

# Comparison of Averaging Methods for Interface Conductivities in One-dimensional Unsaturated Flow in Layered Soils

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## Abstract

The water flow in unsaturated soils is governed by Richards equation, a nonlinear parabolic partial differential equation. In a layered unsaturated soil, enforcing the continuity of both pressure head and flux across the interface of distinct soil materials leads to a non-linear interface equation. This interface equation may exhibit multiple solutions. Using different averaging methods for cell-centered hydraulic conductivities impacts the ill-posedness of this interface problem and therefore affects the numerical simulations of transient unsaturated flow. Four averaging methods for cell-centered conductivities (arithmetic, harmonic, geometric or log-mean) are compared in this study. The choice of averaging schemes impacts the limit of discretization size that is needed to guarantee a unique solution of the interface equation. Numerical experiments confirm that the averaging schemes leading to larger interface conductivity averages (log-mean) are less likely to be affected by the non-uniqueness of solutions to the interface problem.

## 1 Introduction

The vertical infiltration flow in an unsaturated porous medium is described by the one-dimensional Richards equation (in mixed form),

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z}, \quad q = K \left( 1 - \frac{\partial h}{\partial z} \right), \quad (1)$$

where  $\theta = \theta(z, t)$  represents volumetric water content,  $z$  is depth (positive downwards),  $q$  is infiltration flux,  $K$  denotes soil hydraulic conductivity, and  $h$  is capillary pressure head. The effective saturation  $S$  is defined by

$$S = \frac{\theta - \theta_r}{\theta_s - \theta_r}, \quad (2)$$

where  $\theta_r$  is the residual water content and  $\theta_s$  the saturated water content. The soil hydraulic constitutive model describes the hydraulic conductivity  $K$  and the effective saturation  $S$  as functions of the pressure head  $h$ . In this work we focus on the (quasi-linear) Gardner model (Gardner, 1958)

$$S = \begin{cases} e^{\alpha h} & \text{if } h < 0, \\ 1 & \text{if } h \geq 0, \end{cases} \quad (3a)$$

$$K = \beta S, \quad (3b)$$

with  $\alpha > 0$ ,  $\beta > 0$ .

The estimate of cell-centered hydraulic conductivities is required for most numerical methods for solving Richards' equation. These estimates are obtained by taking averages of hydraulic conductivity values at adjacent cell boundaries. Various averaging methods for cell-centered hydraulic conductivities are used in practice. Haverkamp and Vauclin (1979) tested nine different methods of weighting cell-centered hydraulic conductivity values in homogeneous unsaturated soil in terms of the impact on the numerical solution. Baker (2006) uses a three-point grid test to validate some common averaging means. Previous studies show that geometric averaging produces in general better numerical solutions (Haverkamp and Vauclin, 1979; Schnabel and Richie, 1984; Belfort and Lehmann, 2005). However, the impact of averaging methods for cell-centered hydraulic conductivities has not been validated in heterogeneous (layered) soils. In this study, we investigate four commonly used averaging methods in terms of the ill-posedness of the interface problem for unsaturated infiltration in a two-layer soil.

## 2 The interface problem

In one-dimensional simulations, a standard second-order central finite difference method with a staggered scheme (Figure 1a) is used to convert Richards' equation to a system of ordinary differential equations (ODEs),

$$\frac{d\theta_j}{dt} = - \frac{K_{j+\frac{1}{2}} \left(1 - \frac{h_{j+1}-h_j}{\Delta_j}\right) - K_{j-\frac{1}{2}} \left(1 - \frac{h_j-h_{j-1}}{\Delta_{j-1}}\right)}{\frac{1}{2}(\Delta_{j-1} + \Delta_j)}. \quad (4)$$

In this section, the cell-centered conductivities  $K_{j\pm\frac{1}{2}}$  in Eq. (4) are estimated by geometric means of conductivity values of adjacent cell boundaries,

$$K_{j-\frac{1}{2}} = \sqrt{K_{j-1}K_j}, \quad K_{j+\frac{1}{2}} = \sqrt{K_jK_{j+1}}. \quad (5)$$

Using the geometric mean and the Gardner model enables the description of the the interface problem between two different soil layers in terms on only two independent parameters. Other averaging methods for cell-centered hydraulic conductivities do not lead to such simplicity and are discussed in Section 3.

