Notes on Spatial and Temporal Discretization
(when working with HYDRUS)
by
Jirka Simunek

1. Temporal Discretization

Four different time discretizations are used in HYDRUS: (1) time discretizations associated with the numerical solution, (2) time discretizations associated with the implementation of boundary conditions, (3) time discretizations which provide printed output of the simulation results (e.g., nodal values of dependent variables, water, solute mass balance components, and other information about the flow regime), and (4) time discretizations associated with data defining the objective function in the inverse mode of HYDRUS (e.g., measured water contents, pressure heads, concentrations, and/or fluxes).

Discretizations 2, 3, and 4 are mutually independent; they generally involve variable time steps as described in the input data file. Discretization 1 starts with a prescribed initial time increment, Δt_{init}. The time increment, Δt, is automatically adjusted at each time level according to the following rules:

a. Discretization 1 must coincide with time values resulting from time discretizations 2, 3, and 4.
b. Time increments cannot become less than a preselected minimum time step, Δt_{min}, nor exceed a maximum time step, Δt_{max} (i.e., $\Delta t_{min} \leq \Delta t \leq \Delta t_{max}$).
c. If, during a particular time step, the number of iterations necessary to reach convergence is ≤3 (It_{min}), the time increment for the next time step is increased by multiplying Δt by a predetermined constant >1 (k_1, usually between 1.1 and 1.5). If the number of iterations is ≥7 (It_{max}), Δt for the next time level is multiplied by a constant <1 (k_2, usually between 0.3 and 0.9).
d. If, during a particular time step, the number of iterations at any time level becomes greater than a prescribed maximum (It_{crit}, usually between 10 and 50), the iterative process for that time level is terminated. The time step is subsequently reset to $\Delta t/3$, and the iterative process restarted.

Parameters Δt_{init}, Δt_{min}, Δt_{max}, It_{crit}, It_{min}, It_{max}, k_1, and k_2 are be specified by a user at the input. The recommended values for these parameters are as follows:

Parameter	Recommended Value	Comment
Δt_{init}	1 s (15 minutes)	The recommended value for the initial time step depends on the type of simulation and boundary conditions used. When simulating a process that starts with a large initial pressure head or concentration gradient at the boundary (e.g., ponded infiltration or a sudden change of boundary concentration), use a small value of the initial time step (e.g., 1 s). When simulating a long term process with variable boundary conditions (e.g., seasonal or multiyear simulation), start with a larger time step (e.g., 15 min). This is because this initial time step is used whenever time variable boundary conditions significantly change. If needed (if there is no convergence for Δt_{init}), the program will still use a smaller time step than Δt_{init}, but starting with larger Δt_{init} leads to more efficient calculations. In general smaller initial time steps must be used for soil with more nonlinear soil hydraulic properties (e.g., course textured soils) and larger initial time steps can be used for soil with less nonlinear soil hydraulic properties (e.g., loam)
Δt_{min}	1 s	Always specify a small minimum allowed time step, on the order of 1 s. This value may never be used, but it provides the code with flexibility when it may be needed, e.g., when there is a sudden change in boundary fluxes and HYDRUS may not converge with larger time steps.
Δt_{max}	Large	This is relatively unimportant parameter and a large value may be specified. Since HYDRUS automatically selects its optimal time step, there is usually no need to constraint that. The only time when there is a need to constrain the time step is likely for cases when HYDRUS is asked to generate internally intra-daily variations in temperature, or in evaporation and transpiration fluxes. Then there is a need to have time step smaller (e.g., 1 h) so that these daily variations can be properly modeled.
It_{crit}	10	It is usually not helpful to use a larger value than 10. If HYDRUS does not converge in 10 iterations, then there is a relatively small probability that it will do so during more iteration. Even if it does, it is much more efficient to reduce the time step and attempt to find the solution with a smaller time step, which is done automatically by the program when It_{crit} is reached.
It_{mi}	3	Optimal value in most cases.
It_{max}	7	Optimal value in most cases.
k_1	1.3	Optimal value in most cases. Only when there is a saturated zone in the profile, e.g., a perched water layer, the numerical solution may be more stable with smaller k_1 (e.g., 1.1).
k_2	0.7	Optimal value in most cases.

2. Spatial Discretization

2.1. HYDRUS-1D

The finite element mesh is constructed by dividing the soil profile into linear elements whose sizes are defined by the *z*-coordinates of the nodes that form the element corners.

