Math 6008 Numerical PDEs–Lecture 11

Mixed type equations

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1 Nonlinear parabolic problems (continuation of the previous lecture)

For nonlinear problems,

$$\partial_t u = f(x, t, u, \partial_x u, \partial_{xx} u),$$

often the explicit discretization

$$\frac{u_j^{n+1} - u_j^n}{\tau} = f(x_j, t_n, \frac{u_{j+1}^n - u_{j-1}^n}{2h}, D^2 u_j^n)$$

has severe constraints on the time step for stability. Determining the stability conditions is complicated (may even depend on the value of the solution). Moreover, the usual case is that the implicit method is stable:

$$\frac{u_j^{n+1} - u_j^n}{\tau} = f(x_j, t_n, \frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2h}, D^2 u_j^{n+1}).$$

The drawback is that such method is very hard to solve for u^{n+1}.

Below we introduce the **Richtmyer** linearization using an example. Consider

$$\partial_t u = \partial_{xx}(u^5).$$

Note that the right hand side is a function of u, u_x, u_{xx}. In fact $\partial_{xx}(u^5) = 20u^3 u_x^2 + 5u^4 u_{xx}$.

If we use the centered difference for space and the trapezoidal rule for time discretization for better stability, one has

$$\frac{u_j^{n+1} - u_j^n}{\tau} = \frac{1}{h^2}[\theta \delta_x^2 (u^5)_j^{n+1} + (1-\theta)\delta_x^2 (u^5)_j^n].$$

This is a nonlinear equation for u_j^{n+1}. Solving it can be challenging. To solve this problem, Richtmyer introduced the following linearization procedure:

$$u(x_j, t_{n+1})^5 = u(x_j, t_n)^5 + 5\tau u(x_j, t_n)^4 \partial_t u(x_j, t_n) + R(x_j, t_n)\tau^2.$$

Approximating

$$\partial_t u = \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\tau} + \bar{R}(x_j, t_n)\tau,$$

and substituting this back into the equation, the equation becomes linear in u^{n+1} **given** u^n:

$$\frac{u_j^{n+1} - u_j^n}{\tau} - \frac{5\theta}{h^2}[(u_{j+1}^n)^4(u_{j+1}^{n+1} - u_{j+1}^n) - 2(u_j^n)^4(u_j^{n+1} - u_j^n) + (u_{j-1}^n)^4(u_{j-1}^{n+1} - u_{j-1}^n)] = \frac{1}{h^2}\delta^2(u^5)_j^n.$$

The truncation error is

$$O(\tau + h^2).$$

Here, it seems that there is error $O(\tau^2)$ in the numerator so that the error would be τ^2/h^2. The reason that there is no such term because the error in the numerator is of the form $v(x_j)\tau^2$ for smooth function $v(x_j)$. Applying the centered finite difference for it will not give an extra $1/h^2$.

This scheme can be solved by first viewing

$$w_j := u_j^{n+1} - u_j^n$$

as a variable. After this is solved, one can recover u_j^{n+1}.

The PDE is equivalent to the following:

$$\partial_t u = \partial_x(5u^4 \partial_x u).$$

This is a conservative form, with flux

$$J = -5u^4 \partial_x u.$$

The stability of the θ-method above with Richtmyer linearization could be roughly be obtained by the stability condition for the θ-method for this form, by regarding $5u^4$ as the coefficient and the frozen coefficient approach. This of course is only an intuition, not a rigorous method.

The consequence is that: if $\theta \geq 1/2$, it is unconditionally stable while $\theta \leq 1/2$, one needs

$$5\sup_j(u_j^4)\mu \leq \frac{1}{2-4\theta}, \quad \mu = \frac{\tau}{h^2}.$$

Remark 1. *We remark that the method above is not the same by regarding $5u^4$ as the coefficient and applying the θ-method*

$$\begin{aligned}\frac{u_j^{n+1}-u_j^n}{\tau} &= \theta\frac{5(u_{j+1/2}^n)^4 u_{j+1}^{n+1} - 5((u_{j+1/2}^n)^4 + (u_{j-1/2}^n)^4)u_j^{n+1} + 5(u_{j-1/2}^n)^4 u_{j-1}^{n+1}}{h^2} \\ &+ (1-\theta)\frac{5(u_{j+1/2}^n)^4 u_{j+1}^{n} - 5((u_{j+1/2}^n)^4 + (u_{j-1/2}^n)^4)u_j^{n} + 5(u_{j-1/2}^n)^4 u_{j-1}^{n}}{h^2}.\end{aligned}$$

In fact, in this scheme, one in fact has the following

$$\frac{u_j^{n+1}-u_j^n}{\tau} - \theta\tau\delta(5u^4\partial_t\delta u) = \frac{5(u_{j+1/2}^n)^4 u_{j+1}^{n} - 5((u_{j+1/2}^n)^4 + (u_{j-1/2}^n)^4)u_j^{n} + 5(u_{j-1/2}^n)^4 u_{j-1}^{n}}{h^2},$$

but the scheme in the Richtmyer linearization is

$$\frac{u_j^{n+1}-u_j^n}{\tau} - \theta\tau\frac{1}{h^2}\delta^2(5u^4\partial_t u) = \frac{1}{h^2}\delta^2(u^n)^5.$$

The right hand side can be viewed as roughly equivalent. The term for θ are different in the $O(\tau)$ order!