Assume the soil is partitioned into two layers with different soil hydraulic parameters superscripted by  $-$  (upper) and  $+$  (lower) as shown in Figure 1b. At node  $j$  and  $j+1$

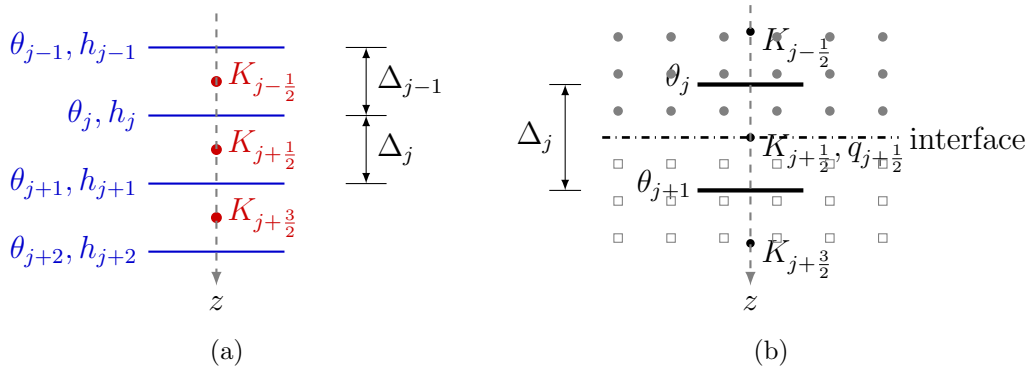


Figure 1: (a) Staggered finite difference scheme. (b) Interface between two distinct soil layers.

in Figure 1b, Eq. (4) no longer holds because it involves quantities across the interface. Also, the conductivity at the interface,  $K_{j+\frac{1}{2}}$ , cannot be estimated by averaging  $K_j$  and

$K_{j+1}$  since these quantities are associated with soils with different hydraulic properties. Instead, the continuity of flux  $q$  at the interface yields an equation

$$q_{j+\frac{1}{2}} := K_{j+\frac{1}{2}}^- \left( 1 - \frac{h_{j+1}^- - h_j}{\Delta} \right) = K_{j+\frac{1}{2}}^+ \left( 1 - \frac{h_{j+1} - h_j^+}{\Delta} \right), \quad (6)$$

where superscripts  $-$  and  $+$  refer to upstream (smaller  $z$ ) and downstream (larger  $z$ ) quantities, resp., and for simplicity we have assume a uniform mesh  $\Delta_{j-1} = \Delta_j = \Delta$ . Taking into account the continuity of pressure head  $h_j$  across the interface, ghost values  $h_{j+1}^-, h_j^+$  can be defined by linear extrapolation into extended layers (Romano et al., 1998),

$$\begin{aligned} h_{j+1}^- &= 2h_{j+\frac{1}{2}} - h_j &= h_{j+1} - \delta h, \\ h_j^+ &= 2h_{j+\frac{1}{2}} - h_{j+1} &= h_j - \delta h, \end{aligned} \quad (7)$$

with

$$\delta h := h_{j+1} + h_j - 2h_{j+\frac{1}{2}}.$$

Interface conductivities  $K_{j+\frac{1}{2}}^\pm$  can be similarly defined in the extended layer, using geometric means,

$$K_{j+\frac{1}{2}}^- = \sqrt{K_j K_{j+1}^-}, \quad K_{j+\frac{1}{2}}^+ = \sqrt{K_j^+ K_{j+1}} \quad (8)$$

with  $K_{j+1}^- = K^-(h_{j+1}^-)$ ,  $K_j^+ = K^+(h_j^+)$ . Substitution of Eq. (7) into (6) then yields

$$\delta h = (\Delta - (h_{j+1} - h_j)) \frac{1-r}{1+r} \quad (9)$$

with

$$r := \frac{K_j^-}{K_j^+} = \sqrt{\frac{K_{j-\frac{1}{2}} K^- (h_{j+\frac{1}{2}} - \delta h)}{K_{j+\frac{1}{2}} K^+ (h_{j-\frac{1}{2}} - \delta h)}} := g(r). \quad (10)$$

