DUE TODAY
Assignment #1 Conceptual Model:
Select a **SINGLE-PHASE, SATURATED, FLOW** modeling project with both a steady and transient aspect, and write a summary describing it to me. If you do not have a place to model, I can help you identify one. Your description should use illustrations and include:

Title
Objective
Problem Description
Geohydrologic Setting

FIGURES (at least one plan and one cross section) ARE REQUIRED TO ILLUSTRATE THE FOLLWING ITEMS

- **location**
- **geometry**
- **boundary conditions**
- **parameter value ranges**
- **Stresses for which you will predict the resulting conditions**

Special considerations (if any)
Calibration Data that are available (head and flow data from the site)
A description of what you envision your final result will be
References

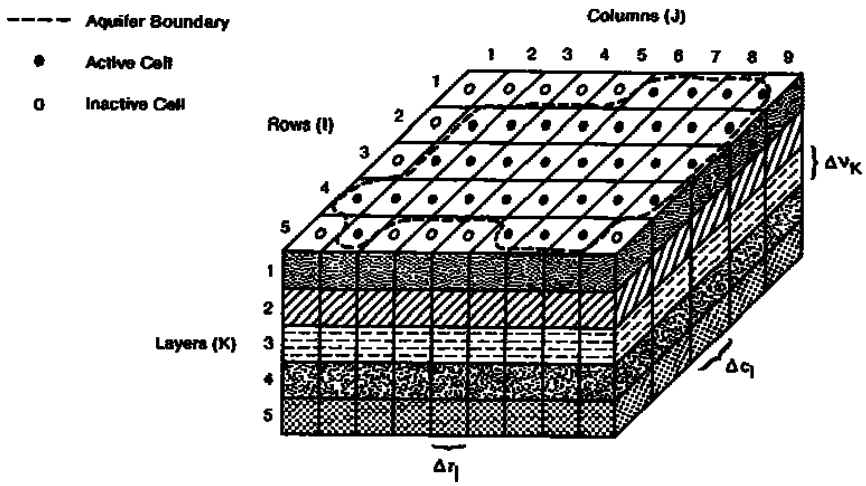
Submit a description and the drawings as hard copy OR as ASSGN1_LASTNAME.ZIP

Overview of Numerical Modeling

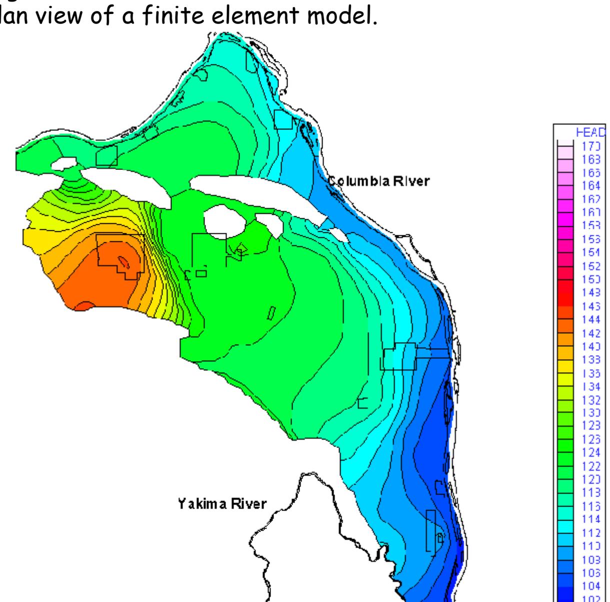
- DISCRETIZE to blocks of constant properties
- Set up FLOW EQUATIONS for each block N EQUATIONS
- Either H or Q will be KNOWN at each block N UNKNOWNS
- SOLVE for H or Q in all blocks SIMULTANEOUSLY (matrix algebra)
- CALIBRATE
- "VALIDATE"
- PREDICT
- EVALUATE UNCERTAINTY

EXAMPLE OF A SIMPLE NUMERICAL MODEL

Complex geologic material distributions are simplified.
Usually properties will vary across the layers.
Some of the model pieces are defined as inactive (open circles).
We use numbers to define a conceptual object like the grid shown below to represent the geometry, properties, boundary conditions, initial conditions and stresses on a groundwater system to build a representation of field conditions.

