Fully implicit, finite-differences resolution of variably saturated flow in 1D with Python.

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1 Soil hydraulic properties

In unsaturated conditions, water content θ can be expressed with the closed-form equation provided by *Van Genuchten* [1980] :

$$\theta(h) = \theta_r + (\theta_s - \theta_r)\left(1 + |\alpha h|^n\right)^{-m} \tag{1}$$

where θ_r, θ_s, α and n are soil characteristics and $m = 1 - 1/n$. h [L] is pressure head,counted as negative in unsaturated conditions. For any $h > 0$, $\theta(h) = \theta_s$.

The derivative of Eq. 1 with respect to h reads :

$$\frac{d\theta}{dh}(h) = mn\alpha^n h^{n-1}(\theta_s - \theta_r)\left(1 + |\alpha h|^n\right)^{-m-1} \tag{2}$$

Though apparently different, this expression is equivalent to Eq. 23 in *Van Genuchten* [1980]. The derivative was obtained with the condition $h < 0$.

Following *Van Genuchten* [1980], the relative permeability K_r is expressed as follows [*Van Genuchten*, 1980] :

$$K_r(h) = \frac{\left(1 - |\alpha h|^{n-1}(1 + |\alpha h|^n)^{-m}\right)^2}{(1 + |\alpha h|^{m/2})} \tag{3}$$

2 Model implementation

We consider the mixed-form equation for variably saturated flow proposed by *Celia et al.* [1990] and modified by *Clement et al.* [1994] :

$$S_s \frac{\theta}{\eta}\frac{\partial h}{\partial t} + \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(-K(\theta)\frac{\partial H}{\partial z}\right) + q \tag{4}$$

where S_s [L^{-1}] is the specific storage, H [L] is the hydraulic head, θ [-] is the water content, η [-] is the porosity, K [LT^{-1}] is the hydraulic conductivity and q [T^{-1}] the source term. Contrary to the original Richards' equation, Eq. 4 accounts for the effect of specific storage, which makes it valid for transient saturated flow.

The hydraulic head is defined by $H = h + z$, where h is the pressure head and z the coordinate along the (Oz) vertical upward axis. Eq. 4 yields :

$$S_s \frac{\theta}{\eta}\frac{\partial h}{\partial t} + \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K \frac{\partial h}{\partial z}\right) + \frac{\partial K}{\partial z} \tag{5}$$

Spatial derivation is obtained with a central differences scheme as follows :

$$\begin{aligned}\frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z}\right) + \frac{\partial K}{\partial z} \approx \frac{1}{dz}\Bigg\{&\left(\frac{K_i^{n+1,m} + K_{i+1}^{n+1,m}}{2}\right)\left(\frac{h_{i+1}^{n+1,m+1} - h_i^{n+1,m+1}}{dz}\right)\\ &- \left(\frac{K_i^{n+1,m} + K_{i-1}^{n+1,m}}{2}\right)\left(\frac{h_i^{n+1,m+1} - h_{i-1}^{n+1,m+1}}{dz}\right)\Bigg\}\\ &+ \frac{1}{dz}\left(\left(\frac{K_i^{n+1,m} - K_{i+1}^{n+1,m}}{2}\right) - \left(\frac{K_i^{n+1,m} + K_{i-1}^{n+1,m}}{2}\right)\right)\end{aligned} \tag{6}$$

where n denotes the nth discrete time level, when the solution is known, dt is the time step, K_i is the value of hydraulic conductivity at the ith node and h_i the value of pressure head at the ith node. The current and previous Picard iteration are denoted as $m + 1$ and m, respectively.

A backward finite-difference expression is used for temporal derivative :

$$S_s \frac{\theta}{\eta}\frac{\partial h}{\partial t} \approx \frac{S_s}{\eta}\theta_i^{n+1,m}\left(\frac{h_i^{n+1,m+1} - h_i^n}{dt}\right) \tag{7}$$

After *Celia et al.* [1990] and *Clement et al.* [1994], time derivative of water content is approximated as follows :

$$\frac{\partial \theta}{\partial t} \approx \left(\frac{\theta_i^{n+1,m} - \theta_i^n}{dt}\right) + C_i^{n+1,m}\left(\frac{h_i^{n+1,m+1} - h_i^{n+1,m}}{dt}\right) \tag{8}$$

where C is the derivative of the water content with respect to the pressure head (Eq. 2)

