Finite Difference Modeling with Spatially Varying Material Properties

In this course we have looked at the diffusion equation for a variety of physical problems. For example, we looked at the transient heat equation:

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}. \tag{1}$$

In all of previous problems, we made the assumption that the material property is constant throughout the medium. For the heat conduction problem, this means we assumed the thermal diffusivity κ does not vary. However, some of the most interesting real-world problems involve material properties that vary as a function of position. For example, consider what happens if the thermal diffusivity varies laterally so that $\kappa \equiv \kappa(x)$. When $\kappa(x)$ is not constant, the heat conduction partial differential equation has the form:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial T}{\partial x}\right) \tag{2}$$

Thus, the thermal diffusivity is now inside the first partial derivative. A similar form of equation governs the transient groundwater flow problem when the hydraulic diffusivity varies laterally.

So let's take a quick look at how the finite difference solution to the diffusion equation when the material properties vary. We will continue using the specific diffusion equation for heat conduction. We start by introducing the temporary variable ϕ:

$$\phi = \kappa(x)\frac{\partial T}{\partial x}, \tag{3}$$

which when substituted into the diffusion equation gives:

$$\frac{\partial T}{\partial t} = \frac{\partial \phi}{\partial x}. \tag{4}$$

The first order derivative on the right hand side is approximated at time t_n and spatial grid point x_i using a central finite difference formula

$$\frac{\partial \phi_i^n}{\partial x} \approx \frac{\phi_{i+\frac{1}{2}}^n - \phi_{i-\frac{1}{2}}^n}{\Delta x} \tag{5}$$

Here $\phi^n_{i+\frac{1}{2}}$ is the value of ϕ at half-spacing grid point $x_{i+\frac{1}{2}}$ and $\phi^n_{i-\frac{1}{2}}$ is the value of ϕ at $x_{i-\frac{1}{2}}$. These values of ϕ are found using finite difference appoximations of equation 3:

$$\phi^n_{i+\frac{1}{2}} \approx \kappa_{i+\frac{1}{2}} \frac{T^n_{i+1} - T^n_i}{\Delta x}, \tag{6}$$

$$\phi^n_{i-\frac{1}{2}} \approx \kappa_{i-\frac{1}{2}} \frac{T^n_i - T^n_{i-1}}{\Delta x}. \tag{7}$$

Inserting these expressions into equation 5 gives:

$$\frac{\partial \phi^n_i}{\partial x} \approx \frac{\kappa_{i+\frac{1}{2}} \frac{T^n_{i+1} - T^n_i}{\Delta x} - \kappa_{i-\frac{1}{2}} \frac{T^n_i - T^n_{i-1}}{\Delta x}}{\Delta x} \tag{8}$$

$$= \frac{\kappa_{i+\frac{1}{2}} \left(T^n_{i+1} - T^n_i\right) - \kappa_{i-\frac{1}{2}} \left(T^n_i - T^n_{i-1}\right)}{\Delta x^2} \tag{9}$$

Note that if κ is uniform (i.e. constant), this equation turns into the 2nd order central finite difference approximation we have already used in this course several times.

Inserting this into equation 4 and using a forward difference formula for the time derivative gives:

$$\frac{T^{n+1}_i - T^n_i}{\Delta t} = \frac{\kappa_{i+\frac{1}{2}} \left(T^n_{i+1} - T^n_i\right) - \kappa_{i-\frac{1}{2}} \left(T^n_i - T^n_{i-1}\right)}{\Delta x^2}, \tag{10}$$

which can be rearranged to give the time stepping update equation:

$$T^{n+1}_i = T^n_i + \frac{\Delta t}{\Delta x^2} \left[\kappa_{i+\frac{1}{2}} \left(T^n_{i+1} - T^n_i\right) - \kappa_{i-\frac{1}{2}} \left(T^n_i - T^n_{i-1}\right)\right] \tag{11}$$

$$= T^n_i + \frac{\Delta t}{\Delta x^2} \left[\kappa_{i+\frac{1}{2}} T^n_{i+1} - \left(\kappa_{i+\frac{1}{2}} + \kappa_{i-\frac{1}{2}}\right) T^n_i + \kappa_{i-\frac{1}{2}} T^n_{i-1}\right] \tag{12}$$

In a typical modeling problem, the values of the material coefficient are defined discretely at the grid points x_i, thus it is not clear what the values at the half-grid points $x_{i+\frac{1}{2}}$ should be. Usually, the value at the half-grid points is approximated by averaging the coefficient values at the neighboring grid points. For example:

$$\kappa_{i+\frac{1}{2}} \approx \frac{\kappa_{i+1} + \kappa_i}{2} \tag{13}$$