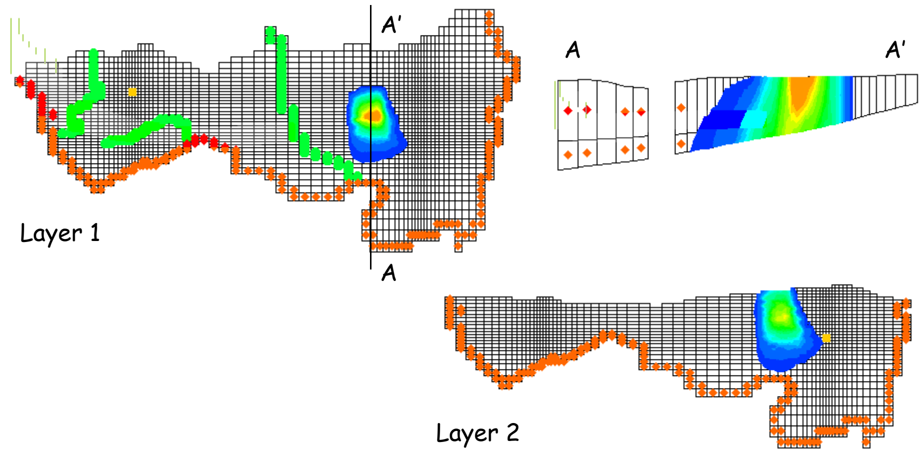


Hanford Reservation flow system from 1943 to 1996 when processing water was discharged to ponds raising the water table and then discontinued so the water table dropped. This is a plan view of a finite element model.



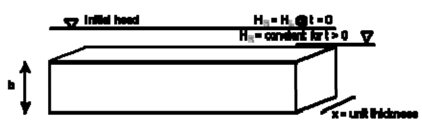
http://inside.mines.edu/~epoeter/583/08/model_example0.htm

This is a plan view of a 2 layer finite difference model. Each grid cell has one value for each relevant material property and one value of head, flow, and concentration associated with it. The north side is no-flow due to the presence of a low permeability rock. The orange dots indicate a river boundary. The green spots are drains representing intermittent streams. The yellow dots represent wells. The plume emanates from a landfill.

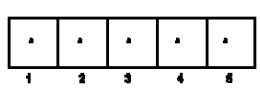


www.mines.edu/~epoeter/583/08/model_example1.htm

To understand how finite differencing works, let us define a simple situation. Consider a one-dimensional confined aquifer, with a constant initial head across its length. Then instantly drop the head on the right end of the aquifer while maintaining a constant head on the left side.



now overlay a grid on it, one unit thickness into the computer screen

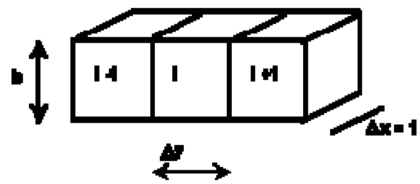


initial head will be the same for each cell

a constant head equal to the initial head, H_L will be defined for cell 1

a constant head equal to the head, H_R that begins the stress on the right will be defined for cell 5

we will solve for the flux at those nodes based on Darcy's Law after the heads are determined for the internal continuity nodes

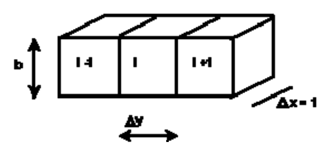


Maintaining simplicity, we define:

n = as the time index to identify increments in time
i = as the space index to identify the increments in space
$h_1 = h_2 = \ldots = h_5$ = initial head
$K_1 = K_2 = \ldots = K_5$ = hydraulic conductivity of the cell
$b_1 = b_2 = \ldots = b_5$ = thickness of the cell
$s_1 = s_2 = \ldots = s_5$ = specific storage of the cell

the flow from cell i-1 to cell i can be calculated as:

$$Q_{i-1-i} = -KA\frac{h_i^n - h_{i-1}^n}{\Delta y} \qquad (1)$$



the area of the flow face between cells is A = b * x

and since x=1, A=b
so we have K * b rather than K *A, so equation 1 can be rewritten as:

