Solving diffusion equations in two dimensions using finite differences

Review of finite differences in 1D

Earlier in this course we looked at a specific finite difference solution to the one dimensional diffusion equation for transient groundwater modeling. The diffusion equation can be written in general form as:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{1}$$

where u is the variable that represents the physical quantity being modeled (for example hydraulic head, concentration, temperature, etc). u is a function of both time t and spatial position x: $u = u(x,t)$. The coefficient α is the material property that controls the rate of diffusion.

In the finite difference method, the unknown function u is discretized using a series of grid points in both time and space, as shown in Figure 1. The first and second order derivatives in the diffusion equation are then approximated using finite differences of neighboring values of u at the grid points in time and space.

The first order partial derivative with respect to time t has the forward finite difference approximation:

$$\frac{\partial u(x,t_k)}{\partial t} \approx \frac{u(x,t_{k+1}) - u(x,t_k)}{\Delta t}, \tag{2}$$

where Δt is $t_{k+1} - t_k$.

The second order partial derivative with respect to position x has the central finite difference approximation:

$$\frac{\partial^2 u(x_i,t)}{\partial x^2} \approx \frac{u(x_{i+1},t) - 2u(x_i,t) + u(x_{i-1},t)}{\Delta x^2}, \tag{3}$$

where Δx is the grid spacing in x.

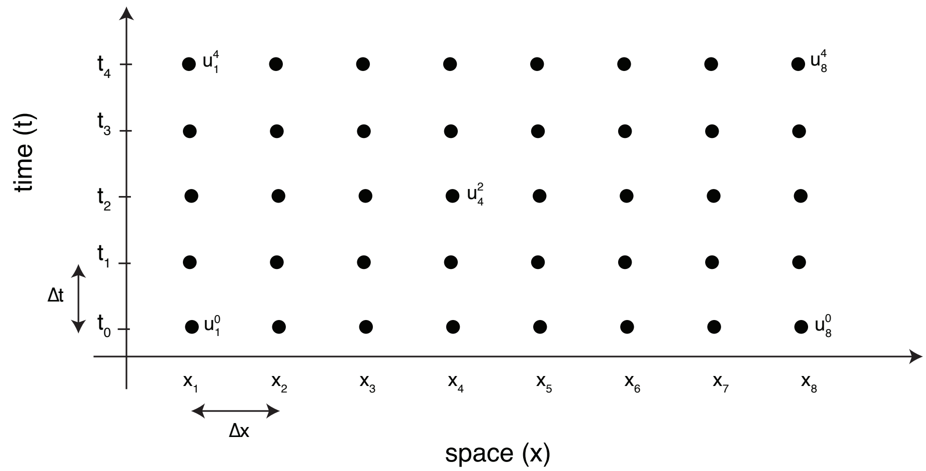

Figure 1: Example finite difference grid in x and t function $u_i^k = u(x_i, t_k)$ using spacings Δx and Δt. In this simplified example, there are 8 grid point in spatial dimension x and 5 grid points in time t.

We can shorten the notation using a subscript to denote the spatial index of a grid point and a superscript to represent the time index. For example $u_i^k = u(x_i, t_k)$. See the labeled grid point examples in Figure 1).

Using this more concise notation, the finite difference approximations for the time and spatial derivatives are then:

$$\frac{\partial u}{\partial t} \approx \frac{u_i^{k+1} - u_i^k}{\Delta t}, \tag{4}$$

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i+1}^k - 2u_i^k + u_{i-1}^k}{\Delta x^2} \tag{5}$$

Inserting these into equation 1 gives:

$$\frac{u_i^{k+1} - u_i^k}{\Delta t} = \alpha \frac{u_{i+1}^k - 2u_i^k + u_{i-1}^k}{\Delta x^2} \tag{6}$$

This expression is then rearranged to solve for u_i^{k+1}, giving:

$$u_i^{k+1} = u_i^k + \frac{\alpha \Delta t}{\Delta x^2}\left(u_{i+1}^k - 2u_i^k + u_{i-1}^k\right) \tag{7}$$

$$= \left(1 - 2\frac{\alpha \Delta t}{\Delta x^2}\right) u_i^k + \frac{\alpha \Delta t}{\Delta x^2}\left(u_{i+1}^k + u_{i-1}^k\right) \tag{8}$$

$$= a u_i^k + b\left(u_{i+1}^k + u_{i-1}^k\right) \tag{9}$$

This equation shows that the values at time t_{k+1} can be found using only values from the previous time step t_k. Thus, given the initial values u^0 at t_0, equation 9 can be used to step the solution forward in time. This process is repeated iteratively until the desired number of time steps has been carried out.