Eq. (10) with  $\delta h$  given by (9) represents a nonlinear equation in  $r$ , which must be solved iteratively, for example using a fixed-point (Picard) iteration

$$r_{n+1} = g(r_n), \quad r_0 \text{ given}, \quad (11)$$

or a Newton iteration

$$r_{n+1} = r_n - \frac{g(r_n) - r_n}{g'(r_n) - 1} := f(r_n), \quad r_0 \text{ given}. \quad (12)$$

With geometric averaging under the Gardner model Eq. (10) reduces to

$$r = g(r) = \lambda \exp \left( \mu \frac{1-r}{1+r} \right) \quad (13)$$

with

$$\lambda = \frac{\beta^-}{\beta^+} \exp \left( (\alpha^- - \alpha^+) \frac{h_{j+\frac{1}{2}} + h_{j-\frac{1}{2}}}{2} \right) > 0 \quad (14)$$

and

$$\mu = \frac{1}{2} (\alpha^+ - \alpha^-) \left( \Delta - (h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}}) \right). \quad (15)$$

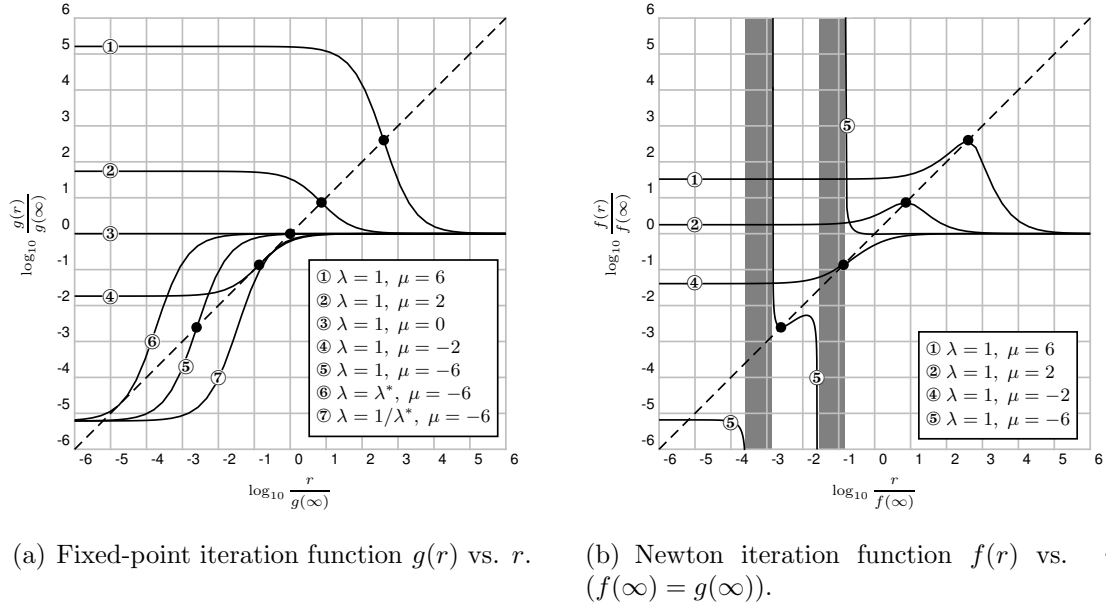


Figure 2: Fixed-point iteration and Newton iteration for interface problem under the Gardner model and the geometric mean for cell-centered hydraulic conductivities. For fixed  $\mu$ , changes in  $\lambda$  correspond to horizontal translations. For  $\mu < -2$  Eq. (13) has multiple roots for a range  $1/\lambda^* \leq \lambda \leq \lambda^*$  ( $\lambda \approx 13.6$  for  $\mu = -6$ ). When  $\lambda = 1$  the value  $r = 1$  is a root of (13) for any  $\mu$ , represented by a  $\bullet$ . For  $\mu \geq -2$  the Newton iteration converges globally, quadratically for  $\mu > -2$  but only linearly (with rate  $\frac{2}{3}$ ) for  $\mu = -2$  due to  $r = 1$  having multiplicity 3. For  $\mu < -2$  the iteration function  $f$  may become negative (shaded areas), leading to non-physical iterated values  $r_n$  and potentially creating problems in the convergence. In each case the root  $r = 1$  is represented by a  $\bullet$ .