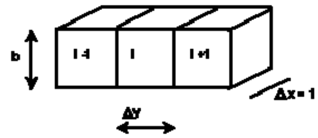
$$Q_{i-1-i} = -Kb\Delta x\frac{h_i^n - h_{i-1}^n}{\Delta y} \qquad (2)$$

similarly, the flow from cell i to cell i+1 can be calculated as:

$$Q_{i-i+1} = -Kb\Delta x\frac{h_{i+1}^n - h_i^n}{\Delta y} \qquad (3)$$

the rate of change of storage in grid block i over time t

$$\frac{\Delta V_i}{\Delta t}=sb\Delta y\Delta x\frac{h_i^{t+\Delta t}-h_i^t}{\Delta t} \qquad (4)$$



by continuity, the difference in flow into a cell and outflow from the cell equals the change in storage in the cell

$$Q_{i-1\to i}-Q_{i\to i+1}=\frac{\Delta V_i}{\Delta t} \qquad (5)$$

Notice we could add other flows from recharge, wells, head dependent flux boundaries etc, but we will keep this simple.

substituting equations 2, 3, and 4 into equation 5, we obtain:

$$(-Kb\Delta x\frac{h_i^n-h_{i-1}^n}{\Delta y})-(-Kb\Delta x\frac{h_{i+1}^n-h_i^n}{\Delta y})=sb\Delta y\Delta x(\frac{h_i^{t+\Delta t}-h_i^t}{\Delta t}) \qquad (6)$$

we can substitute transmissivity, T, for Kb because T = K * b, so equation 6 can be rewritten as:

$$(-T\frac{h_i^n-h_{i-1}^n}{\Delta y})-(-T\frac{h_{i+1}^n-h_i^n}{\Delta y})=S\Delta y(\frac{h_i^{t+\Delta t}-h_i^t}{\Delta t}) \qquad (7)$$

rearranging to place the spatial variation of head on the left and the time variation of head on the right, along with the aquifer constants, we obtain:

$$h_{i+1}^n-2h_i^n+h_{i-1}^n=\frac{S}{T}\frac{(\Delta y)^2}{\Delta t}(h_i^{t+\Delta t}-h_i^t) \qquad (8)$$

IF we set n = t, EXPLICIT, FORWARD DIFFERENCE

IF we set n = t+ Δt IMPLICIT, BACKWARD DIFFERENCE to take the EXPLICIT approach, SET n = t and rearrange so that the only unknown head is on the left

$$h_i^{t+\Delta t} = \frac{T\Delta t}{S\Delta y^2}(h_{i+1}^t + h_{i-1}^t) + h_i^t\left(1 - \frac{2T\Delta t}{S\Delta y^2}\right) \qquad (9)$$

notice that the expression will be stable as long as:

$$\frac{T\Delta t}{S\Delta y^2} < \frac{1}{2}$$

Because the second term will always be positive.

to take the IMPLICIT approach, SET n = t+Δt

$$h_{i+1}^{t+\Delta t} - 2h_i^{t+\Delta t} + h_{i-1}^{t+\Delta t} = \frac{S\Delta y^2}{T\Delta t}(h_i^{t+\Delta t} - h_i^t) \qquad (10)$$

and rearrange the unknown heads to be on the left

$$h_{i+1}^{t+\Delta t} - \left(2 + \frac{S\Delta y^2}{T\Delta t}\right)h_i^{t+\Delta t} + h_{i-1}^{t+\Delta t} = -\frac{S\Delta y^2}{T\Delta t}h_i^t \qquad (11)$$

For homework you will work through this by hand
both explicitly and implicitly on a small problem.
There is a link on the class page and description in the syllabus.
Let's look at that now

http://inside.mines.edu/~epoeter/583CSM/index.shtml

http://inside.mines.edu/~epoeter/583/06/exercise/finite_diff_exer.htm

A variety of matrix solution techniques are utilized to solve the finite difference equations. These techniques iteratively approximate the solution. There are a few essential concepts you need to grasp in order to use a solution wisely

DIRECT - EXACT SOLUTION
ITERATIVE - APPROXIMATE SOLUTION

We rarely use direct solutions because the problems we solve are so large it is not likely that we can solve the entire matrix within the available memory.