This technique above is known an *explicit* finite difference method since only the current time values are used to find the values one step forward in time. More specifically, the method outlined above is know as the forward-in-time, center-in-space, or FTCS finite difference scheme since it uses a central different for the space derivative and a forward difference for the time derivative. There are other finite difference methods that are more complicated to derive (and which are computationally more intensive) that can be used for more complicated differential equations. However, the basic FTCS method is easy to implement and suitably accurate to handle a wide range of diffusion modeling problems. The key limitation, is that the time step Δt and spatial grid spacing Δx need to be carefully chosen. For the 1D FTCS method to be stable, the time step and grid spacing need to satisfy:

$$\alpha \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2} \tag{10}$$

This requirement comes from Von Neumann stability analysis. We don't have time to cover this in this course, but a useful starting point for learning more about this can be found here: `https://en.wikipedia.org/wiki/Von_Neumann_stability_analysis`

Two dimensional Partial Differential Equations

Now let's expand the finite difference method to two dimension so we can model the behavior of function u in both the x and y directions: $u = u(x, y)$.

Three commonly encountered two-dimensional partial differential equations are:

$$\alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0 \qquad \text{Laplace's equation} \tag{11}$$

$$\alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = \frac{\partial u}{\partial t} \qquad \text{Diffusion equation} \tag{12}$$

$$\alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = \frac{\partial^2 u}{\partial t^2} \qquad \text{Wave equation} \tag{13}$$

where α is a constant depending on the material properties. Notice how these equations are all nearly the same. The differences are in the time derivative terms on the right hand side. Laplace's equation has no time dependence, and can be thought of as the steady state solution to either the diffusion of wave equations. The diffusion equation has a first order time derivative and the wave equation has a second order time derivative.

When applying these equations to real problems, the material properties of the problem are represented by the diffusion parameter α. For example, in the transient groundwater problem considered earlier in this course, α depended of a few hydraulic properties of the aquifer. The variable u will correspond to some physical behavior, such as pressure, velocity, temperature, electric potential, groundwater head, etc, depending on the particular system being studied.

Two dimensional Finite Difference Solution

In two dimensions (2D) we divide up the (x,y) plane into a grid of points with spacings Δx and Δy, as shown in Figure 2. Now we will use two subscripts to represent a grid point, with i for the x index and j for the y index. We will use the shorthand notation $u_{i,j} = u(x_i, y_j)$.

Laplace's equation in 2D

First let's consider Laplace's equation, since it is the simplest of the three equations shown above. The finite difference expression for the second-order partial derivative with respect to x is:

$$\frac{\partial^2 u_{i,j}}{\partial x^2} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \tag{14}$$

and similarly, the second-order partial derivative with respect to y has the finite difference approximation:

$$\frac{\partial^2 u_{i,j}}{\partial y^2} \approx \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} \tag{15}$$

where we have omitted the superscript k since Laplace's equation has no time dependence (and thus represents a steady-state solution).

Inserting these into Laplace's equation gives:

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = 0. \tag{16}$$

If we assume our grid spacing is even in the x and y directions so $\Delta x = \Delta y$, we can factor out the Δx and Δy terms. Rearranging the resulting expression for u_i yields:

$$u_{i,j} = \frac{1}{4} \left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} \right). \tag{17}$$

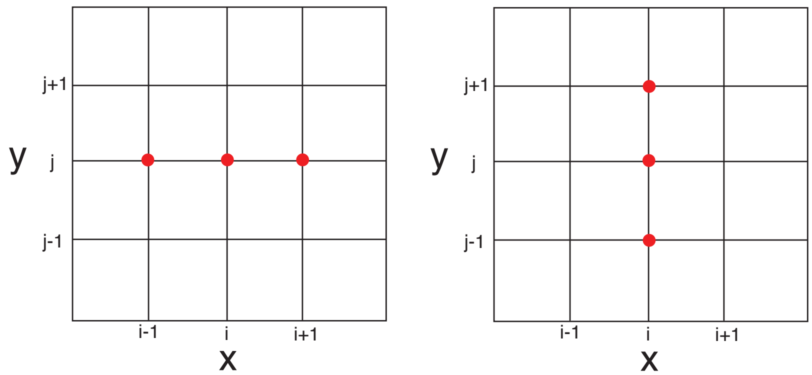

Figure 2: Finite differences in the x and y directions for a two dimensional grid.

This equation reveals a surprising result—the finite difference solution to Laplace's equation says that the value at a grid point shall simply be the average of all its neighbors!

See Figure 3 for a visualization of the 2D finite difference stencil for Laplace's equation.