2.2. HYDRUS (2D/3D)

The finite element mesh is constructed by dividing the flow region for two-dimensional problems into quadrilateral and/or triangular elements or for three-dimensional problems into tetrahedral, hexahedral and/or triangular prismatic elements whose shapes are defined by the coordinates of the nodes that form the element corners. The program automatically subdivides the quadrilaterals into triangles (or hexahedrals and triangular prisms into tetrahedrals), which are then treated as subelements.

2.3. Common Rules

Finite element dimensions must be adjusted to a particular problem. They should be made relatively small at locations where large hydraulic gradients are expected. Such a region is usually located close to the soil surface where highly variable meteorological factors can cause rapid changes in the soil water content and corresponding pressure heads. Similarly, regions with sharp gradients can be located in the vicinity of the internal sources or sinks. Hence, we recommend normally using relatively small elements at and near the soil surface. The size of elements can gradually increase with depth to reflect the generally much slower changes in pressure heads at deeper depths. We also recommend using elements having approximately equal sizes to decrease numerical errors. The ratio of the sizes of two neighboring elements is not recommended to exceed about 1.5.

The required size of finite elements close to the soil surface depends very much on how boundary conditions are specified. When boundary conditions are specified for daily, or shorter, time intervals, usually resulting in short-duration fluxes of a large magnitude, spatial discretization needs to be finer (on the order of cm) than when boundary conditions are specified for longer time intervals (e.g., weekly or monthly).

The element dimensions should also depend upon the soil hydraulic properties. For example, coarse-textured soils having relatively high n- and α-values generally require a finer discretization than fine-textured soils. That is because their soil hydraulic functions are more nonlinear and thus the numerical solution may be less stable. To demonstrate this issue, we have carried out simulations of ponded infiltrations into sand and clay soil profiles (see figures below). Notice that the pressure head front for a sandy profile is very sharp and the entire front is only about 5 cm thick. To be able to describe this front using our numerical model, we need several FE nodes at the front, implying that our spatial discretization must be on the order of 1 cm or less. On the other hand, the pressure head (and correspondingly water content) front for a clay profile is relatively smooth and consequently our spatial discretization can be much coarser.

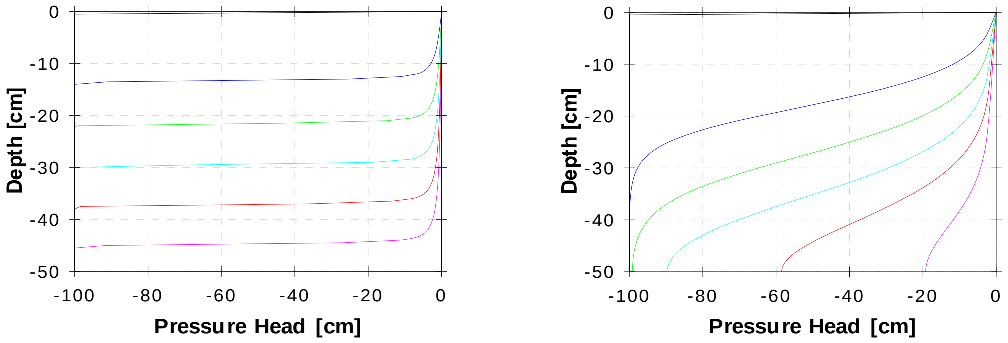

Figure 1. Pressure head profiles for ponded infiltration into sand and clay soil profiles.

2.4. HYDRUS (2D/3D)

In higher dimensions, it is often recommended that in order to obtain smooth solutions, FE elements should have approximately all sides equal. This recommendation is not valid for most applications involving fluxes in the vadose zone. Since in the vadose zone vertical fluxes usually dominate over horizontal fluxes, the spatial discretization must be much finer in the vertical direction than in the horizontal direction. In general, the spatial discretization should reflect the expected gradients in the transport domain; it should be fine in the direction of large gradients and can be coarser in the direction of small gradients.

HYDRUS offers several tools to adjust the spatial discretization to expected flow and transport conditions. The two most important tools are the **Smoothing Factor** and **Mesh Stretching** (both parameters can be specified in the FE Mesh Parameters dialog window. The smoothing factor is the ratio of the maximum and minimum height of a finite element triangle. For a triangle with equal sizes this factor is equal to 1 (which is theoretically not achievable for finite element meshes). The smoothing factor can be decreased to a value of about 1.1 when a highly smooth finite element mesh is required and, vice-versa, can be increased when a course mesh can be tolerated. The smoothing factor significantly affects the final number of elements, with the number of elements decreasing dramatically for larger values of the smoothing factor (e.g., 3). We recommend keeping the smoothing factor at its default value (i.e., 1.3) for relatively small transport domains (e.g., simulations of irrigation details), and increase its value to about 2-3 for larger transport domains (e.g., soil transects, field scale simulations).

