SawSim

In this study, I introduce a new groundwater scheme to Noah-MP; Sawsan's Simulation (SawSim, Figure 20), which consists of two fixed thickness layers (unconfined and confined) separated by a confining unit that does not store water. SawSim simulates the groundwater dynamics in a three-dimensional system, the interaction between groundwater and surface water, the interaction between soil layers and the unconfined aquifer, and the effect of pumping on groundwater dynamics. Groundwater fluxes are simulated vertically and laterally based on Darcy's law in both the unconfined and confined aquifer layers.

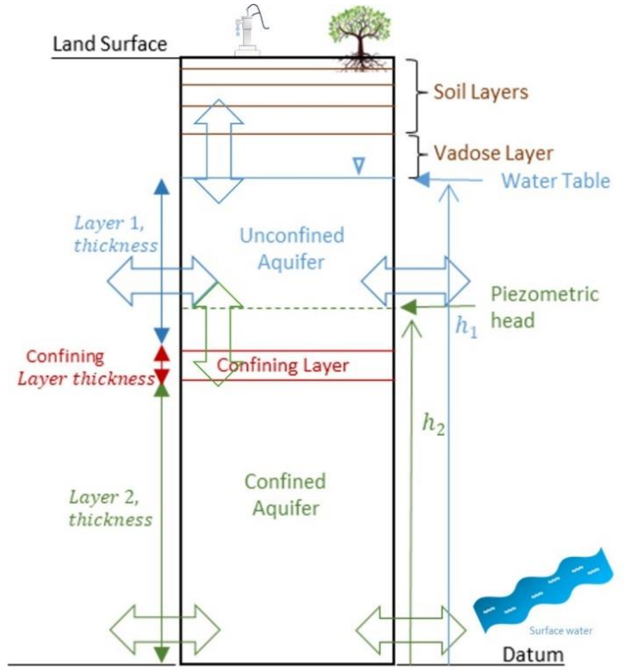

Figure 20: Schematic of the new groundwater option; the existing Noah MP's soil and vadose layers (in brown). The blue represents the unconfined layer and its interactions, while the green represents the confined aquifer and its interaction. The confining layer is shown in red.

Detailed Approach

The governing equation of groundwater dynamics is the combination of the groundwater balance equation and Darcy's law, where equations (2 and 3) show the governing equation of groundwater flow in non-equilibrium condition, the heterogenous and anisotropic medium

$$\frac{\partial}{\partial x}(q_x) + \frac{\partial}{\partial y}(q_y) + \frac{\partial}{\partial z}(q_z) + W = S_S \frac{\partial h}{\partial t} \qquad \text{Equation 2}$$

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right) + W = S_S \frac{\partial h}{\partial t} \qquad \text{Equation 3}$$

Where h is piezometric head (L), x,y and z are coordinate directions, t is time (T), K is hydraulic conductivity (L/T), W is external source/sink, Ss is Specific Storage (1/L), $\partial h/\partial t$ is the change in head over time (L/T), and $Ss\ \ \partial h/\partial t$ is the volume of water taken into storage per unit volume of aquifer per unit change in head over a time interval.

The inter-cell flows are based on Dary's Law; for example, equation (4) shows the flow equation in the x-direction through a block of aquifer extending from node $i, j-1, k$ to node i, j, k

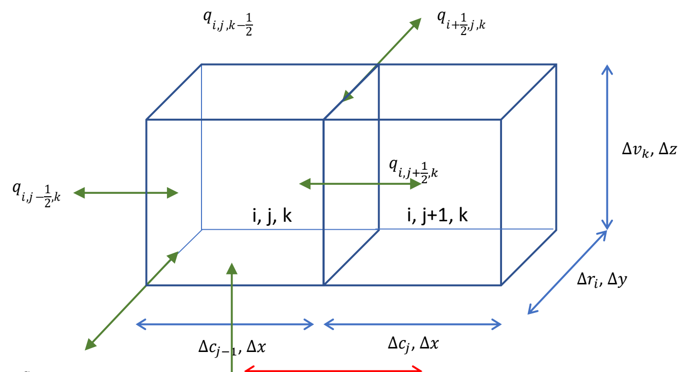

Figure 21: The flow between i,j,k cell and its surroundings

$$q_{i,j-\frac{1}{2},k} = K_{x,i,j-\frac{1}{2},k} \Delta c_i \Delta v_k \left(\frac{h_{i,j-1,k} - h_{i,j,k}}{\Delta r_{j-\frac{1}{2}}} \right) \qquad \text{Equation 4}$$