2 Mixed equations

In practice, several physical processes could take place simultaneously. The PDE model would not be a pure equation of the type we have investigated. Instead, it would be a mixed equaiton.

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.

Other examples is the following advection-reaction equation:

$$u_t + au_x = -\lambda u,$$

or the reaction-diffusion equation

$$u_t = \Delta u - \lambda f(u).$$

A more general advection-diffusion-reaction equation could be

$$\partial_t u + f(u)_x = \kappa u_{xx} + R(u).$$

Other famous models include the KdV equation

$$\partial_t u + uu_x = \nu u_{xxx},$$

where the dispersion effect and the nonlineary take place at the same time. The dispersion term is very stiff and has strong dispersion effects (eigenvalues are imaginary). The interplay between them would result in the so-called solitons (a very stable nonlinear wave, like the tsunami).

There are many approaches developed for these models, and some of them are specialized for particular problems. In this lecture, we will take a brief look at some typical approaches. Roughly speaking, we will introduce the following methods.

- The IMEX method, including the convex-concave splitting for gradient flows.
- Time splitting, or fractional step methods. This has been explained and we omit it here.
- The exponential differentiation.

3 The implicit-explicit methods

We first check the method of lines type methods and understand why sometimes it is not suitable for mixed type problems. Then, we move to the IMEX methods.

3.1 Method of lines, Direct methods

We 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 us say $\lambda = a\tau/h$, $\mu = \nu\tau/h^2$. The LTE is $O(\tau + h^2)$. The growth factor using von-Neumann analysis is

$$G(\xi) = 1 - i\lambda\sin(h\xi) - 2\mu(1 - \cos(h\xi)).$$

Explicit computation shows that

$$|G|^2 = 1 - (1 - \cos(\xi h))[4\mu - 4\mu^2(1 - \cos\xi h) - \lambda^2(1 + \cos\xi h)].$$

Hence, if

$$4\mu - 4\mu^2(1 - \cos\xi h) - \lambda^2(1 + \cos\xi h) \geq 0,$$

one has $|G| \leq 1$. Since $\zeta := \cos(\xi h) \in [-1, 1]$, the requirement is thus (by taking $\zeta = -1$ or $\zeta = 1$ as the formula linearly depends on ζ)

$$4\mu - 8\mu^2 \geq 0,\ 4\mu - 2\lambda^2 \geq 0.$$

Hence,

$$2\mu \geq \lambda^2, \quad 2\mu \leq 1.$$

$\nu\tau/h^2 \leq 1/2$ and $\tau \leq 2\nu/a^2$.

We see that the second constraint is not good for ν small. For example, if the temperature is low and the diffusion effect is small, then τ must be small. The reason is that the advection term is not discretized suitably. In fact, the modified equation of this numerical scheme to the leading order is given by

$$u_t + au_x = (\nu - \frac{1}{2}a^2\tau)u_{xx}.$$

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

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_{j+1}^n - u_{j-1}^n}{2h} = (\nu + \frac{1}{2}a^2\tau)\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}.$$

For this modified method, the accuracy is still $O(\tau + h^2)$. The stability condition is obtained by replacing ν with $\nu + \frac{1}{2}a^2\tau$. The constraint for small ν is improved!

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

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_j^n - u_{j-1}^n}{h} = \nu\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}.$$

This is equivalent to adding the numerical viscosity $ah/2$ for the centered difference. The stability condition is obtained by replacing ν with $\nu + \frac{1}{2}ah$.

$$(\nu + \frac{1}{2}ah)\frac{\tau}{h^2} \leq 1/2.$$

This condition is slightly better than the above constraints and there is no much constraint for small ν. However, one still needs $\tau \sim h^2$.

If we use the implict method like Cranck-Nicolson, the advection is also treated implicitly. In the MOL type schemes, all the terms are made explicit or implicit at the same time.

- If we use explicit schemes, the stiff terms put severe contraints as we have seen.
- If we use implicit schemes, some other non-stiff terms are also implicit, which is not necessary.