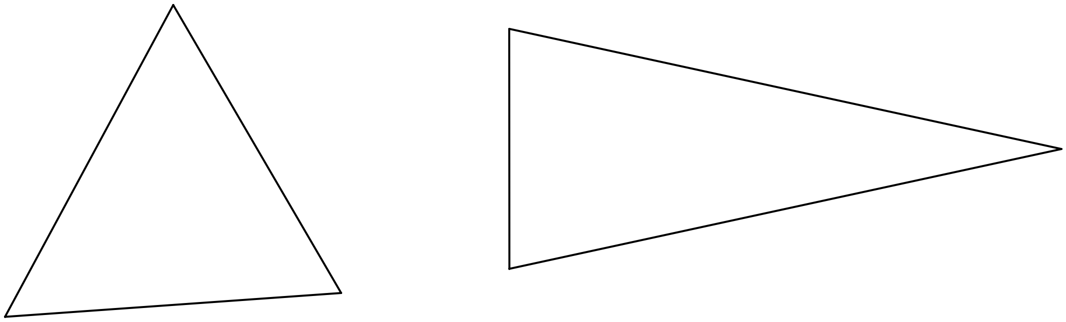

Figure 2. Triangle with a smoothing factor equal to 1 (left) and 3 (right).

Stretching of the finite element mesh (i.e., the degree of mesh anisotropy in a certain direction) is defined using the **Stretching Factor** and **Stretching Direction**. The finite elements are made larger in the particular **Stretching Direction** if the **Stretching Factor** is larger than one, and smaller if less that one. The result of this transformation is a mesh deformed in the given direction, which can be desirable for problems that, for example, require different spatial steps (mesh sizes) in the *X* and *Y* directions. As discussed above, in the vadose zone vertical fluxes usually dominate over horizontal fluxes, and thus the spatial discretization must be much finer in the vertical direction than in the horizontal direction. If vertical fluxes are expected to be many times larger (e.g., 10-100 times) in the vertical direction than in the horizontal direction, the **Stretching Factor** can also be very large (e.g., 10-100).

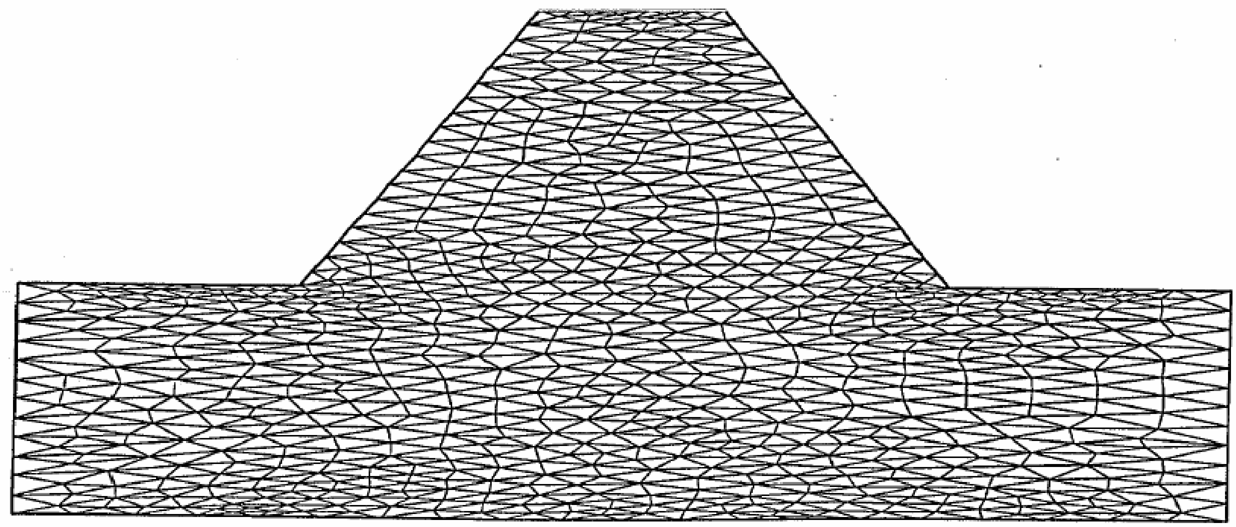

Figure 3. Example of mesh stretching using a stretching factor of 3 in the *y*-direction.