

## COMPUTATIONAL EFFICIENT MODELLING OF SOIL-COUPLED 3D ROOT WATER UPTAKE FOR MULTIPLE ROOT SYSTEMS

T. Kalbacher<sup>1</sup>, C. L. Schneider<sup>2</sup>, W. Wang<sup>1</sup>,  
A. Hildebrandt<sup>2</sup>, S. Attinger<sup>2,3</sup> and O. Kolditz<sup>1,4</sup>

<sup>1</sup> Dept. of Environmental Informatics, Helmholtz Centre for Environmental Research - UFZ  
Permoserstrasse 15, Leipzig 04318, Germany  
e-mail: thomas.kalbacher@ufz.de, web page: <http://www.ufz.de>

<sup>2</sup> Dept. of Computational Hydrosystems, Helmholtz Centre for Environmental Research - UFZ  
Permoserstrasse 15, Leipzig 04318, Germany

<sup>3</sup> Institute for Geosciences, University of Jena, Jena, Germany

<sup>4</sup> Technical University of Dresden, Dresden, Germany

**Key words:** adaptive time stepping, coupling, HPC, Richards flow, root water uptake

**Summary.** Numerical modelling of interacting flow processes between roots and soil is essential for understanding the influence of different root geometries and types on the hydro-system and remains a challenging task especially for multiple interacting root systems. This is mainly due to the geometric complexity, the coupled physical processes, scale differences and the required computational resources. These days, coupled 3D-soil-root models at the plant scale are available simulating the water flow along potential gradients within root as well as in soil. Although the biological, chemical and physical processes along the soil-root interface have not been fully investigated yet, current models suggest strong gradients in water potential at the soil-root interface. We develop high-precision models, which capture the main small scale features of plant-water uptake (aRoot) but run on the bulk soil scale coupled to soil water infiltration (OpenGeoSys). This requires an appropriate combination of the geometric models and time stepping schemes to solve both, the plant-water uptake and the soil water flow. The three-dimensional root architectures are embedded into bulk soil and the water flow is modeled along a network of resistances from the bulk soil along radial soil discs towards the root system up to the root collar. The non-linear dynamics of water flow within the soil surrounding the roots are covered by a 3D-Richards model. The numerical analysis of such coupled multiple-root-soil problems with a high precision involves significant computational resources and parallel computing is a way to enable the use of the necessary computer power of SMP machines or clusters. Moreover, we apply adaptive time stepping with automatic control, which assures model stability and a shorter total run-time as compared to a static and steady time-step scheme.

## 1 INTRODUCTION

Previous research using small scale models for water uptake, e.g. [1][2], indicates that both water flow in the soil near the root, but also within the root system itself shape the uptake behavior of the plant. Due to the high nonlinearity of radial flow in the unsaturated zone, steep gradients of water potential evolve in the immediate vicinity of the root that extracts water from the soil. As shown in Schröder et al. 2009 [3], a refined spatial discretization of the numerical soil domain around the root can represent the local gradients in soil water potential. For an efficient computing performance, Schneider et al. 2009 [4] separated the microscopic soil water flow towards the root segment from the water flow in the bulk soil by the use of cylinder elements and applied an approximated analytical solution of the Richards equation [5][6][7]. We couple this model, in the following called aRoot [4], with the parallelized 3D-Richards model of OpenGeoSys (OGS) [8][9] to simulate the non-linear dynamics of water flow within the soil together with the root water uptake.

The coupling of such existing source code requires an interdisciplinary knowledge in computer science such as an understanding of the basic program structure, data and control dependencies, and most important the awareness of the governing scientific processes. However, all are indispensable for a tool coupling project to be successful and an interdisciplinary collaboration is essential to enable efficient coupled code interactions, especially in terms of high performance computing (HPC) and when three-dimensional problems on complex geometries are faced. In this paper, we present a straightforward software coupling technique of two independent code structures, for HPC environments of coupled water flow in and around a root network (Section 2).

In cases that numerical simulations are limited by the required computational resources, a parallel processing can help to overcome this limitation. However, parallelization is a way to improve performance but doesn't guarantee necessarily robust and stable results or efficient solution procedures and memory management. We introduce theory based automatic controls for nonlinear equations such as P (proportional feedback) or PI (proportional and integral feedback), which permit stable and efficient time stepping [10,11] for numerical solver. Technically, the primary aim of the present work is to investigate the functionality and performance of such PI controls (Section 3) applied to the governing Richards equation for coupled root-soil models.