where $q_{i,j-\frac{1}{2},k}$ is the flow rate across the cell interface; $K_{x,i,j-\frac{1}{2},k}$ is effective hydraulic conductivity at the cell interface calculated as a harmonic mean;Δc_i is the cell dimension in the x-direction (width), Δv_k is the cell dimension in the z-direction (thickness of the layer), $h_{i,j-1,k}, h_{i,j,k}$ is the hydraulic heads in the neighboring cell and the active cell; $\Delta r_{j-\frac{1}{2}}$ is the distance between cell centers in the flow direction.

As per MODFLOW principles, I used conductance to describe the ease with which water can flow between cells or between cells and an external source such as a river. Conductance (C) is the product of hydraulic conductivity, and the area of the interface is divided by the length of the flow path. So that equation (4) will become equation (5)

$$q_{i,j-\frac{1}{2},k} = C_{R,i,j-\frac{1}{2},k}\left(h_{i,j-1,k} - h_{i,j,k}\right) \qquad \text{Equation 5}$$

External processes

External processes (n) to the aquifer include flow to and from rivers, recharge, and wells. These flows may be dependent on the head in the receiving cell but independent of all other heads in the aquifer, according to Equation (6),

$$\sum_{n=1}^{N} q_{i,j,k,n} = \sum_{n=1}^{N} p_{i,j,k,n} h_{i,j,k} + \sum_{n=1}^{N} b_{i,j,k,n} \qquad \text{Equation 6}$$

where $q_{i,j,k,n}$ is the flow from an nth external source into cell i, j, k (L^3/T), $p_{i,j,k,n}$ is constant (L^2/T), $and\ b_{i,j,k,n}$ is constant (L^3/T)

There are two cases to consider for external processes affecting the aquifer: when n=1, representing discharge from a well (pumping), when n=2, representing recharge from upper soil layers, and when n=3, representing groundwater – river exchange

1. n =1; a cell receives discharge from a well (Pumping). The flow is assumed to be independent of the head. $b_{i,j,k,1}$: pumping rate for the well, then $q_{i,j,k,1} = b_{i,j,k,1}$, the cell is releasing water through the well (out of the cell, the sign is negative)
2. n=2, A cell is receiving recharge from upper soil layers, using the same approach as recharge in MMF (Fan et al., 2007; Miguez-Macho et al., 2007; Zhang et al., 2020). The flow will be independent of the head (constant) and depend on the water table (WT) level. WT can be within soil layers (4 layers with total depth =2 m) (RECH in existing Noah MP scripts), or WT is below the soil layers; if it is below soil layers, an auxiliary soil layer (Vadose Zone in Figure (1)) will be added to the scheme and varies in space and time. The reason for adding this layer is to get more accurately calculated fluxes between the four soil layers and the aquifer(Zhang et al., 2020). The auxiliary layer depth (Z_{aux}) can be calculated by

$$Z_{aux} = \begin{cases} 1, & WTD \leq 3 \\ WTD - 2, & WTD > 3 \end{cases} \qquad \text{Equation 7}$$

The recharge ($q_{i,j,k,2}$) equation (8) is the flow from/to the layer above the WTD and can be measured based on Richard's equation as in MMF, (Zhang et al., 2020)

$$q_{i,j,k,2} = \begin{cases} K_k \left[\frac{(\psi_i - \psi_k)}{Z_i - Z_k}\right] - 1, & WTD \leq 2; \boldsymbol{in\ Noah\ MP \gg RECH} \\ K_{aux} \left[\frac{(\psi_i - \psi_{aux})}{3 - 2}\right] - 1, & 3 \geq WTD > 2; \boldsymbol{I\ didn't find\ it\ is\ Noah\ MP\ scripts} \\ K_{sat} \left[\frac{(\psi_{aux} - \psi_{sat})}{WTD - 2}\right] - 1, & WTD > 3; \boldsymbol{In\ Noah\ MP \gg DEEPRECH} \end{cases} \qquad \text{Equation 8}$$