Consequently, we employ a mathematical scheme that repeatedly approximates the solution to the matrix, until there is very little change from the previous approximation. **The approximation is repeated (this is called iterating) until the change is less than a specified tolerance. When this point is reached, we say that the solution has converged.** Generally the tolerance is specified by the user. Sometimes subsequent approximations change very slowly and we would like to speed the process up, other times the approximation causes large changes that repeatedly overshoot the answer in opposite directions, so we want to slow the process down. **Often the code provides the user the opportunity to specify an acceleration or relaxation (two terms for the same variable) parameter to speed up or stabilize the convergence process.** Occasionally a particular solver requires specific input items and you will need to carefully read the manual to understand your options, but nearly all solvers require a tolerance and relaxation.

CONVERGENCE IS "ARBITRARY" i.e. it depends on the tolerance value:

GENERALLY we assume that the user specified a reasonable tolerance and that the solution will be fairly accurate (have a small mass balance) at that precision level

For heads A REASONABLE TOLERANCE is small relative to the total head change across the system and small relative to the head difference between cells in low gradient areas

IF TOLERANCE IS VERY SMALL, LACK OF CONVERGENCE MAY NOT BE SIGNIFICANT because the solution may be very precise, that is the mass balance may be very small.

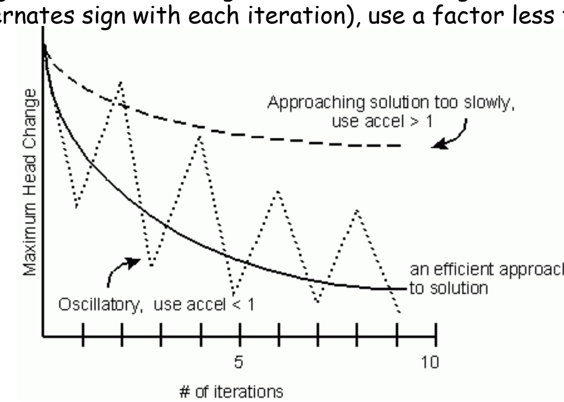
For example, a user may specify a tolerance for head change between iterations that is smaller than the precision of the computer ... this tolerance could never be met but the solution would be very precise. In a case like this, it is usually desirable to increase the tolerance so that the problem converges to avoid the unfounded concerns of those who feel uncomfortable with the words "did not converge!" In reality the solution will not be any better. One could simply look at the model output to see how much head change occurred for the last iteration and use a value just slightly larger. Then the solution would be identical but the output would say "solution converged!"

IF TOLERANCE IS VERY LARGE, PRESENCE OF CONVERGENCE MAY NOT BE SIGNIFICANT because the solution may be very imprecise, that is, the mass balance may be large.

For example, a user may specify a tolerance for head change between iterations that is large compared to the total head change across the model or to the difference in head between cells in areas of low gradient. The model would converge after a small number of iterations but the flow field may appear erratic, even with flow apparently generated out of "nowhere" because one cell ends with a high head and flow moves out to all surrounding cells and there is no source to "feed" that radial outflow. Such conditions result in a poor mass balance.

Acceleration or Relaxation

If progress toward convergence is proceeding too slowly, use a factor larger than one. If progress toward convergence is over shooting the answer (maximum head change alternates sign with each iteration), use a factor less than one.



Typically the maximum head change varies in location. A good code will report the node at which the maximum occurred. If your model is not converging efficiently, it can be useful to note where the maximum head change is occurring. Sometimes evaluation of your input will reveal that you have a "typo", for example you may have typed the exponent on a hydraulic conductivity incorrectly resulting in a large contrast of conductivity between adjacent cells, or you may have added an extra "0" to a boundary head for one cell causing a huge influx at one cell.

MASS BALANCE

ULTIMATELY THE SOLUTION MUST CONSERVE MASS

Although your conceptual model may be based on a balanced hydrologic budget, the numerical model will have mass imbalances if the heads are not calculated accurately. The fluxes will be based on gradients between cells. If the heads are not accurate, the gradients will produce inconsistent fluxes, thus the inflows and outflows (note that flow into storage is an outflow and flow in from storage is an inflow) will not balance.