Plant root systems vary greatly in form and morphology, not only between species, but also between individuals of the same species. This paper contributes to answer the question, how this variety influences the expected uptake pattern at the plant community scale. By combining the local features of root water uptake and the dynamics of water flow in soil, several hypotheses on soil-plant-interaction can be tested at the scale of interest. Studying these processes at such a high level of complexity, we aim to investigate the validity of common root water uptake approaches at the community scale. Neglecting the local flow processes around and within individual root segments, such water uptake models rely namely on the spatial distribution of roots and a simplistic water stress function [12].

## 2 COUPLING OF THE ROOT AND SOIL WATER MODEL FOR HPC

In this section we describe the coupling between two software tools, one simulating the root water uptake (aRoot) and the other one simulating flow in soil by the use of the 3D Richards equation (OGS). Furthermore we extend the coupling procedure to simulate systems with multiple roots on different locations to be able to analyze root systems with multiple roots.

### 2.1 The Richards flow model

We make use of the classic Richards equation to model the unsaturated flow in soil, which can be written as

$$\phi \rho^l \frac{\partial S^l}{\partial p^c} \frac{\partial p^w}{\partial t} + \nabla \cdot \left[ \rho^l \frac{\mathbf{k} k_{rel}^l}{\mu^l} (\nabla p^w - \rho^l \mathbf{g}) \right] = Q_w \quad (1)$$

with  $\phi$  porosity,  $\rho^l$  liquid density,  $\mu^l$  liquid viscosity,  $p^c$  capillary pressure,  $p^w$  water pressure,  $S^l$  saturation,  $\mathbf{k}$  the intrinsic permeability,  $k_{rel}$  relative permeability and  $\mathbf{g}$  gravity constant.

### 2.2 The hydraulic root water uptake model

The root water uptake model calculates the sink term for the bulk soil water flow model that is based on the Richards Equation (previous section). Within our root water uptake approach two specific flow domains are modeled: (a) the radial soil water flow from the bulk soil towards the root segment and (b) the water flow along the root system up to the root collar. These two domains are coupled by the fluxes at the soil root interface where the water entering the root segment is equal to the soil water discharge from the soil disc.

Within the root system, our hydraulic model approach distinguishes two pathways: the radial flow entering the roots through the root cortex and the epidermis ( $J_r$ ) and the axial flow ( $J_a$ ) along the root xylem tubes (Fig.1). Both paths are characterized by their specific hydraulic properties where each root segment is modeled as a series of radial and axial conductances. The outer boundary conditions are the bulk soil water potential and the transpirational demand at the root collar. The whole system is solved for the soil water potential at the soil-root-interface for all root segments. Solving such nonlinear systems with  $n$  equations in  $n$  unknowns requires a multidimensional root-finding algorithm that is provided by the free GNU Scientific Library.

### 2.3 The coupling scheme

The plant-water uptake model operates on a fine and precise line element network which represents the detailed geometry of the root system (Fig.1, left). The root system itself is created using a 3D root generator [13]. These roots are not growing anymore after the generation and geometrically static during the simulation. Obviously, modelling can therefore only be applied to shorter time periods where the growth of plants and roots can be neglected.

Beside the plant and root specific parameters, aRoot requires the information of the bulk soil water content which is the result provided by OGS but for the complete finite element mesh, i.e. pressure values for each mesh node of the soil model domain. Therefore, we developed a mapping function which links the geometric root network with the geometric soil model. The box-shaped soil model itself is a structured finite element mesh with hexahedral elements (Fig.1) and is created around the roots at the very beginning when the coupled simulation is executed. After mapping, the geometric relations between both models are stored i.e.

- nearest node of the soil model for each node of the root model,
- in which element of the soil model a root voxel is placed as well as
- how many and which root segments cross each element of the soil model (Fig.1 right).

The latter is needed for the effect of root segments occupying a certain soil volume, which decrease the porosity by the corresponding fraction of volumetric root content. Therefore we create a new material group for each cell with a decreased porosity. After the geometric coupling, it is unproblematic to assign spatial distributed data from and on both sides.

Figure 1 illustrates that the two software tools only have to exchange source/sink terms and soil water potential  $h_s$ , which is done for each time step (Section 4.1).