Hence, in practice, we do not always use MOL type schemes, we would consider the following IMEX schemes

3.2 Implicit-explicit methods (IMEX)

In the diffusion-advection equation, we do not want the requirement $\tau = O(h^2)$ 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.

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_j^n - u_{j-1}^n}{h} = \nu\frac{1}{2}\left\{\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} + \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{h^2}\right\}.$$

Now, let us now 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 $F(u) = \int^u f(s)ds = (\frac{1}{4}u^4 - \frac{1}{2}u^2)$. The equation is clearly

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

The energy E is a Lyapunov functional and

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

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:

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

Let us 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

$$\sum h\Delta_h u^{n+1}(u^{n+1}-u^n)=-\sum hD_-u^{n+1}(D_-u^{n+1}-D_-u^n)$$
$$=-\|D_-u^{n+1}\|^2+\frac{1}{2}(\|D_-u^{n+1}\|^2+\|D_-u^n\|^2-\|D_-u^{n+1}-D_-u^n\|^2)$$

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

$$(\frac{1}{2}\|D_-u^{n+1}\|^2+\lambda\sum_j hF(u^{n+1}))-(\frac{1}{2}\|D_-u^n\|^2+\lambda\sum_j hF(u^n))$$
$$\le -\frac{1}{2}\|D_-u^{n+1}-D_-u^n\|^2+(\frac{1}{2}\lambda\sup_{|\xi|\le M}|f'(|\xi|)|-\frac{1}{\tau})\|u^{n+1}-u^n\|^2.$$

where M is the bound for the solution u. The method is stable if $\tau\le \frac{2}{\lambda}(\sup|f'|)^{-1}$. This condition is much better. However, if λ is big such that the nonlinear term is also stiff? One would consider other methods.

The concave-convex splitting**(Free reading)

The restriction $\tau\le\frac{2}{\lambda}(\sup|f'|)^{-1}$ 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 $\tilde{B}(u^n)=\frac{\delta\tilde{E}_e}{\delta u}|_{u=u^n}$. Under this splitting,

$$\frac{1}{\tau}(u^{n+1}-u^n)=-\frac{\delta E_c}{\delta u}|_{u=u^{n+1}}+\frac{\delta\tilde{E}_e}{\delta u}|_{u=u^n}$$

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

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

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

$$E_h(u^{n+1}) - E_h(u^n) = (E_{c,h}(u^{n+1}) - E_{c,h}(u^n)) - (\tilde{E}_e(u^{n+1}) - \tilde{E}_e(u^n))$$
$$\le \langle \frac{\delta E_c}{\delta u}|_{u=u^{n+1}}, u^{n+1} - u^n \rangle - \langle \frac{\delta \tilde{E}_e}{\delta u}|_{u=u^n}, u^{n+1} - u^n \rangle = -\langle \frac{1}{\tau}(u^{n+1} - u^n), u^{n+1} - u^n \rangle \le 0.$$

□

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, $|u| \le M$ is bounded. Hence, if μ is sufficiently large ($\mu \ge \lambda \sup_{|\xi| \le M} |f'(\xi)|$), the second term will be concave. The numerical scheme is

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

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

4 Time splitting method (fractional step method)

4.1 The basic splitting

Consider the equation

$$u_t = A(u) + B(u),$$

where A, B are two spatial operators. The idea of the fractional step method is to solve the following two equations from t^n to t^{n+1}:

$$u_t = A(u) \Rightarrow u^n \to u^*$$
$$u_t = B(u) \Rightarrow u^* \to u^{n+1}.$$

Theorem 1. *If A and B are linear bounded, constant operators, then the splitting error is of first order.* **If A and B commute, then there's no splitting error.**

The argument is easy to make. By the methods, we have

$$u^* = e^{\tau A}u^n, \quad u^{n+1} = e^{\tau B}u^* = e^{\tau B}e^{\tau A}u^n.$$

For the original equation, we should have

$$u(t^{n+1}) = e^{\tau(A+B)}u(t^n).$$

By the definition of exponential of operators, we have

$$\begin{aligned}
e^{\tau(A+B)} &= I + \tau(A+B) + \frac{1}{2}\tau^2(A+B)^2 + O(\tau^3) \\
&= I + \tau(A+B) + \frac{1}{2}\tau^2(A^2 + AB + BA + B^2) + O(\tau^3)
\end{aligned}$$

Similarly,

$$\begin{aligned}
e^{\tau A} &= I + \tau A + \frac{1}{2}\tau^2 A^2 + O(\tau^3) \\
e^{\tau B} &= I + \tau B + \frac{1}{2}\tau^2 B^2 + O(\tau^3).
\end{aligned}$$