Eqs. 6, 7 and 8 can be re-arranged to form a system of linear algebraic equations :

$$m_1 h_{i-1}^{n+1,m+1} + m_2 h_i^{n+1,m+1} + m_3 h_{i+1}^{n+1,m+1} = -b_1 h_i^{n+1,m} - b_2 h_i^n + b_3 + b_4 \quad (9)$$

with :

$$m_1 = \left(\frac{K_i^{n+1,m} + K_{i-1}^{n+1,m}}{2dz^2} \right) \quad (10)$$

$$m_3 = \left(\frac{K_i^{n+1,m} + K_{i+1}^{n+1,m}}{2dz^2} \right) \quad (11)$$

$$b_1 = \frac{C_i^{n+1,m}}{dt} \quad (12)$$

$$b_2 = \frac{S_s \theta_i^{n+1,m}}{\eta dt} \quad (13)$$

$$b_3 = -\left(\frac{K_{i-1}^{n+1,m} - K_{i+1}^{n+1,m}}{2dz} \right) \quad (14)$$

$$b_4 = \left(\frac{\theta_i^{n+1,m} - \theta^n}{dt} \right) \quad (15)$$

$$m_2 = -(m_1 + m_3 + b_1 + b_2) \quad (16)$$

The following system should then be solved iteratively :

$$\mathbf{M}^{n+1,m} \mathbf{h}^{n+1,m+1} = \mathbf{B}^{n+1,m} \quad (17)$$

where $\mathbf{M}$ is a sparse matrix containing in its central diagonals the coefficients m_1,m_2,m_3 and vector $\mathbf{B}$ gather the second member of Eq. 9.

The resolution of the system is obtained with the Python `scipy.sparse.spsolve` or `scipy.sparse.cg` function, or `numpy.linalg.solve`. This remains an issue. . .

3 Boundary conditions

We consider a soil column subject to infiltration at the top. The boundary condition at the bottom is either a fixed-head or free drainage.

3.1 Fixed pressure head

For a fixed pressure head boundary condition at the **bottom** of the column, the boundary condition is expressed as follows :

$$h_1^{n+1,m} = h_{bot}^{n+1} \tag{18}$$

where h_{bot} is the value of the imposed pressure head at $t = t_{n+1}$. On the left side of Eq. 9, we have $m_1 = m_3 = 0$ and m_2=1. The right side of Eq. 9 is h_{bot}^{n+1}.

Similarly, for a fixed pressure head boundary condition at the **top** of the column, the boundary condition is expressed as follows :

$$h_I^{n+1,m} = h_{top}^{n+1} \tag{19}$$

where h_{top} is the value of the imposed pressure head at $t = t_{n+1}$. On the left side of Eq. 9, we have $m_1 = m_3 = 0$ and m_2=1. The right side of Eq. 9 is h_{top}^{n+1}.

3.2 Fixed flow

With a flux q_z [LT^{-1}] imposed to one of the boundaries of the soil column, Darcy law yields :

$$\begin{aligned} q_z = -K\frac{\partial H}{\partial z} &\iff q_z = -K\left(\frac{\partial h}{\partial z} + 1\right) \\ &\iff \frac{\partial h}{\partial z} = -\frac{q_z}{K} - 1 \end{aligned} \tag{20}$$

If the flux q_{top} is imposed to the **bottom** of the column, Eq. 20 yields :

$$h_0 = h_1 + \frac{q_{bot}}{K_1} + 1 \tag{21}$$

where h_0 is pressure head at a virtual node out of the system. Inserting Eq. 21 into Eq. 9 yields :

$$(m_1+m_2)h_1^{n+1,m+1}+m_3h_2^{n+1,m+1} = -b_1h_1^{n+1,m}-b_2h_1^n+b_3+b_4+m_3dz\left(\frac{q_{bot}}{K_1}+1\right) \tag{22}$$

In turn, if the flux q_{top} is imposed to the **top** of the column, Eq. 20 yields :

$$h_{I+1} = h_I - \frac{q_{top}}{K_I} - 1 \tag{23}$$

where I is the total number of nodes and h_{I+1} is a virtual node out of the system. Inserting Eq. 23 into Eq. 9 yields :

$$m_1h_{I-1}^{n+1,m+1}+(m_2+m_3)h_I^{n+1,m+1} = -b_1h_I^{n+1,m}-b_2h_I^n+b_3+b_4+m_3dz\left(\frac{q_{top}}{K_I}+1\right) \tag{24}$$

Note that infiltration into the soil column is simulated with a negative q_{top}.

No flow boundary condition is a special case of the fixed flow boundary condition with $q_z = 0$.

3.3 Free drainage at the bottom of the column

Free drainage is expressed with a unit vertical hydraulic head gradient :

$$\begin{aligned} \frac{\partial H}{\partial z} = 1 &\iff \frac{\partial}{\partial z}(z+h) = 1 \\ &\iff \frac{\partial h}{\partial z} = 0 \\ &\iff \frac{(h_1 - h_0)}{dz} = 0 \\ &\iff h_0 = h_1 \end{aligned} \tag{25}$$

Where h_0 is pressure head at a virtual node out of the system. In these conditions, Eq. 9 becomes :

$$(m_1 + m_2)h_1^{n+1,m+1} + m_3 h_2^{n+1,m+1} = -b_1 h_1^{n+1,m} - b_2 h_1^n + b_3 + b_4 \tag{26}$$