Diffusion equation in 2D

Now consider the 2D diffusion equation which builds on the Laplace's equation by adding a first-order time derivative term. Using the finite difference expressions from above, we have:

$$\frac{u_i^{k+1} - u_i^k}{\Delta t} = \alpha \left(\frac{u_{i+1,j}^k - 2u_{i,j}^k + u_{i-1,j}^k}{\Delta x^2} + \frac{u_{i,j+1}^k - 2u_{i,j}^k + u_{i,j-1}^k}{\Delta y^2} \right). \tag{18}$$

Then we rearrange this into the FTCS update equation for u_i^{k+1}. This is easiest if an even grid spacing is used so that $\Delta x = \Delta y$, we then have:

$$u_{i,j}^{k+1} = u_{i,j}^k + \frac{\alpha \Delta t}{\Delta x^2} \left(u_{i+1,j}^k + u_{i-1,j}^k + u_{i,j+1}^k + u_{i,j-1}^k - 4u_{i,j}^k \right). \tag{19}$$

We can further simplify this equation by rearrangement into:

$$u_{i,j}^{k+1} = a u_{i,j}^k + b \left(u_{i+1,j}^k + u_{i-1,j}^k + u_{i,j+1}^k + u_{i,j-1}^k \right), \tag{20}$$

where

$$a = 1 - 4\frac{\alpha \Delta t}{\Delta x^2}, \tag{21}$$

$$b = \frac{\alpha \Delta t}{\Delta x^2}. \tag{22}$$

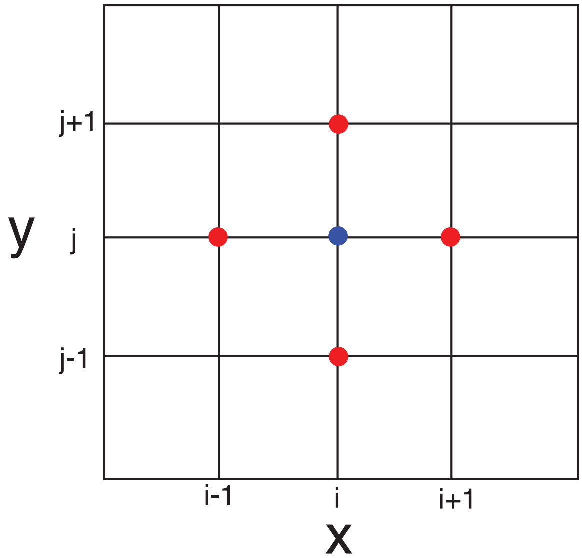

Figure 3: Finite difference stencil for Laplace's equation at point x_i, y_j. The values are the red dots are used to compute the solution at the blue dot.

Equation 20 is very similar to the 1D solution, except now it includes additional terms for the neighboring points in the 2nd spatial dimension y, Further, the 2nd term in the coefficient a has a factor of 4 instead of 2. A graphical illustration of this 2D FTCS time step is shown in Figure 4.

Von Neumann stability analysis for 2D FTCS methods shows a stable solution is possible when the values of Δt and Δx satisfy the relation:

$$\alpha \frac{\Delta t}{\Delta x^2} \leq \frac{1}{4} \tag{23}$$

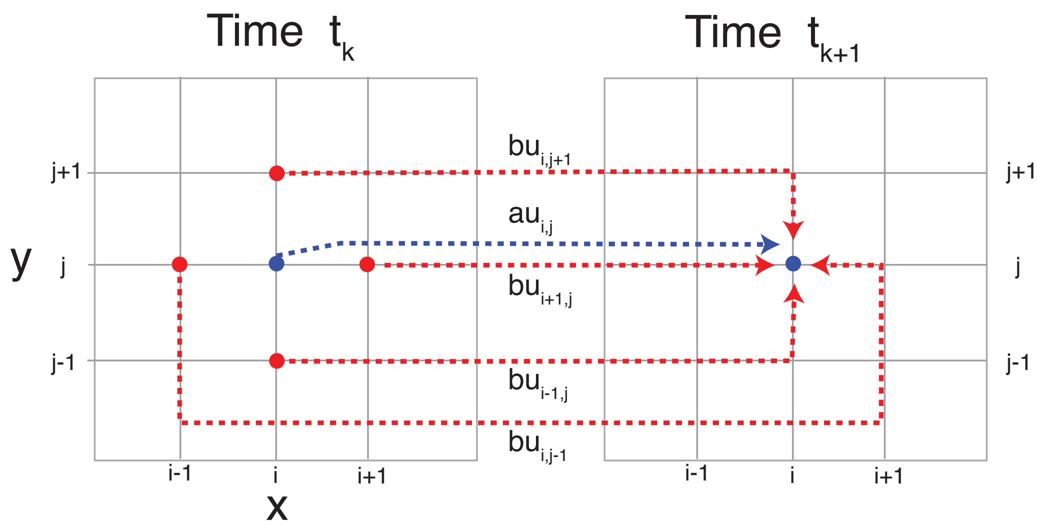

Figure 4: Finite difference stencil for the diffusion equation at point x_i, y_j. The values of u^k at the red dots and the central blue dot at time t_k (shown on the left) are used to compute the solution at the blue dot ($u_{i,j}^{k+1}$) at time t_{k+1} (shown on the right).