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 somewhat difficult to obtain with the $|h|$.

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 :

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

Références

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