In this case the interface problem Eq. (13) depends on two parameters  $\lambda$  and  $\mu$ , which depend on the jump in soil hydraulic properties accross the interface, as well as differences in pore water pressure accross the interface. For identical layers these values become  $\lambda = 1$ ,  $\mu = 0$ , regardless of pore water pressure levels.

Figure 2 shows the functions  $g(r)$  and  $f(r)$  in terms of  $r$  in scaled logarithmic axes, indicating that for certain choices of the parameters  $\lambda$  and  $\mu$ , multiple solutions of Eq. (13) exist. Figure 3 identifies the specific regions in  $(\lambda, \mu)$  parameter space where multiple (namely three) solutions of (13) exist. Note that a unique solution to the interface problem is guaranteed for small enough  $|\mu|$ , which can always be achieved by reducing the mesh size  $\Delta$ .

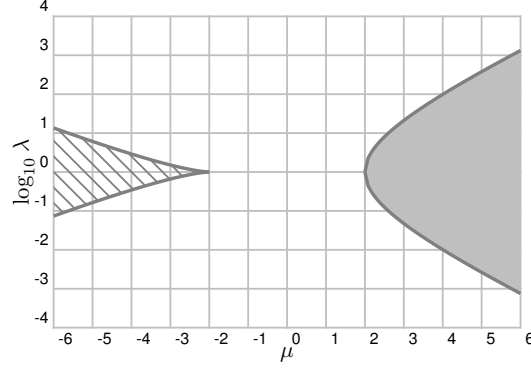


Figure 3: For  $|\mu| \leq 2$  the iteration (11) converges for any choice of  $r_0$  (locally). For  $\mu > 2$  (shaded region) the iteration (11) converges to a 2-cycle (oscillates between two distinct values), while the iteration (12) converges to the single root. For  $\mu < -2$  the iteration (11) or (12) converges to a solution of (13). When Eq. (13) has multiple roots (hatched region) the iteration (11) converges to a solution which may be non-physical.

### 3 Averaging methods for cell-centered hydraulic conductivities

Four commonly used averaging methods are investigated for the numerical solutions of water infiltration in one-dimensional unsaturated layered soils,

$$\text{harmonic mean: } K_{j+\frac{1}{2}}^{(h)} = \frac{2K_j K_{j+1}}{K_j + K_{j+1}}, \quad (16)$$

$$\text{geometric mean: } K_{j+\frac{1}{2}}^{(g)} = \sqrt{K_j K_{j+1}}, \quad (17)$$

$$\text{log mean: } K_{j+\frac{1}{2}}^{(l)} = \begin{cases} \frac{K_{j+1} - K_j}{\ln(K_{j+1}/K_j)} & \text{if } K_j \neq K_{j+1}, \\ K_j & \text{if } K_j = K_{j+1}, \end{cases} \quad (18)$$

$$\text{arithmetic mean: } K_{j+\frac{1}{2}}^{(a)} = \frac{1}{2}(K_j + K_{j+1}). \quad (19)$$

The arithmetic mean corresponds to “parallel flow” and may be more adapted to two or three-dimensional settings, favoring large values of hydraulic conductivities (path of least resistance). The harmonic mean is equivalent to “serial flow” in stacked up soil layers or cells, and may be more adapted to the one-dimensional setting, favoring small conductivity values (associated to bottlenecks in the water flow). The geometric mean is based on the arithmetic mean of pressure heads assuming a Gardner type constitutive relation, while the log mean is derived from the cell-average conductivity

$$K_{j+\frac{1}{2}} = \frac{1}{h_{j+1} - h_j} \int_{h_j}^{h_{j+1}} K(h) dh = \frac{1}{h_{j+1} - h_j} \int_{h_j}^{h_{j+1}} e^{\alpha h} dh = \frac{K_{j+1} - K_j}{\ln(K_{j+1}/K_j)}, \quad (20)$$

also making use of the Gardner relation. It can be easily verified that

$$K_{j+\frac{1}{2}}^{(h)} \leq K_{j+\frac{1}{2}}^{(g)} \leq K_{j+\frac{1}{2}}^{(l)} \leq K_{j+\frac{1}{2}}^{(a)}, \quad (21)$$

with equalities whenever  $K_j = K_{j+1}$ .