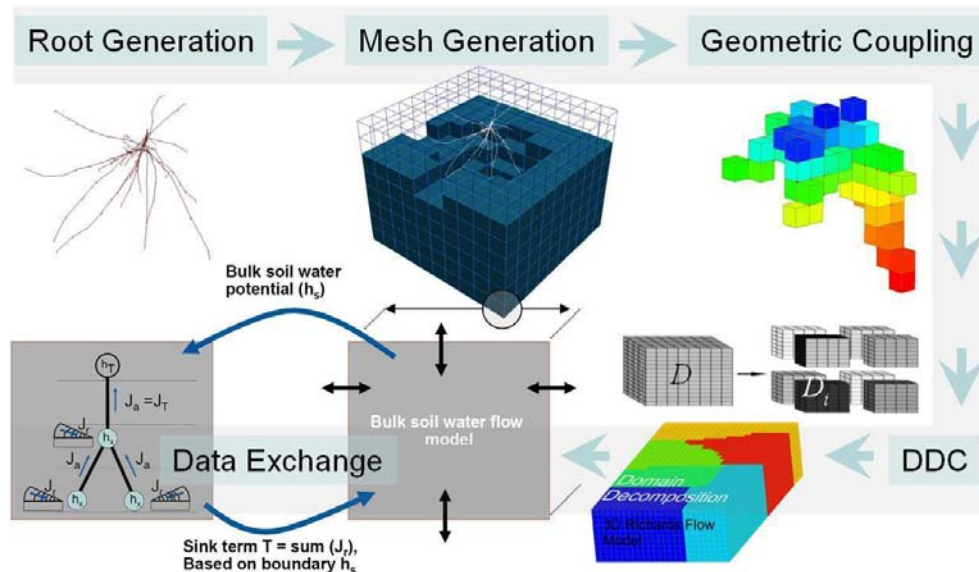


Figure 1: Coupling Concept between aRoot (serial) and OGS (parallel).

## 2.4 The coupling interface

The coupling interface is designed for a multithreading environment and needs at least a dual core CPU to ensure a robust “forking” of the processes. When a process forks, it creates a copy of itself by generating a child thread from the parent thread with a separate address space. Under Linux-like operating systems, the parent and the child processes can tell each other apart by examining the return value of the fork() call ( $pid = \text{fork}()$ ,  $pid=0$  for the child process). Both the parent and child processes include the same code segments, but execute

independently of each other. We use these characteristics to handle the work flow of both tools as shown in Fig. 2.

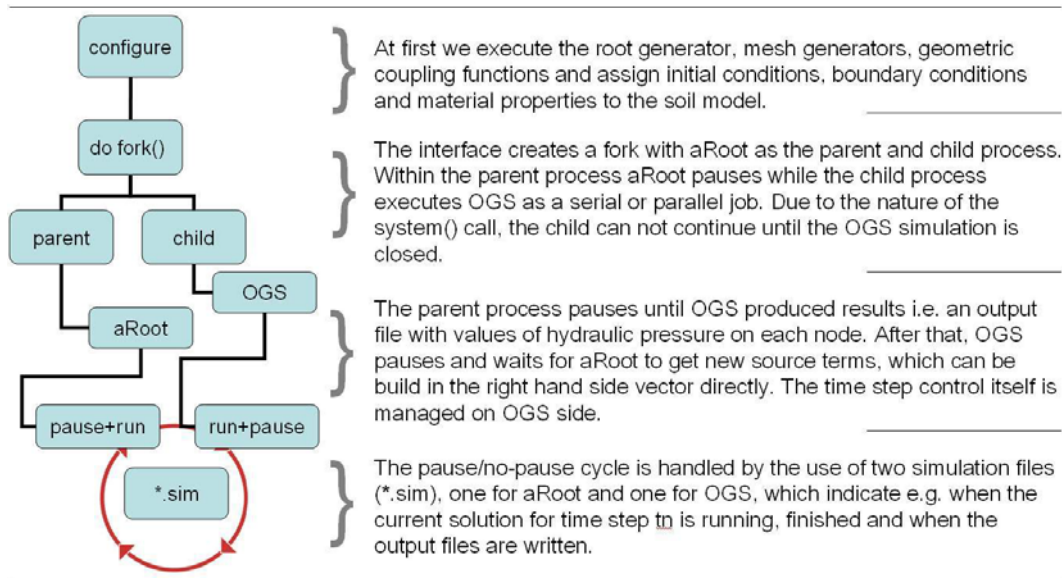


Figure 2: Work flow of the coupling interface for HPC environments.

