1 MAT 228B - Feb/3/2009

The CN method for solving the two-dimensional diffusion equation can be written as follows

$$\left(I - \frac{b\Delta t}{2}L_x - \frac{b\Delta t}{2}L_y\right)u^{n+1} = \left(I + \frac{b\Delta t}{2}L_x + \frac{b\Delta t}{2}L_y\right)u^n.$$

The standard ADI method approximately solves this problem in 2 steps:

$$\begin{aligned}\left(I - \frac{b\Delta t}{2}L_x\right)u^* &= \left(I + \frac{b\Delta t}{2}L_y\right)u^n\\ \left(I - \frac{b\Delta t}{2}L_y\right)u^{n+1} &= \left(I + \frac{b\Delta t}{2}L_x\right)u^*.\end{aligned}$$

Last time, we showed that this numerical scheme is unconditionally stable and second order accurate in time. The ADI system is equivalent to

$$\left(I - \frac{b\Delta t}{2}L_x\right)\left(I - \frac{b\Delta t}{2}L_y\right)u^{n+1} = \left(I + \frac{b\Delta t}{2}L_x\right)\left(I + \frac{b\Delta t}{2}L_y\right)u^n.$$

Assume that we are given some boundary data. To use the ADI scheme, we also need the left and right boundary values of u^*. What to use for u^*? In general fractional step methods, the value of u^* may not have any physical meaning. However, in the ADI scheme, u^* does have a physical meaning. To see this, examine the first step of the ADI scheme. Rearranged, this is

$$\frac{u^* - u^n}{\Delta t/2} = b\left(L_x u^* + L_y u^n\right).$$

This looks like a mix of 1/2-step BE and FE schemes. In fact, u^* approximates the solution at the half time level, $t_{n+1/2}$ and $u^* = u^{n+1/2} + O(\Delta t^2)$. We can use $u^*_{0j} = u^{n+1/2}_{0j}$ and $u^*_{N+1,j} = u^{n+1/2}_{N+1,j}$ for the boundary conditions to have a second order accurate scheme. Another way to find boundary conditions is by deriving an equation for u^* that relates it to the values of the solution. Adding the two equations,

$$\left(I - \frac{b\Delta t}{2}L_y\right)u^{n+1} + \left(I + \frac{b\Delta t}{2}L_y\right)u^n = 2u^*,$$

which holds for any grid points inside the domain. Now we apply this equation at the boundary of the domain to obtain:

$$\begin{aligned}u^*_{0,j} &= \frac{1}{2}\left(I - \frac{b\Delta t}{2}L_y\right)u^{n+1}_{0,j} + \left(I + \frac{b\Delta t}{2}L_y\right)u^n_{0,j}\\ &= \frac{u^n_{0,j} + u^{n+1}_{0,j}}{2} + \frac{b\Delta t}{2}L_y(u^n_{0,j} - u^{n+1}_{0,j}).\end{aligned}$$

which gives us a more accurate boundary condition than simply using the half time level values. However, these two different approaches both give a second-order accurate solution. To show that the two approaches use similar values, compute the Taylor expansion of this last equation in time about the half time level to get

$$u^*_{0,j} = u^{n+1/2}_{0,j} + \mathcal{O}(\Delta t^2).$$

Note that the u^* in LOD scheme does not have a physical interpretation. The LOD scheme is

$$\begin{aligned}\left(I - \frac{b\Delta t}{2}L_x\right) u^* &= \left(I + \frac{b\Delta t}{2}L_y\right) u^n \\ \left(I - \frac{b\Delta t}{2}L_y\right) u^{n+1} &= \left(I + \frac{b\Delta t}{2}L_x\right) u^*.\end{aligned}$$

There are other ADI schemes, e.g. schemes based on backward Euler. In 3D, we have Douglas-Gunn scheme which replaces

$$\left(I - \frac{b\Delta t}{2}L_x - \frac{b\Delta t}{2}L_y - \frac{b\Delta t}{2}L_z\right) u^{n+1} = \left(I + \frac{b\Delta t}{2}L_x + \frac{b\Delta t}{2}L_y + \frac{b\Delta t}{2}L_z\right) u^n$$

by

$$\left(I - \frac{b\Delta t}{2}L_x\right)\left(I - \frac{b\Delta t}{2}L_y\right)\left(I - \frac{b\Delta t}{2}L_z\right) u^{n+1} = \left(I + \frac{b\Delta t}{2}L_x\right)\left(I + \frac{b\Delta t}{2}L_y\right)\left(I + \frac{b\Delta t}{2}L_z\right) u^n.$$

One can show that this approximate factorization introduces a second order error.