The analysis of the interface problem Eq. 13 in terms of two parameters  $\lambda$  and  $\mu$  conducted in Section 2 is only possible for the case of geometric averaging (and for the Gardner hydraulic model). In the next section we therefore investigate the occurrence of multiple roots of the interface problem numerically for other conductivity averaging schemes, and the impact on the simulation of infiltration flows.

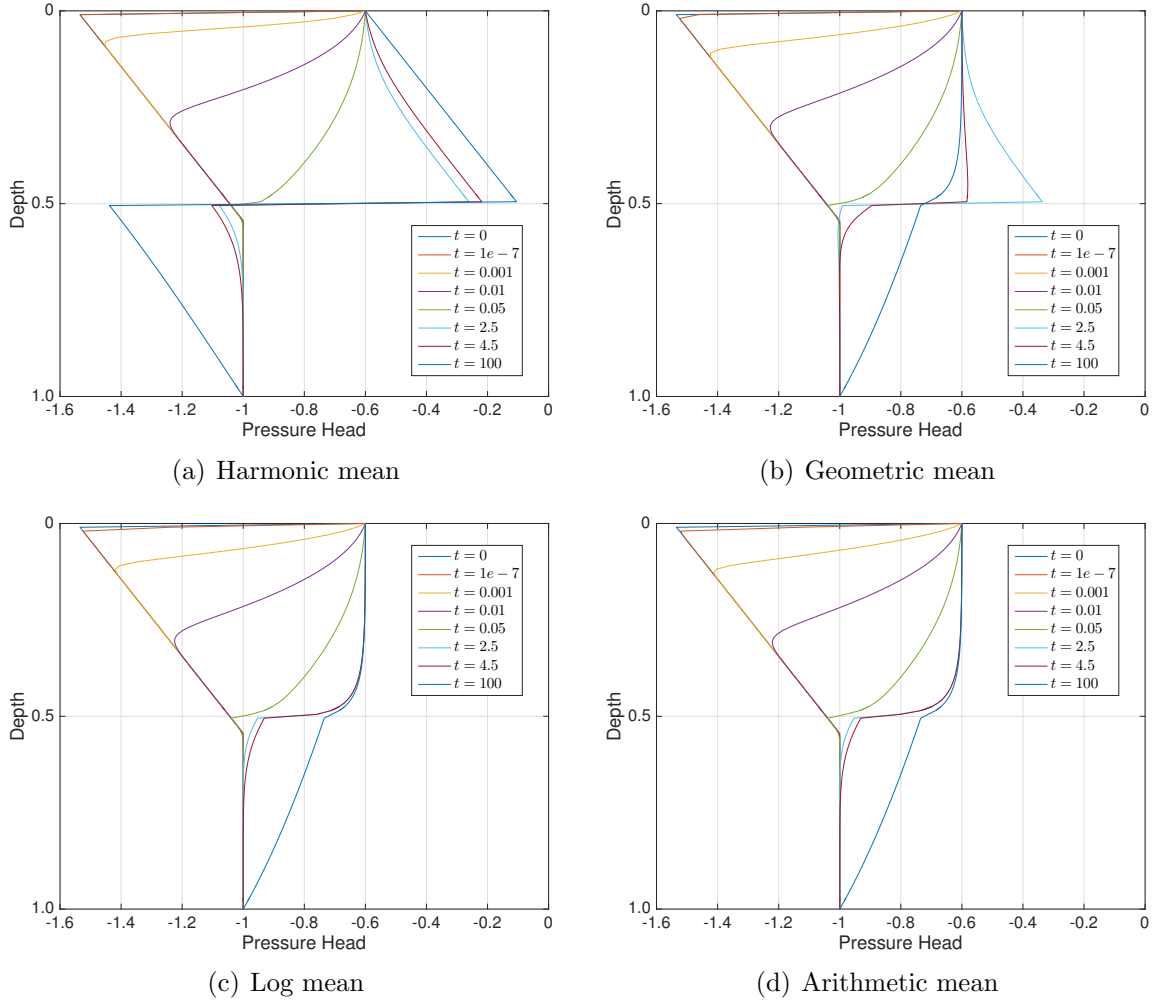


Figure 4: Numerical solutions of unsaturated flow in a two-layer soil using different averaging methods for cell-centered hydraulic conductivities.