For dealing multiple plants we use additionally a modified copy of the aRoot source code called “mRoots”. This maps an additional root network for each additional plant with its parameters and properties at a different position within the soil. The parent, i.e. aRoot, calls the mRoots executable consecutively for each additional root network. The source term file created by aRoot will be extended with the new sources. As long as the multiple root networks are modeled one after each other, no special handler is required to manage the mRoots implementation. The coupling procedure between mRoots and OGS is equivalent to the description in section 2.3.

### 3 ADAPTIVE TIME STEPPING WITH AUTOMATIC CONTROL

Practically, fixed time step sizes usually does not satisfy the stability and efficiency requirements in solving problems that exhibit nonlinearity in material properties and boundary conditions. As long as aRoot provides OGS with time-dependent source terms a static time step model is difficult to predict, especially because the complex root network geometries provide distributed and varying sink terms of same complexity within the domain of the soil model. The time step scheme itself is provided and organized on the OGS side since the results of root model only change when the soil water pressure changes.

For the Richards model, different kinds of time stepping methods can be found in the literature like e.g. heuristic stepping methods [14] or empirically based adaptive scheme with high order time integration for their transformed Richards equation [15]. The first mathematically based time stepping method for Richards equation was developed by Kavetski et al. [16] using the approximation of the local truncation error.

The PI time control method is originally developed for the numerical method for solving time dependent nonlinear PDEs with high-order finite difference schemes for time discretization and with the Newton-Raphson method for the solution of nonlinear PDEs [10,11]. In the following, we will briefly describe the implemented adaptive time stepping with automatic control for solving the nonlinear partial differential equation (PDEs) of Richards flow for soil models. A more detailed description is given by Wang et al. 2009 [17].

The fluid mass balance equation can be derived from the mass conservation law. Moreover, Wang et al 2009 [17] derived a corresponding weak form and discretized it in the finite element space with Galerkin procedure, which leads to the ordinary differential equation

$$\mathbf{M}\dot{\mathbf{p}} + \mathbf{K}\mathbf{p} = \mathbf{f} \quad (2)$$

where the mass matrix is denoted by  $\mathbf{M}$ , the Laplace matrix by  $\mathbf{K}$ , and the right hand side vector by  $\mathbf{f}$ , and their definition can be find in [17].

For the implementation of the automatic time stepping with automatic control for hydraulic processes, we use the backward Euler method to approximate the solutions of ordinary differential equations (2). The temporal discretization can be written like

$$\mathbf{M}(\mathbf{p}_{n+1} - \mathbf{p}_n) / \Delta t + \mathbf{K}[\alpha \mathbf{p}_{n+1} + (1 - \alpha) \mathbf{p}_n] = \mathbf{f} \quad (3)$$

where  $\alpha \in [0, 1]$  indicates a relaxation parameter,  $n$  the current time step and  $\Delta t$  the time step size.

With the Picard method we can linearize the equation and for each Picard iteration  $i+1$ . The solution of equation (3) is related to the previous Picard iteration  $i$  and given by

$$\mathbf{p}_{n+1}^{i+1} = [\mathbf{M}^i / \Delta t + \alpha \mathbf{K}^i]^{-1} (\mathbf{f}^i + \mathbf{M}^i \mathbf{p}_n / \Delta t - (1 - \alpha) \mathbf{K}^i \mathbf{p}_n) \quad (4)$$

Now we make use of the PI (proportional and integral feedback) [18] classic time control method, which should provide a stable and efficient time stepping. The idea of automatic PI bases on the elementary local error control theory [18,11] and in combination with the predictive control presented by Gustafsson [18] the next time step size  $\Delta t+1$ , can be predicted by the use of a time step size factor  $\eta$  with

$$\frac{\Delta t_{n+1}}{\Delta t_n} = \max(\eta_1, \eta_2) \quad (5)$$

Restrictions are introduced in modern controls to handle exceptions and we employ the restrictions presented in RODAS, the Rosenbrock solver for stiff ODEs (c.f. [11]) to apply them for our model equations (4). The first time step size factor  $\eta_1$  with restrictions is given by (c.f.[11]) as

$$\eta_1 = \max \left( c_1 \frac{\min(c_2, \sqrt[4]{\zeta})}{c_f} \right) \quad (6)$$

with default restrictions for step size selection  $c_1=1/6$ ,  $c_2=5.0$  and a safety factor in step size prediction with a default value  $c_f=0.9$ .  $\zeta$  denotes the error excess, i.e.

$$\zeta = \left( \frac{\varepsilon}{e_A + e_r \max(p_{n+1}^{i+1}, p_n)} \right) \quad \text{with} \quad \varepsilon = |p_{n+1}^{i+1} - p_{n+1}^i| \quad (7)$$

where  $\varepsilon$  is the error between the current and previous solution of a Picard iteration  $i+1$ ,  $e_r$

the relative tolerance and  $e_A$  the absolute tolerance to avoid zero entries.

