

# 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 is to solve 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. To use the ADI scheme is equivalent to solve

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

Assume that we are given some boundary data. To use ADI scheme, we also need the left and right boundary values of  $u^*$ . What to use for  $u^*$ ? Usually,  $u^*$  may not be physical. In ADI scheme,  $u^*$  has its physical meaning and we can find out the physical interpretation of  $u^*$ . To see this, let us look at the first step of ADI scheme. Write

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

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  $u_{0,j}^* = u_{0,j}^{n+1/2}$  and  $u_{N+1,j}^* = u_{N+1,j}^{n+1/2}$  for the boundary conditions to have a second order accurate scheme. Another way to derive boundary conditions for  $u^*$  is adding both of the equations. We find

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

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

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

which gives us not only a more accurate boundary condition but also a second order error. Taylor series of  $u^*$  in time about the half time level shows that

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

Note that the  $u^*$  in LOD scheme is not physical. Here the LOD scheme is presented as follows

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

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

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

by

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

## 1.1 Fractional Step Scheme

Now let us introduce a new scheme, the fractional step scheme. The spirit of the fractional step scheme is that to solve the PDE, we take a step including some terms,  $u^*$ , and then take another step with other terms to get  $u^{n+1}$ . Now we take a look at an example of where this scheme is useful-reaction diffusion equation, i.e. the equation of the form

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

$b\Delta u$  presents the transportation of the heat/concentration by diffusion and  $R(u)$  presents chemical reaction.

**Example 1.1.** Fisher's equation:

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

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

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

where  $D = \text{diag}(D_1, \dots, D_N)$  is a diagonal matrix whose diagonals  $D_j \geq 0$  and  $D_i \neq 0$  for some  $i$ . How to solve this equation numerically? Let us try 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 that we can use the Newton's method. Let us solve the scalar problem  $f(u) = 0$  by Newton's method. The Newton's method is presented in the following recursive relation

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

Rearranging this equation we find

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

Now we can generalize Newton's method to high dimensional cases:

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

for some  $\delta$  to be determined and  $J^k$  is the Jacobian matrix of  $f$  at  $u^k$ . Let's go back to our reaction-diffusion equations. We want to solve  $F(u^{n+1}) = 0$ , where

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

The linearization of  $F$  can be easily calculated and equals to

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

which requires one iteration for each time step. Hence we need to solve

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

which loop 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 are  $\mathcal{O}(h^{-2})$ . What if the reactions are not stiff? We update  $u^n \rightarrow u^*$  by solving the diffusion equation,

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

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

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

Now we can use a non-stiff method e.g. RK and 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.