#### 4 Numerical experiments

Numerical simulations of one-dimensional infiltration flow in a two-layer soil are used here to compare the different hydraulic conductivity averaging methods and their impact in the interface problem. The computational domain  $0 \leq z \leq 1$  is partitioned into two layers, with the interface located at a depth  $z = 0.5$ . The upper and lower layer are associated with soil hydraulic parameters  $\alpha^- = 13, \beta^- = 1$  and  $\alpha^+ = 1, \beta^+ = 0.0006$ , resp. The boundary conditions are fixed pressure head values,  $h_{\text{top}} = -0.6, h_{\text{bottom}} = -1$  (non-dimensionalized). The initial pressure head profile is assumed to be constant within the range  $0.55 \leq z \leq 1$  (lower layer) and linear within the range  $0 \leq z \leq 0.55$  (upper layer plus a small piece of the lower layer). This initial steady state can be interpreted as a forced drainage at the bottom of the soil. The soil is uniformly discretized into 100 spatial cells. The interface problem is solved via a fixed-point iteration using previous values of interface conductivities ratio  $r$  as initial guess.

Figure 4 shows the numerical simulations of unsaturated flows in a two-layer soil using the four hydraulic conductivities averaging methods described in Section 3 (used throughout the domain and not simply at the interface). The harmonic mean leads to a non-physical solution as soon as the water front reaches the interface, and the ponding

occurring at the interface persists later on because of underestimated interface conductivity. The root of the problem can be attributed to the existence of multiple solutions to the interface problem when variations of pore water pressure start increasing at the passage of the water front, a lower than physical root being selected in the numerical iteration. The simulation with the geometric mean temporarily exhibits a similar behavior, with the existence of multiple solutions, but the problem is only temporary as the pressure head profile seems to correctly adjust itself once operating conditions cease to lead to multiple solutions to the interface problem (after the water front had passed). Both log and arithmetic means lead in this example to an interface problem with a unique root at all times. The corresponding head profiles can be verified to be correct by using a finer spatial discretization.

## 5 Discussions and conclusions

Continuity of pressure head flux across the interface of soils is often neglected in numerical (including commercial) software. Our results highlight numerical difficulties in properly enforcing continuity of flux.

Several factors affect in particular the well-posedness of the resulting interface problem. In this study we show that the choice of averaging schemes for hydraulic conductivities in staggered formulations of Richards equations can substantially impact the solution on the downstream side of the interface. As expected, averaging schemes leading to larger conductivities, such as log-mean or arithmetic averaging, offer less numerical resistance and are less likely to trigger multiple solutions to the interface problem, yielding acceptable solutions in this illustration. Numerical experiments conducted on more sophisticated setups, which will be reported elsewhere, show that arithmetic averaging may however grossly overestimate appropriate physical ranges. The log-mean model seems to be appropriate, both physically and numerically, at least for one-dimensional simulations such as those conducted here.

The size of the spatial discretization around the interface between soil layers is certainly an important factor affecting the occurrence of multiple roots of the interface problem. In the case of geometric averaging with the Gardner hydraulic model, Eq. 15 shows that the parameter  $\mu$  can be made small enough by reducing the cell size  $\Delta$ , and, according to Fig. 3, eliminate the multiplicity of roots. In more complex examples with more realistic hydraulic models, such as the Mualem-van Genuchten model (Van Genuchten, 1980) or the Fredlund & Xing-Leong & Rahardjo model (Leong and Rahardjo, 1997), and in multilayered soils, mesh refinement has been shown to help reduce, but not always eliminate, temporary instabilities in pressure head profiles (Liu et al., 2016).

The multiplicity of roots of the interface problem at small (but finite) discretization sizes is ultimately related to the fact that Richards equation is not far from being ill-posed. Another instance of instabilities triggered by small perturbations (via third-order pore pressure derivatives) of the continuous Richards equation has for example been used to model the so-called viscous fingering effect.

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