Math 660-Lecture 9: FDM for mixed type equations

In practice, the physical models contain several effects. For example, the advection-diffusion equation
\[ u_t + au_x = \nu u_{xx} \]
is parabolic, but besides the diffusion effect due to the parabolic equations, it also contains the advection effect owned by the hyperbolic equations.

Another example is the following advection-reaction equation:
\[ u_t + au_x = -\lambda u. \]

Reaction-diffusion equation
\[ u_t = \Delta u - \lambda f(u). \]

The numerical methods for these equations can generally be classified into unsplitting methods and time-splitting methods (also called fractional step methods). We first discuss the unsplitting methods.

1 Unsplit methods for mixed type equations

1.1 Method of lines, Direct methods

We’ll take the advection-diffusion equation as the example
\[ u_t + au_x = \nu u_{xx}. \]

If we apply the centered difference in space and forward Euler in time, we have
\[ \frac{u_j^{n+1} - u_j^n}{k} + a\frac{u_{j+1}^n - u_{j-1}^n}{2h} = \nu\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}. \]

Let’s say \( \lambda = ak/h, \mu = \nu k/h^2 \). The LTE is \( O(k + h^2) \). The amplification factor using von-Neumann analysis is
\[ g(\xi) = 1 - i\lambda \sin(h\xi) - 2\mu(1 - \cos(h\xi)). \]

The conditions for \( |g| \leq 1 \) are given by
\[ 2\mu \geq \lambda^2, \quad 2\mu \leq 1. \]
\( \nu k/h^2 \leq 1/2 \) and \( k \leq 2\nu/a^2 \). The modified equation of this numerical scheme to the leading order is given by

\[
 u_t + au_x = (\nu - \frac{1}{2}a^2k)u_{xx}.
\]

Hence, the numerical diffusion is less than the real diffusion. One can instead use

\[
 \frac{u_{j}^{n+1} - u_{j}^{n}}{k} + a\frac{u_{j+1}^{n} - u_{j-1}^{n}}{2h} = (\nu + \frac{1}{2}a^2k)\frac{u_{j+1}^{n} - 2u_{j}^{n} + u_{j-1}^{n}}{h^2}.
\]

For this modified method, the stability condition is \( \nu k/h^2 + \frac{1}{2}(ak/h)^2 \leq 1/2 \).

Another method is to use the upwind scheme for advection and centered difference for diffusion. Consider \( a > 0 \). We have:

\[
 \frac{u_{j}^{n+1} - u_{j}^{n}}{k} + a\frac{u_{j}^{n} - u_{j-1}^{n}}{h} = \nu\frac{u_{j+1}^{n} - 2u_{j}^{n} + u_{j-1}^{n}}{h^2}.
\]

This is equivalent to adding the numerical viscosity \( ah/2 \) for the centered difference. The stability condition is

\[
 (\nu + \frac{1}{2}ah)\frac{k}{h^2} \leq 1/2.
\]

Comments on the MOL.

### 1.2 Implicit-explicit methods (IMEX)

In the diffusion-advection equation, we don’t want the requirement \( k = O(h^2) \) caused by the stiffness of diffusion. Consider generally that

\[
 u_t = A(u) + B(u),
\]

where \( A \) is stiff while \( B \) is not stiff. Then, we can apply implicit schemes for \( A \) and explicit schemes for \( B \). This is convenient if \( A \) is linear and easy to invert. For example, for the advection-diffusion equation, we can apply Crank-Nicolson for the diffusion term and upwind for the advection term.

\[
 \frac{u_{j}^{n+1} - u_{j}^{n}}{k} + a\frac{u_{j}^{n} - u_{j-1}^{n}}{h} = \nu\frac{1}{2}\left\{ \frac{u_{j+1}^{n} - 2u_{j}^{n} + u_{j-1}^{n}}{h^2} + \frac{u_{j+1}^{n+1} - 2u_{j}^{n+1} + u_{j-1}^{n+1}}{h^2} \right\}.
\]

Now, let’s focus on the following Allen-Cahn equation as the example, which is a diffusion-reaction equation

\[
 u_t = \Delta u + \lambda u(1 - u^2) = \Delta u - \lambda f(u).
\]
The term \( Au = \Delta u \) is linear but stiff. The term \( B(u) = -\lambda u(1 - u^2) \) is not stiff but nonlinear.

Define the energy functional

\[
E(u) = \frac{1}{2} \int |\nabla u|^2 dx + \int \lambda F(u) dx,
\]

where \( F(u) = \int u f(s) ds = (\frac{1}{3} u^4 - \frac{1}{2} u^2) \). The equation is clearly

\[
 u_t + \frac{\delta E}{\delta u} = 0.
\]

The energy \( E \) is a Lyapunov functional and

\[
\frac{dE}{dt} = \int \delta E \delta u_t dx = - \int (\frac{\delta E}{\delta u})^2 dx \leq 0.
\]

According to the stiffness of the diffusion property, we hope to make \( A \) implicit while keep \( B \) explicit. Besides, we want to make sure that the discrete energy also decreases. To start with, let’s try the following scheme:

\[
\frac{1}{k}(u^{n+1} - u^n) = \Delta_h u^{n+1} - \lambda f(u^n).
\]