Hence,

$$\begin{aligned}
e^{\tau B}e^{\tau A} &= (I + \tau B + \frac{1}{2}\tau^2 B^2 + O(\tau^3))(I + \tau A + \frac{1}{2}\tau^2 A^2 + O(\tau^3)) \\
&= I + \tau A + \tau B + \frac{1}{2}\tau^2 A^2 + \frac{1}{2}\tau^2 B^2 + \tau^2 BA + O(\tau^3)
\end{aligned}$$

Assuming that $u^n = u(t^n)$, we find the local truncation error is

$$LTE = \frac{1}{\tau}(u^{n+1} - u(t^{n+1})) = \frac{1}{\tau}\Big(I + \tau A + \tau B + \frac{1}{2}\tau^2 A^2 + \frac{1}{2}\tau^2 B^2 + \tau^2 BA + O(\tau^3)$$
$$-(I + \tau(A+B) + \frac{1}{2}\tau^2(A^2 + AB + BA + B^2) + O(\tau^3))\Big)u^n = \frac{1}{2}\tau(BA - AB)u^n + O(\tau^2).$$

Splitting method decouples the problem into two problems and each may be solved easily. Also, spitting makes the numerical method much easier and we may have less constraints for the stability requirement.

A disadvantage of fractional step method is that we may have issue for the boundary conditions of u^*. If the boundary conditions for u is 0 for all time $t = 0$, then we may apply the same boundary condition for u^*. For other cases, we should treat this problem carefully, as u^* is not a physical quantity.

These features can be seen by the LOD method for the 2D heat equation.

One example

Consider the advection-reaction equation:

$$u_t + a(x)u_x = -\lambda u, \quad a(x) \geq 0.$$

If we don't split, we probably want to do

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a_j \frac{u_j^n - u_{j-1}^n}{h} = -\lambda u_j^{n+1}.$$

If we do splitting, then we have:

- Problem A: $u_t + a(x)u_x = 0$.
- Problem B: $u_t = -\lambda u$.

The first can be solved using the upwind scheme while the second can be solved exactly:

$$\begin{aligned} \frac{u_j^* - u_j^n}{\tau} &= -a_j \frac{u_j^n - u_{j-1}^n}{h}, \\ u_j^{n+1} &= \exp(-\tau\lambda) u_j^*. \end{aligned}$$

Another example is the viscous Burger's equation:

$$u_t + uu_x = \nu u_{xx}.$$

Then, we can split it into two subproblems.

$$u_t = \nu u_{xx}$$

and

$$u_t + uu_x = 0.$$

For the diffusion part, the term is stiff but linear, we can use implicit scheme like the Cranck-Nicolson method. For the advection term, it is the Burger's equation, a nonlinear hyperbolic conservation law. To capture the correct physics when the shock forms, we use the conservative form and the finite volume method

$$\partial_t u + (\frac{u^2}{2})_x = 0$$

and use certain flux to approximate.

4.2 Strang splitting

To improve the accuracy of the splitting method, we may use the following Strang splitting:

$$\begin{aligned} u_t &= A(u), \text{ for time } \tau/2, \\ u_t &= B(u), \text{ for time } \tau, \\ u_t &= A(u), \text{ for time } \tau/2. \end{aligned}$$

By direct Taylor expansion, one can show that the local truncation error for this method is $O(\tau^2)$.

In real implementation, we do not solve the three steps for one time interval with length τ. The observation

$$\begin{aligned} &(\exp(\frac{1}{2}\tau A)\exp(\tau B)\exp(\frac{1}{2}\tau A))^n \\ &\qquad = \exp(\frac{1}{2}\tau A)\exp(\tau B)(\exp(\tau A)\exp(\tau B))^{n-1}\exp(\frac{1}{2}\tau A), \end{aligned}$$

allows us to solve two steps essentially for one time interval.

5 Exponential time differencing methods **(free reading)

In the IMEX method, we make one of the operators implicit. As well-known, the implicit method often introduce numerical viscosity that is non-physical diffusion. Sometimes people want less non-physical diffusion, so the exponential time differencing methods might be used.

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 consant, linear operator and B_n only depends on the state at time t. Then Duhamel's principle gives

$$u(t^{n+1}) = e^{A_n \tau} u^n + \int_{t^n}^{t^{n+1}} e^{A_n(t^{n+1}-s)} B_n(u(s)) ds.$$

The simplest method is to approximate $B_n(u(s)) \approx B_n(u^n)$ and have

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

One typical choice is

$$A_n = f'(U^n).$$

ETD could be suitable for stiff problems. Compared implicit methods, it has less non-physical numerical dissipation, which is sometimes desired.

Read P240 of the book by Leveque for more discussions.