EXAMPLES of MODELING PROBLEMS THAT CAN LEAD TO MASS IMBALANCE INCLUDE:

- **large convergence tolerance**
- **poor conceptual model formulation (i.e. set up is hydraulic nonsense)**
- **large contrasts in properties between adjacent cells**
- **large difference in size of adjacent cells**
- **large time steps or time steps so small that the defined flows are below the accuracy of the computer solution**

MOST CODES PROVIDE A TABLE TO ASSESS MASS BALANCE

Generally the table includes a summary of inflow and outflow to and from various types of features as well as the overall flow. This is another good place to pause and assess the model results to be sure everything makes sense to you. It is also valuable to evaluate the inflow or outflow to each cell where a head or head dependent flux has been specified. Such evaluation can reveal errors that could otherwise go unnoticed yet have negative repercussions on your results. The mantra for this is: always monitor the flow at fixed head nodes and the flux at fixed flux nodes.

A SMALL MASS BALANCE IS REQUIRED

substantially <1% (0.5% is the high end of acceptable)

SOMETIMES A LARGE MASS BALANCE IS NOT A PROBLEM:

for example, if there is a large imbalance for an early time step, perhaps even 200%, it may not be important, because as you will learn later we generally start with very small time steps and gradually increase the length of each time step, so a 200% error in the first time step may only reflect lost accounting for a gallon of water while the problem as a whole involves 10s of thousands of gallons and subsequent time steps have reasonable mass balances.

MOST IMPORTANTLY ONE MUST CAREFULLY EVALUATE THE MODEL OUTPUT TO DETERMINE WHERE WATER ENTERS AND LEAVES THE MODEL AND ASSESS IF THE FLOW PATTERN AND VOLUMES ARE REASONABLE

ALWAYS MONITOR:

Q @ FIXED H NODES
AND
H @ FIXED Q NODES

Discretization

Once the problem is defined and you have conceptualized the model and made preliminary analytical assessments, it is time to design the numerical model and consider how to discretize space and time.

You may find that designing your grid is the most difficult task you undertake in your modeling project.

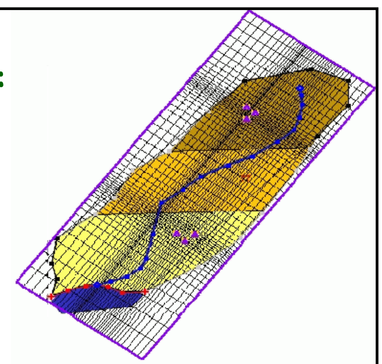
It probably doesn't help to know that the success of your project is dependent on a good grid design and that redesign of the grid is a major undertaking (unless you use a GUI …more later).

You may feel the equivalent of writer's block.

Let's look at issues to keep in mind when building a grid

Then "go for it!"
Do not worry about making mistakes
Mistakes can be used as learning experiences

DESIGNING PLAN VIEW OF GRID
balance the following considerations:



INCLUDE PROBLEM DOMAIN

MINIMIZE # OF CELLS

MINIMIZE EXTERNAL INACTIVE GRIDS

ORIENT WITH FLOW DIRECTION

ORIENT WITH ANISOTROPY

ACCOMMODATE BOUNDARIES BETWEEN FEATURES/HIGH CONTRAST IN MATERIAL PROPERTIES

FINER GRIDS IN STRESS AREAS WITH STEEP GRADIENTS

FINER GRIDS NEAR AREAS OF INTEREST / OBSERVATION POINTS

OMIT PART OF THE SYSTEM IF IT IS SYMMETRICAL

MAINTAIN RELATIVE SIZE OF ADJACENT GRIDS (1:1.5)

MAINTAIN ASPECT RATIO ORTHOGONAL DIRECTIONS (100:1)

CONSIDER FINER GRID FOR FUTURE SOLUTE TRANSPORT

Smaller cell sizes provide more accuracy, sizes are small enough when the ANSWER REMAINS THE SAME FOR SMALLER CELL SIZES

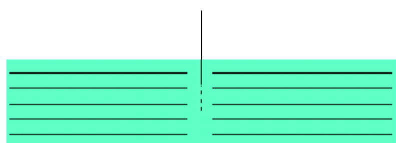
DESIGNING Cross-Sectional VIEW OF GRID

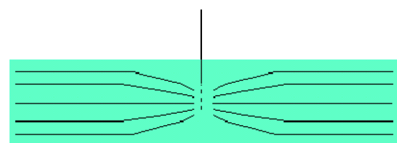
If you have only one layer in a model, then flow is always parallel to the layer. There will be NO potential for VERTICAL flow no matter how you stress the model.