Let’s investigate the stability of this method using energy strategy. Multiplying \( h(u^{n+1} - u^n) \) and taking the sum. The summation by parts \( \langle D_+ u, v \rangle = -\langle u, D_- v \rangle \) gives

\[
\sum h \Delta_h u^{n+1}(u^{n+1} - u^n) = -\sum h D_- u^{n+1}(D_- u^{n+1} - D_- u^n)
\]

\[
= -\|D_- u^{n+1}\|^2 + \frac{1}{2}(\|D_- u^{n+1}\|^2 + \|D_- u^n\|^2 - \|D_- u^{n+1} - D_- u^n\|^2)
\]

For the other term:

\[
f(u^n)(u^{n+1} - u^n) = F(u^{n+1}) - F(u^n) - \frac{1}{2} f'(\xi)(u^{n+1} - u^n)^2.
\]

Hence, we obtain

\[
(\frac{1}{2}\|D_- u^{n+1}\|^2 + \lambda \sum_j h F(u^{n+1})) - (\frac{1}{2}\|D_- u^n\|^2 + \lambda \sum_j h F(u^n))
\]

\[
\leq -\frac{1}{2}\|D_- u^{n+1} - D_- u^n\|^2 + \frac{1}{2} \lambda \sup_{|\xi| \leq M} |f'(\xi)| - \frac{1}{k}\|u^{n+1} - u^n\|^2.
\]
where $M$ is the bound for the solution $u$. The method is stable if $k \leq \frac{2}{\lambda}(\sup |f'|)^{-1}$.

Exercise: What if $\lambda$ is big such that the nonlinear term is also stiff? See the homework.

The restriction $k \leq \frac{2}{\lambda}(\sup |f'|)^{-1}$ may be too serious sometimes. Another idea is to use the so-called convex-concave splitting. The idea is to decompose the energy functional $E$ into two parts $E = E_c - E_e$ such that both $E_c$ and $E_e$ are convex. Then, define $\tilde{A}(u^{n+1}) = -\frac{\delta E_c}{\delta u}|_{u=u^{n+1}}$ and $\tilde{B}(u^n) = \frac{\delta E_e}{\delta u}|_{u=u^n}$. Under this splitting,

$$\frac{1}{k}(u^{n+1} - u^n) = -\frac{\delta E_c}{\delta u}|_{u=u^{n+1}} + \frac{\delta E_e}{\delta u}|_{u=u^n}.$$

The method then is unconditionally stable (in the energy norm sense).

Proof. For a convex energy functional $\tilde{G}$, we have

$$\{\frac{\delta \tilde{G}}{\delta u}|_{u=u^n}, u^{n+1} - u^n\} \leq \tilde{G}(u^{n+1}) - \tilde{G}(u^n) \leq \{\frac{\delta \tilde{G}}{\delta u}|_{u=u^{n+1}}, u^{n+1} - u^n\}.$$

$$E_h(u^{n+1}) - E_h(u^n) = (E_{c,h}(u^{n+1}) - E_{c,h}(u^n)) - (\tilde{E}_e(u^{n+1}) - \tilde{E}_e(u^n))$$

$$\leq \{\frac{\delta E_c}{\delta u}|_{u=u^{n+1}, u^{n+1} - u^n} - \frac{\delta \tilde{E}_e}{\delta u}|_{u=u^n, u^{n+1} - u^n}\} = -\frac{1}{k}(u^{n+1} - u^n, u^{n+1} - u^n) \leq 0.$$

\hfill\Box

In our case, we can split the energy into $\frac{1}{2} \int (|\nabla u|^2 + \mu u^2)dx + \int (\lambda F(u) - \frac{1}{2}\mu u^2)$. By the maximum principle of parabolic theory, $|u| \leq M$ is bounded. Hence, if $\mu$ is sufficiently large ($\mu \geq \lambda \sup_{|\xi| \leq M} |f'(\xi)|$), the second term will be concave. The numerical scheme is

$$\frac{1}{k}(u^{n+1} - u^n) = (\Delta_h u^{n+1} - \mu u^n) + (\mu u^n - \lambda f(u^n)).$$

Remark 1. By the proof above, we actually only need $\mu \geq \frac{\lambda}{2} \sup_{|\xi| \leq M} |f'(\xi)|$ for it to be stable but the second energy functional may not be concave.

1.3 Exponential time differencing methods

For the equation $u_t = f(u)$, on $[t^n, t^{n+1}]$, decompose $f(u) = A_n u(t) + B_n(u(t))$ where $A_n$ is a constant, linear, Markovian operator, and $B_n$ only depends on the state at time $t$. Then Duhamel’s principle gives

$$u(t^{n+1}) = e^{A_n t^{n+1}} + \int_{t^n}^{t^{n+1}} e^{A_n (t^{n+1} - \tau)} B_n(u(\tau)) d\tau.$$
The simplest method is to approximate $B_n(u(\tau)) \approx B_n(u^n)$ and have

$$u^{n+1} = u^n + A_n^{-1}(e^{A_n k} - I)f(u^n).$$

Read P240 for more discussions.