} \left( e^{\sqrt{c}l_{seg}} (\psi_0 - \psi_s) + 1 \right), \quad (30)$$

where  $d$  is the determinant of above matrix

$$d = e^{-\sqrt{c}l_{seg}} - e^{\sqrt{c}l_{seg}}. \quad (31)$$