Where q is water flux between two adjacent layers (m/s), Kk is the hydraulic conductivity (m/s) at a particular soil layer that contains WTD while i is the layer above, ψ is the soil matric potential (m). The subscript "sat" denotes saturation, while aux is for the auxiliary layer

3. n= 3; A cell is receiving water from the river, representing river-aquifer interaction

$$q_{i,j,k,3} = p_{i,j,k,3} h_{i,j,k} + b_{i,j,k,3} \qquad \text{Equation 9}$$

Where $p_{i,j,k,3} = -C_{River,i,j,k}$; $b_{i,j,k,3} = C_{river,i,j,k}\, h_{river}$; and $C_{river,i,j,k}$ represents river-aquifer interconnection (river conductance). It is a product of vertical hydraulic conductivity of the riverbed material and the area of the riverbed as it crosses the cell, divided by riverbed material thickness.

With all external sources, the governing equation (2, or 3), can be written as equation 10 and in more the detailed parameterization as in equation 11.

$$q_{i,j-\frac{1}{2},k} + q_{i,j+\frac{1}{2},k} + q_{i-\frac{1}{2},j,k} + q_{i+\frac{1}{2},j,k} + P_{i,j,k}h_{i,j,k} + B_{i,j,k} = Ss_{i,j,k}\Delta r_j \Delta c_i \Delta v_k \frac{\Delta h_{i,j,k}}{\Delta t} \quad \text{Equation 10}$$

$$\begin{aligned} C_{R,i,j-\frac{1}{2},k}\left(h^m_{i,j-1,k} - h^m_{i,j,k}\right) &+ C_{R,i,j+\frac{1}{2},k}\left(h^m_{i,j+1,k} - h^m_{i,j,k}\right) \\ &+ C_{C,i-\frac{1}{2},j,k}\left(h^m_{i-1,j,k} - h^m_{i,j,k}\right) + C_{C,i+\frac{1}{2},j,k}\left(h^m_{i+1,j,k} - h^m_{i,j,k}\right) \\ &+ C_{V,i,j,k-\frac{1}{2}}\left(h^m_{i,j,k-1} - h^m_{i,j,k}\right) + C_{V,i,j,k+\frac{1}{2}}\left(h^m_{i,j,k+1} - h^m_{i,j,k}\right) \\ &+ P_{i,j,k}h^m_{i,j,k} + B_{i,j,k} = Ss_{i,j,k}\Delta r_j \Delta c_i \Delta v_k \frac{h^m_{i,j,k} - h^{m-1}_{i,j,k}}{t^m - t^{m-1}} \end{aligned} \quad \text{Equation 11}$$

where h is piezometric head (L), i, j and k are coordinate directions, t is time (T), C is conductance (L^2/T), Ss is Specific Storage (1/L),m is the current step,;Δc_i is the cell dimension in the x-direction (width), Δv_k is the cell dimension in the z-direction (thickness of the layer), $h_{i,j-1,k}, h_{i,j,k}$ i; Δr_j is the distance between cell centers in the flow direction; $P_{i,j,k} = \sum_{n=1}^{N} p_{i,j,k,n}$; $B_{i,j,k} = \sum_{n=1}^{N} b_{i,j,k,n}$; and $\frac{\Delta h_{i,j,k}}{\Delta t} = \frac{h^m_{i,j,k} - h^{m-1}_{i,j,k}}{t^m - t^{m-1}}$

In equation (11) all seven head terms are unknowns at time m, all coefficients are knowns, $B_{i,j,k}$ is known, and $h^{m-1}_{i,j,k}$ is known, this equation cannot be solved directly because it represents a single equation with seven unknowns. It needs to be written as a system of equations as equation (12) that can be solved numerically,