The second time step factor presented by Gustafsson [18] can be calculated by

$$\eta_2 = \max \left( c_1, \min \left( c_2, \frac{\Delta t_{n-1}}{\Delta t_n} \sqrt[4]{\frac{\zeta^2}{\max(\zeta_{n-1}, 10^{-2})}} / c_f \right) \right) \quad (8)$$

In the present study, the backward Euler method and the Picard method are utilized for the temporal discretization and linearization. The error  $\varepsilon$  (7) is calculated during each Picard iteration step but only the value of the converged Picard iteration is applied to predict the time step size. Within the finite element context, nodal solutions are obtained and the error excess  $\zeta$  is calculated at each element node as well. Finally, we apply the Euclidean or energy norm to replace  $\zeta$  with the norm of  $\zeta$ .

#### 4 RESULTS AND CONCLUSIONS

A coupled root-soil model, combining a serial root model and a parallelized soil model controlled by automatic adaptive time stepping, was developed to provide a computational effective insight into the below ground interaction of water uptake between multiple root systems sharing the soils water resources. To assign appropriate tolerance factors ( $e_r$ ,  $e_A$ ), it has be taken into account that the time step model has to suit both, the soil water model (3D-Richards flow) and the temporal variability of the source/sink terms to ensure an appropriate water withdrawal. Fig. 3 exemplarily shows on the left side a model result (saturation) after half day of water uptake in a sandy soil with three different roots. The right side of Fig. 3 depicts the according automatically produced time step scheme. The time step sizes  $\Delta t$  decrease due to growing sharp gradients next to the roots and slow convergence of the solution, respectively. During the relaxation periods of the soil water pressure, i.e. less or no contribution of sources to the pressure depressions,  $\Delta t$  increases.

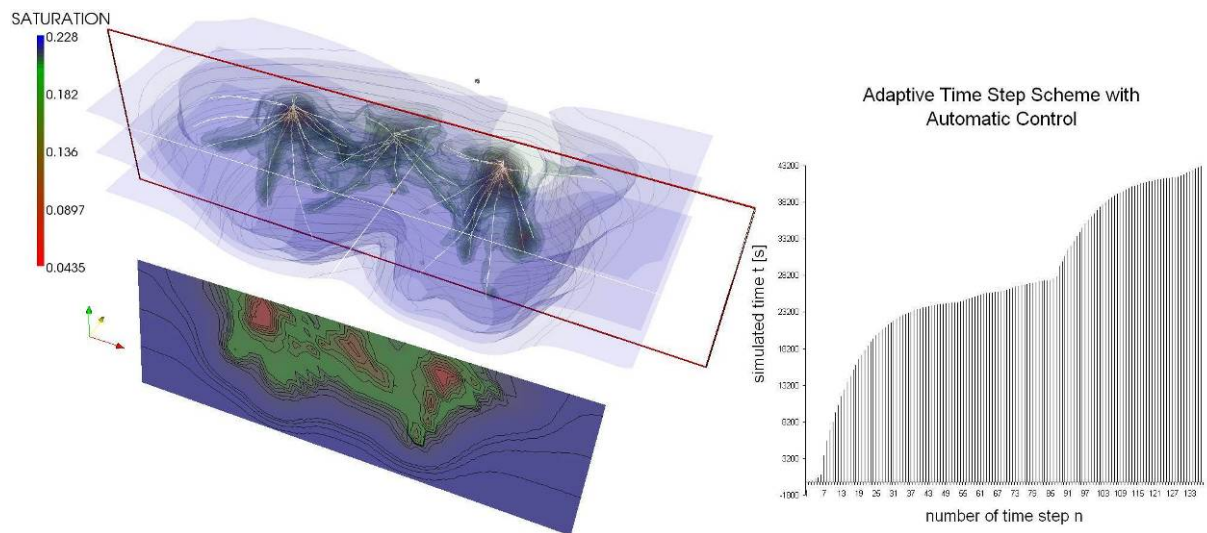


Figure 3: Left: Saturation distribution in sandy soil after  $\frac{1}{2}$  day root water uptake (s.[19]). Right: The appropriate result of the adaptive generated time step scheme ( $e_r = 1.0e-6$   $e_A = 1.0e-9$ ).



