Notes on diffusion

These summarize methods for solving the diffusion equation.

1 Elliptic equations

The diffusion equation is

$$\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial \phi}{\partial x}\right) \tag{1}$$

This can describe thermal diffusion (for example, as part of the energy equation in compressible flow), species/mass diffusion for multispecies flows, or the viscous terms in incompressible flows. In this form, the diffusion coefficient (or conductivity), k, can be a function of x, or even ϕ. We will consider a constant diffusion coefficient:

$$\frac{\partial \phi}{\partial t} = k \frac{\partial^2 \phi}{\partial x^2} \tag{2}$$

2 Explicit differencing

The simplest way to difference this equation is *explicit* in time (i.e. the righthand side depends only on the old state):

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = k \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} \tag{3}$$

This is second-order accurate in space, but only first order accurate in time (since the righthand side is not centered in time).

As with the advection equation, when differenced explicitly, there is a constraint on the timestep required for stability. The timestep constraint in this case is

$$\Delta t < \frac{1}{2} \frac{\Delta x^2}{k} \tag{4}$$

Note the Δx^2 dependence—this constraint can become really restrictive.

To complete the solution, we need boundary conditions at the left (x_l) and right (x_r) boundaries. These are typically either Dirichlet:

$$\phi|_{x=x_l} = \phi_l \tag{5}$$
$$\phi|_{x=x_r} = \phi_r \tag{6}$$

or Neumann:

$$\phi_x|_{x=x_l} = \phi_x|_l \tag{7}$$
$$\phi_x|_{x=x_r} = \phi_x|_r \tag{8}$$

3 Implicit with direct solve

A backward-Euler implicit discretization would be:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = k \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2} \tag{9}$$

This is still first-order in time, but is not restricted by the timestep constraint (although the timestep will still determine the accuracy). Defining:

$$\alpha \equiv k \frac{\Delta t}{\Delta x^2} \tag{10}$$

we can write this as:

$$-\alpha \phi_{i+1}^{n+1} + (1+2\alpha)\phi_i^{n+1} - \alpha \phi_{i-1}^{n+1} = \phi_i^n \tag{11}$$

This is a set of coupled algebraic equations. We can write this in matrix form. Using a cell-centered grid, spanning $[\mathrm{lo}, \mathrm{hi}]$, and Neumann BCs on the left:

$$\phi_{\mathrm{lo}-1} = \phi_{\mathrm{lo}} \tag{12}$$

the update for the leftmost cell is:

$$(1+\alpha)\phi_{\mathrm{lo}}^{n+1} - \alpha \phi_{\mathrm{lo}+1}^{n+1} = \phi_{\mathrm{lo}}^n \tag{13}$$

If we choose Dirichlet BCs on the right ($\phi|_{x=x_l} = A$), then:

$$\phi_{\mathrm{hi}+1} = 2A - \phi_{\mathrm{hi}} \tag{14}$$

and the update for the rightmost cell is:

$$-\alpha \phi_{\mathrm{hi}-1}^{n+1} + (1+3\alpha)\phi_{\mathrm{hi}}^{n+1} = \phi_{\mathrm{hi}}^n + \alpha 2A \tag{15}$$

For all other interior cells, the stencil is unchanged. The resulting system can be written in matrix form and appears as a *tridiagonal* matrix.

$$\begin{pmatrix} 1+\alpha & -\alpha & & & & & \\ -\alpha & 1+2\alpha & -\alpha & & & & \\ & -\alpha & 1+2\alpha & -\alpha & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & -\alpha & 1+2\alpha & -\alpha \\ & & & & & -\alpha & 1+3\alpha \end{pmatrix} \begin{pmatrix} \phi_{\mathrm{lo}}^{n+1} \\ \phi_{\mathrm{lo}+1}^{n+1} \\ \phi_{\mathrm{lo}+2}^{n+1} \\ \vdots \\ \vdots \\ \phi_{\mathrm{hi}-1}^{n+1} \\ \phi_{\mathrm{hi}}^{n+1} \end{pmatrix} = \begin{pmatrix} \phi_{\mathrm{lo}}^{n} \\ \phi_{\mathrm{lo}+1}^{n} \\ \phi_{\mathrm{lo}+2}^{n} \\ \vdots \\ \vdots \\ \phi_{\mathrm{hi}-1}^{n} \\ \phi_{\mathrm{hi}}^{n} + \alpha 2A \end{pmatrix} \tag{16}$$

This can be solved by standard matrix operations, using a tridiagonal solvers (for example).

> *Exercise 1: Write a one-dimensional implicit diffusion solver for the domain $[0, 1]$ with Neumann boundary conditions at each end and $k = 1$. Your solver should use a tridiagonal solver and initialize a matrix like that above. Use a timestep close to the explicit step, a grid with N = 128 zones.*
>
> *If we begin with a Gaussian, the resulting solution is also a Gaussian. Initialize using the following with $t = 0$:*
>
> $$\phi(x,t) = (\phi_2 - \phi_1)\sqrt{\frac{t_0}{t+t_0}}\, e^{-\frac{1}{4}(x-x_c)^2/k(t+t_0)} + \phi_1 \tag{17}$$
>
> *with $t_0 = 0.001$, $\phi_1 = 1$, and $\phi_2 = 2$, and x_c is the coordinate of the center of the domain. Run until $t = 0.01$ and compare to the analytic solution above.*
>
> *(Note: the solution for two-dimensions differs slightly)*

4 Implicit multi-dimensional diffusion via multigrid

Consider a second-order accurate time discretization (this means that the RHS is centered in time), for the multi-dimensional diffusion equation:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{1}{2}\left(k\nabla^2\phi_i^n + k\nabla^2\phi_i^{n+1}\right) \tag{18}$$

This time-discretization is sometimes called *Crank-Nicolson*. Grouping all the $n+1$ terms on the left, we find:

$$\phi_i^{n+1} - \frac{\Delta t}{2}k\nabla^2\phi^{n+1} = \phi^n + \frac{\Delta t}{2}k\nabla^2\phi^n \tag{19}$$

This is in the form of a constant-coefficient Helmholtz equation,

$$(\alpha - \beta\nabla^2)\phi = f \tag{20}$$

with

$$\alpha = 1 \tag{21}$$

$$\beta = \frac{\Delta t}{2}k \tag{22}$$

$$f = \phi_i^n + \frac{\Delta t}{2}k\nabla^2\phi_i^n \tag{23}$$

This can be solved using multigrid techniques with a Helmholtz operator. The same boundary conditions described above apply here. Note: when using multigrid, you do not need to actually construct the matrix.

5 Going Further

non-constant coefficient, how do we put k on edges? average 1/k