4 Runoff estimation

When the rainfall rate exceeds the soil infiltration capacity, a pounding condition occurs at the top of a plane terrain. In time, the pounded water will infiltrate to the soil. Contrary, on sloping terrains the pounding condition is negligable while water is loss as runoff. Following *Herrada et al.* [2014], the pounding condition is reached when the upper soil surface saturates. A transient *fixed flow* is prescribed at the upper boundary [*Herrada et al.*, 2014] :

$$In_n \equiv q(I,n) \equiv q_{rainfall} \equiv q_{top} \tag{27}$$

where Inf_n is the infiltration rate. According to *Herrada et al.* [2014], this condition applies when $\theta(I,n) < \theta_s$, if $\theta(I,n)$ reaches saturation, the boundary condition in Eq. 28 is replaced by $\theta(I,n) = \theta_s$. In our case, as we use the mixed form of the Richard's equation, our boundary conditions are different and the system resolution complex. Following the approach of *Herrada et al.* [2014], we use the saturation condition from the pressure head h to modify the upper boundary condition. When $h_I^{n+1} < 0$, the upper boundary condition is the Eq. 24. In the case where $h_I^{n+1} \geq 0$, the fixed flux upper boundary condition switches to a fixed head condition (Eq. 19), where $h_{top}^{n+1} = 0$. On this scenario, the linear system is resolved again with the new conditions to obtain h^{n+1}. If we solve the Eq. 24 for q_{top} using $h_I^{n+1,m} = h_I^{n+1,m+1} = 0$ (a valid assumption after h_I^{n+1} is already known), Eq. 24 yields :

$$In = q_{top} = K\left[\frac{\left(m_1 h_{I-1}^{n+1} + b_2 h_{I-1}^{n} - b_3 - b_4\right)}{(m_3 dz)} - 1\right] \tag{28}$$

where h_{I-1} is obtained from the solution of the linear system with the new conditions. Finally, surface runoff is calculated as [*Herrada et al.*, 2014] :

$$q_{runoff} = q_{rainfall} - In \tag{29}$$

5 Root water uptake and actual transpiration

Root water uptake from the soil is used by the plants for transpiration purposes. Total potential transpiration is calculated independently and it is redistributed over the soil profile as follows :

$$S_p = b(z)T_p \tag{30}$$

where S_p [T^{-1}] is the potential water uptake rate in a soil unit, T_p [LT^{-1}] is the total potential transpiration rate and $b(z)$ is the normalized water uptake distribution [L^{-1}]. We considered two types of the $b(z)$ functions :

– Equally distributed over the root zone :

$$b(z) = \frac{1}{L_R} \tag{31}$$

– Using the function proposed by *Hoffman and Van Genuchten* [1983] similar to a trapezoid :

$$b(z) = \begin{cases} \frac{1.667}{L_R} & x \geq L - 0.2L_R \\ \frac{2.0833}{L_R}(1 - \frac{L-z}{L_R}) & L - L_R < z < L - 0.2L_R \\ 0 & x \leq L - L_R \end{cases} \tag{32}$$

where L is the soil depth and L_R is the root zone depth which is assummed constant. The water uptake rate is related to the available water in the soil unit. When not enough water is available, the potential rate cannot be achieved. The actual water uptake is defined by *Feddes et al.* [1978] as follows :

$$S = \alpha(h)S_p \tag{33}$$

where S [T^{-1}] (known in Eq. 4 as q) is the actual water uptake and $\alpha(h)$ is a dimensionless stress response function. We used this function related to the water content instead of the pressure head and followed the approach proposed by *Food and Agriculture Organization of the United Nations* [1998] modified to soil units :

$$\alpha(\theta) = \begin{cases} 1 & \theta \geq \theta_{RWC} \\ \frac{\theta - \theta_{WP}}{\theta_{RAW}} & \theta_{WP} < \theta < \theta_{RWC} \\ 0 & \theta \leq \theta_{WP} \end{cases} \tag{34}$$

where θ_{wp} is the water content of the soil unit at the *wilting point* and θ_{RWC} is the readily extracted water content of the soil unit by the roots, obtained with the equation :

$$\theta_{RWC} = \rho(\theta_{FC} - \theta_{WP}) \tag{35}$$

where θ_{FC} is the water content of the soil unit at the *field capacity*, and ρ is the average fraction of the available extracted water content of the soil unit that can be deplected before moisture stress, and its usually 0.5 for many crops. Finally the actual transpiration rate T_p [LT^{-1}] is calculated with the following equation :

$$T_p = \sum_{i=1}^{I} \alpha(\theta)b(z)T_p \tag{36}$$

Note that T_p in Eq. 36 do not consider the effect of osmotic stress by the soil salinity nor the compensation by the root adaptability to increase the uptake from other parts when moisture stress occurs.

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