1.1 Fractional Step Schemes

Next we discuss the general idea of the fractional step schemes. Both ADI and LOD are examples of fractional step schemes. The spirit of a fractional step scheme is to include some terms of the PDE to solve for an intermediate solution, u^*, and then take another step with other terms to get u^{n+1}. Fractional stepping is useful for equations such as reaction-diffusion equations:

$$u_t = b\Delta u + R(u).$$

The term $b\Delta u$ represents the transportation of the heat/concentration by diffusion and $R(u)$ represents chemical reactions. We know how to solve diffusion equations and we know how to handle the reactions (just ODEs), and fractional stepping allows us to use these solvers separately to solve this type of equation.

Example 1.1. Fisher's equation:

$$u_t = bu_{xx} + ku(1-u).$$

If we have a multiple chemical species, let $\underline{q} = (u_1, \cdots, u_N)$ denote the vector whose components represent different species, then we have the system

$$\underline{q}_t = D\Delta\underline{q} + R(\underline{q}),$$

where $D = \mathrm{diag}(D_1, \cdots, D_N)$ is a diagonal matrix whose diagonals $D_j \geq 0$ and $D_i \neq 0$ for some i. How to solve this equation numerically? Try the CN scheme:

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{b}{2}(Lu^{n+1} + Lu^n) + \frac{1}{2}(R(u^{n+1}) + R(u^n)).$$

Then

$$\left(I - \frac{b\Delta t}{2}L\right) u^{n+1} - \frac{\Delta t}{2}R(u^{n+1}) = \left(I + \frac{b\Delta t}{2}L\right) u^{n+1} + \frac{\Delta t}{2}R(u^n).$$

In general, we get a nonlinear equation. How to solve the nonlinear equation? One idea is to use Newton's method. Consider the scalar problem $f(u) = 0$. Newton's method is an iterative scheme in which the problem is linearized about the current solution, and the zero of the linearized problem gives the next approximate solution. Specifically, the iteration is

$$u^{k+1} = u^k - \frac{f(u^k)}{f'(u^k)}.$$

Rearranging this equation,

$$f'(u^k)(u^{k+1} - u^k) = -f(u^k).$$

Now we can generalize Newton's method to systems:

$$J^k \delta = -f(u^k), \quad u^{k+1} = u^k + \delta,$$

where J^k is the Jacobian matrix of f at u^k. Returning to the reaction-diffusion equations. We want to solve $F(u^{n+1}) = 0$, where

$$F(v) = \left(I - \frac{b\Delta t}{2} L\right) v - \frac{\Delta t}{2} R(v) - \left(I + \frac{b\Delta t}{2} L\right) u^n - \frac{\Delta t}{2} R(u^n).$$

The linearization of F can be easily calculated as

$$J(v) = \left(I - \frac{b\Delta t}{2} L\right) - \frac{b\Delta t}{2} R'(v) I.$$

To solve $F(v) = 0$, we must iterate

$$\begin{aligned} J^k \delta &= -F(u^{n+1,k}) \\ u^{n+1,k+1} &= u^{n+1,k} + \delta \end{aligned}$$

until $|\delta| < \text{tol}$.

Another way to solve this nonlinear equation is to use so-called fractional stepping. The idea behind this scheme is that we alternate updating diffusion and reaction. The diffusion equation is stiff; eigenvalues range from $\mathcal{O}(1)$ to $\mathcal{O}(h^{-2})$. What if the reactions are not stiff? We update $u^n \to u^*$ by solving the diffusion equation,

$$\frac{du}{dt} = Lu$$

for one time step and then $u^* \to u^{n+1}$ by including only the reactions

$$\frac{du}{dt} = R(u).$$

Now we can use a non-stiff method e.g. RK or AB. What if we use a second order scheme to find u^* and u^{n+1}? Is the solution second order accurate? In general, the answer is no. The solution is first order accurate because the splitting of the scheme introduces a first order error.