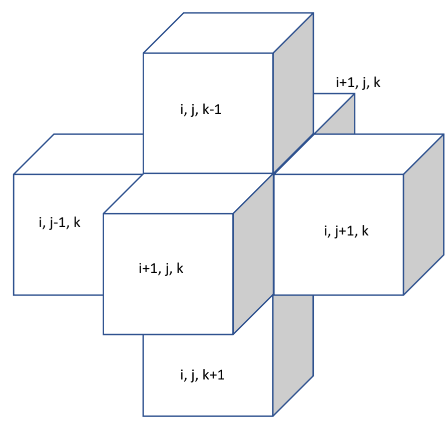

Figure 22:Discretized system using finite difference; Cell i,j,k and its surrounding 6 cells

$$\begin{aligned} &\overbrace{C_{C,i-\frac{1}{2},j,k}}^{B} h^m_{i-1,j,k} + \overbrace{C_{R,i,j-\frac{1}{2},k}}^{D} h^m_{i,j-1,k} + \overbrace{C_{V,i,j,k-\frac{1}{2}}}^{Z} h^m_{i,j,k-1} \\ &+ \Big(\overbrace{-C_{C,i-\frac{1}{2},j,k} - C_{C,i+\frac{1}{2},j,k} - C_{R,i,j-\frac{1}{2},k} - C_{R,i,j+\frac{1}{2},k} - C_{V,i,j,k-\frac{1}{2}} - C_{V,i,j,k+\frac{1}{2}} + G_{i,j,k}}^{E}\Big) h^m_{i,j,k} \\ &+ \underbrace{C_{C,i+\frac{1}{2},j,k}}_{H} h^m_{i+1,j,k} + \underbrace{C_{R,i,j+\frac{1}{2},k}}_{F} h^m_{i,j+1,k} + \underbrace{C_{V,i,j,k+\frac{1}{2}}}_{S} h^m_{i,j,k+1} \\ &= -B_{i,j,k} - Ss_{i,j,k}\Delta r_j \Delta c_i \Delta v_k \frac{h^{m-1}_{i,j,k}}{t^m - t^{m-1}} \end{aligned} \quad \text{Equation 12}$$

where $G_{i,j,k} = P_{i,j,k} - \frac{Ss_{i,j,k}\Delta r_j \Delta c_i \Delta v_k}{t^m - t^{m-1}}$, and $-B_{i,j,k} - Ss_{i,j,k}\Delta r_j \Delta c_i \Delta v_k \frac{h_{i,j,k}^{m-1}}{t^m - t^{m-1}}$ is the right side of the equation (RHS).

Give a name to each coefficient of the head $[A]\vec{h} = RHS$, as shown in Equation 12, the matrix can be illustrated in Figure (23), where $[A]$ is a square matrix and has the coefficients of h, $[A]$ is symmetric which means B=H, D= F , and Z=S

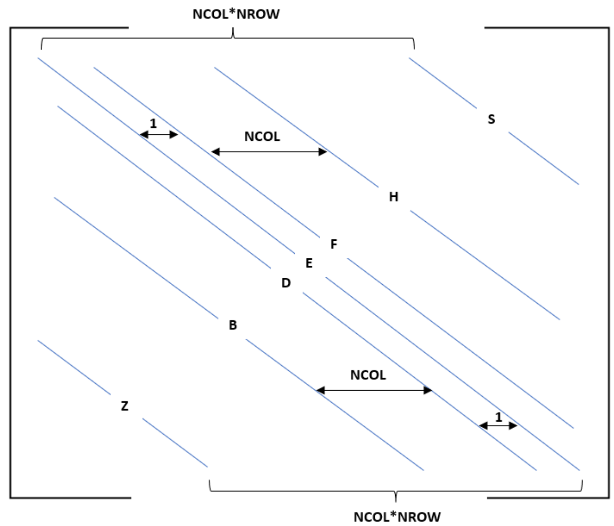

Figure 23: The coefficient matrix of the groundwater system of equations

Numerical solver

SawSim is written in the Fortran programming language and adopts MODFLOW principles to solve the groundwater flow equation (number) numerically. It uses a finite difference method with the generalized minimal residual (GMRES) solver (Saad, 1986) using the Portable, Extensible Toolkit for Scientific Computation (PETSc; Balay et al., 1998). PETSc has a large suite of scalable parallel linear and nonlinear equation solvers, ODE integrators, and optimization algorithms for application codes written in C, C++, Fortran, and Python.

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