## ACKNOWLEDGEMENT

The authors want to thank particularly the German Ministry of Education and Research (BMBF) for funding "IWAS – International Water Research Alliance Saxony" (Project No. 02WM1027).

## REFERENCES

- [1] C. Doussan, A. Pierret, E. Garrigues, E. and L. Pagès, *Water uptake by plant roots: II –Modelling of water transfer in the soil root-system with explicit account of flow within the root system – comparison with experiments*, Plant Soil, 283(1–2), 99–117, (2006)..
- [2] M. Javaux, T. Schröder, J. Vanderborght, and H. Vereecken, *Use of a three-dimensional detailed modeling approach for predicting root water uptake*, Vadose Zone J., 7, 1079–1089 (2008).
- [3] T. Schröder, M. Javaux, J. Vanderborght, B. Körfgen and H. Vereecken, *Implementation of a Microscopic Soil-Root Hydraulic Conductivity Drop Function in a Three-Dimensional Soil-Root Architecture Water Transfer Mode*, Vadose Zone J., 8, 783-792, (2009).
- [4] C.L. Schneider, S. Attinger, J.O. Delfs, A. Hildebrandt, *Implementing small scale processes at the soil-plant interface - the role of root architectures for calculating root water uptake profiles*, Hydrol. Earth Syst. Sci., 14, 279-289, (2009).
- [5] B. Jacobsen, *Water and phosphate transport to plant roots*, Acta Agricult. Scand., 24, 55–60,(1974).
- [6] P. De Willigen, and M. van Noordwijk, *Root, Plant. Production and Nutrient Use Efficiency*, Ph.D. thesis, Agricultural University, Wageningen, Netherlands, (1987).
- [7] Q. de Jong van Lier, J.C. van Dam, K. Metselaar, R. de Jong, and W.H.M. Duijnisveld, *Macroscopic root water uptake distribution using a matric flux potential approach*, Vadose Zone J., 7, 1065–1078, (2008).
- [8] O. Kolditz, J.-O. Delfs, C. Bürger, M. Beinhorn and C.-H. Park, *Numerical analysis of coupled hydrosystems based on an object-oriented compartment approach*, J. Hydroinf., 10(3), 227–244, (2008).
- [9] W. Wang, G. Kosakowski and O. Kolditz, *A parallel finite element scheme for thermo-hydro-mechanical (THM) coupled problems in porous media*. Computers & Geosciences, vol 35(8) 1631-1641 (2009).
- [10] G. Söderlind and K. Gustafsson, *Control strategies for the iterative solution of nonlinear equations in ODE solvers*. SIAM Journal on Scientific Computing, 18(1):23–40 (1997).
- [11] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic problems*, 2nd Revised Edition, Computational Mathematics, Vol. 14. 2nd rev. ed., Springer-Verlag, Berlin (1996).
- [12] R. A. Feddes, H. Hoff, M. Bruen, T. Dawson, P. de Rosnay, P. Dirmeyer, R.B. Jackson, P. Kabat, A. Kleidon, A. Lilly and A.J. Pitman, *Modeling root water uptake in hydrological and climate models*, B. Am. Meteorol. Soc., 82, 2797–2809, (2001).
- [13] L. Pagès, G. Vercambre, J.-L. Drouet, F. Lecompte, C. Collet and J.L. Bot, *Root Typ: a generic model to depict and analyse the root system architecture*, Plant Soil, 258, 103–119, (2004).
- [14] K. Rathfelder and L.M. Abriola, *Mass conservative numerical solutions of the head-based Richards equation*. Water Resources Research, 30(9):2579–2586 (1994).
- [15] G.A. Williams and C.T. Miller *An evaluation of temporally adaptive transformation approaches for solving Richards' equation*. Advances in Water Resources, 22(8):831 – 840, (1999).
- [16] D. Kavetski, P. Binning, and S.W. Sloan, *Adaptive time stepping and error control in a mass conservative numerical solution of the mixed form of Richards equation*. Advances in water resources, 24(6):595–605 (2001).
- [17] W. Wang and O. Kolditz, *Time stepping with automatic control in the finite element analysis*, submitted to International J. for num. Methods in Engineering (2009).
- [18] K. Gustafsson, M. Lundh and G. Söderlind, *A PI step size control for the numerical solution of ordinary differential equations*. BIT, 28(2):270–287 (1988).
- [19] Kolditz O. et al., OpenGeoSys project, [www.opengeosys.net](http://www.opengeosys.net) (2010).