In order to define vertical components of flow, you need vertical "stacks" of cells.

If you have only two layers, you can calculate either an upward or downward gradient of one magnitude (that is you cannot calculate a stronger gradient at one level versus another). With only 2 layers, you cannot calculate convergent flow.

If you want a detailed map of complicated vertical flow patterns, you need to have numerous nodes in the vertical direction.





DESIGNING Cross-Sectional VIEW OF GRID, consider:

PURPOSE

REGIONAL / LOCAL?

PARTIAL PENETRATION?

AQUITARD STORAGE?

FUTURE TRANSPORT MODELING?

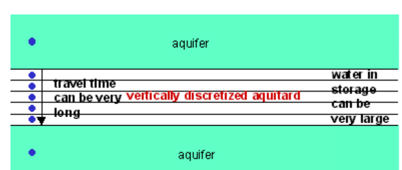
HYDROSTRATIGRAPHIC UNITS

- GEOLOGIC LOGS
- GEOPHYSICS

VERTICAL HYDRAULIC GRADIENTS

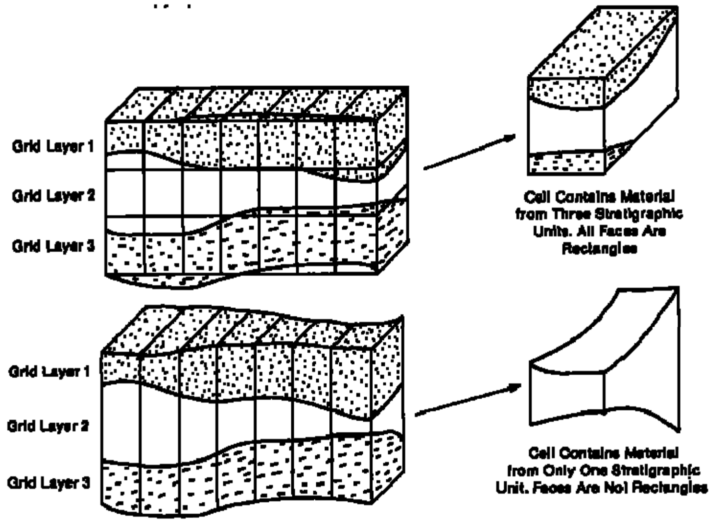
DEWATERING

- RELATIVE SIZE OF ADJACENT GRIDS IS NOT AN ISSUE IN THE VERTICAL DIRECTION



DESIGNING Cross-Sectional VIEW OF GRID, consider:

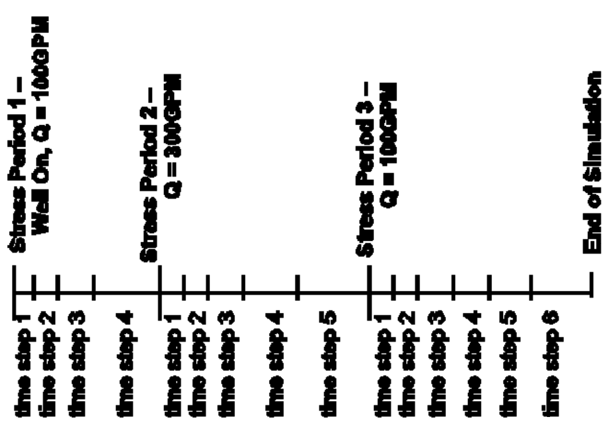
LAYER REPRESENTATION OPTIONS:
CONSTANT LAYER THICKNESS/VARIABLE PROPERTIES
VARIABLE LAYER THICKNESS/CONSTANT PROPERTIES



DESIGNING TIME STEPS (temporal equivalent of grid cells), consider:

Time steps should be small when stresses change and increase in length to a constant, convenient size until the stresses change

STRESS PERIODS
groups of time steps during which the stresses do not change



DESIGNING TIME STEPS (temporal equivalent of grid cells) consider:

It may be difficult to decide on the initial time step size. One can always try one step of a size that seems reasonable given the overall length of the simulation and look at the mass balance to see if it will be small enough. A rule of thumb is to calculate the maximum step size for an explicit formulation of the problem. In a two-dimensional plan view problem with a constant grid spacing in the x and y direction equal to "a":

$$\text{Estimate of initial time step size} = \frac{S\,a^2}{4\,T}$$

In MODFLOW you enter parameters describing the time period, number of steps and a multiplier to gradually increase steps. These parameter are related as follows. The equation can be rearranged to solve for any parameter. Here it is arranged to solve for initial step size:

$$\text{initial time step size} = \text{period length} * \frac{1 - \text{time step multiplier}}{1 - (\text{time step multiplier})^{\text{number of steps}}}$$

The multiplier is typically 1.1 to 1.5

Smaller time step sizes provide more accuracy, sizes are small enough when the ANSWER REMAINS THE SAME FOR SMALLER STEP SIZES

DUE NEXT WEEK Assignment #2 a) Finite Difference Calculation & b) Grid

a) Calculation: For the problem using 5 finite difference grid blocks numbered 1 to 5 left to right and with the following parameters:
confined flow ; y = 3 ft ; b = 3 ft ; K = 0.02 ft/day ; T= 0.06 ft2/day ; s = 0.00033 ft-1 ; S = 0.001
initially, h1=h2=h3=h4=h5=8.2ft ; constant head left h1=8.2ft ; for t>0 constant head h5=3.6ft
as posed on: http://inside.mines.edu/~epoeter/583/06/exercise/finite_diff_exer.htm
using the explicit approach on http://inside.mines.edu/~epoeter/583/06/exercise/explicit_exer.htm
and the implicit approach on http://inside.mines.edu/~epoeter/583/06/exercise/implicit_exer.htm
For both approaches:

1. Calculate h4 @ 0.07 day increments to 0.7 days using the implicit approach
2. Repeat #1 @ 0.14 day increments to 0.7 days using the implicit approach
3. Compare the mass balance at each step for the 0.07 and the 0.14 day time steps.
4. Graph your results as head vs. time
5. Compare your result to those from the explicit method **YOU MAY USE A SPREAD SHEET IF YOU PROVIDE A HAND CALCULATION AS A CHECK FOR EACH TYPE OF CALCULATION**

b) Grid: Layout the finite difference grid over a map of the model area for your problem and in a vertical cross-section. Discuss why you chose to grid the problem as shown. Keep your grid small (e.g. less than 20rows x 20col would be best, but absolutely no larger than 40x40) in order to make the project manageable such that you optimize your learning about modeling. The goal is for you to learn about modeling, not to produce a detailed model of your system. Use at least 2 layers so you can become familiar with issues related to multiple layers. Even if you are only simulating one geologic unit you can break it into an upper and lower portion which will give you a bit of information about vertical gradients in the system. Label the diagrams to describe the initial properties and boundary conditions you will use. These will be adjusted later in the calibration process. Your submission should include:
Drawing of plan view of each layer with properties & boundary conditions labeled
Drawing of cross section view of grid with properties & boundary conditions labeled
submit a description and the drawings as hard copy OR as ASSGN2_LASTNAME.ZIP

ALSO DUE NEXT WEEK

Assignment #3 Analytical Model: Choose an analytical model to represent some aspect of your modeling project and implement it with your model conditions. Describe the problem set-up and solution in a concise and clear manner. If you use a spreadsheet, mathcad, or other code for calculation, provide at least one hand calculation to confirm that your results are correct. Your submission should use illustrations to describe the conceptual model and how it fits your problem. It should include the following items:

Title
Objective
Problem Description
Analytical Model Description
Simplification of System in order to use the analytical model
Parameter values used
Calculations
Results
References

submit the write-up as hard copy and if you have electronic files include it in your zip file labeled: ASSGN3_LASTNAME.ZIP