Math 6008 Numerical PDEs–Lecture 9
More on FDM for hyperbolic equations

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1 Second order hyperbolic equations: wave equation

Consider the wave equation

$$u_{tt} = a^2 u_{xx},$$
$$u(x,0) = f(x), \quad u_t(x,0) = g(x).$$

Previously, we introduced the equivalent system

$$\partial_t u + \frac{a^2}{\rho_0}\partial_x \rho = 0,$$
$$\partial_t \rho + \rho_0 \partial_x u = 0.$$

To solve this, the initial condition should be given as

$$\rho(x,0) = \int^x g(y)dy.$$

This is not very convenient for multi-dimension cases.

If we introduce $v = u_t, w = au_x$, we have the first order system of equations

$$v_t - aw_x = 0$$
$$w_t - av_x = 0.$$

We introduce

$$A = \begin{bmatrix} 0 & -a \\ a & 0 \end{bmatrix}, \quad \boldsymbol{u} = \begin{bmatrix} v(x,t) \\ w(x,t). \end{bmatrix}$$

We can solve the system. After this is solved, we may integrate of v in time t to recover u.

1.1 Discretizing the equivalent system

We discretize the first order system using L-F, Lax-Wendroff, Upwind schemes direction. These can be performed directly except that for upwind schemes we need to look at the eigen-directions.

For example, the Lax-Friedrichs scheme is given by

$$\boldsymbol{u}_j^{n+1} = \frac{1}{2}(\boldsymbol{u}_{j+1}^n + \boldsymbol{u}_{j-1}^n) - \frac{1}{2}\lambda A(\boldsymbol{u}_{j+1}^n - \boldsymbol{u}_{j-1}^n).$$

The stability condition has been discussed,

$$a\lambda \leq 1.$$

1.2 Discretizing directly

Here, we use the simplest scheme:

$$\frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{\tau^2} - a^2\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} = 0.$$

The boundary condition u_t can be approximated by the **ghost point** method.

First of all, let us consider the CFL condition. The PDE has two characteristic speeds. One is $dx/dt = a$ and one is $dx/dt = -a$. By D'Alembert formula, the interval of dependence is $[x - an\tau, x + an\tau]$ on the initial axis. Consider the numerical solution, the interval of dependence is between $[x_j - nh, x_j + nh]$. Hence, the CFL condition implies

$$a\tau \leq h \Rightarrow a\lambda \leq 1.$$

Let's derive the accurate condition using von-Neumann analysis, which is $\frac{a\tau}{h} < 1$.

The growth matrix

Introducing

$$v_j^n = \frac{u_j^n - u_j^{n-1}}{\tau}, \qquad w_{j+1/2}^n = a\frac{u_{j+1}^n - u_j^n}{h}.$$

The the scheme can be rewritten as

$$\begin{aligned}\frac{v_j^{n+1}-v_j^n}{\tau}-a\frac{w_{j+1/2}^n-w_{j-1/2}^n}{h}&=0\\ \frac{w_{j-1/2}^{n+1}-w_{j-1/2}^n}{\tau}-a\frac{v_j^{n+1}-v_{j-1}^{n+1}}{h}&=0.\end{aligned}$$

By doing so, we have a two-time level scheme. Then, $v_j^n = v^n e^{ix_j\xi}$ and $w_j^n = w^n e^{ix_j\xi}$. Then, we have

$$\begin{aligned}\frac{v^{n+1}-v^n}{\tau}-a\frac{w^n 2i\sin(\frac{1}{2}\xi h)}{h}&=0\\ \frac{w^{n+1}-w^n}{\tau}-a\frac{v^{n+1}2i\sin(\frac{1}{2}\xi h)}{h}&=0.\end{aligned}$$

Letting $c=\frac{2a\tau}{h}\sin(\frac{1}{2}\xi h)$, we have

$$\begin{aligned}v^{n+1}&=v^n+icw^n\\ w^{n+1}&=icv^n+(1-c^2)w^n.\end{aligned}$$

The growth matrix is

$$G(\xi)=\begin{bmatrix}1 & ic\\ ic & 1-c^2\end{bmatrix}. \tag{1}$$

The e-vals satisfy $\mu^2-(2-c^2)\mu+1=0$. We need $|\mu|\le 1$. The product is 1 hence both eigenvalues must have magnitude 1. $(2-c^2)=\mu+\mu^{-1}=2\cos(\theta)$. Hence, we must require

$$|2-c^2|\le 2\Rightarrow a\lambda\le 1.$$

If $\mu=\mu^{-1}$, then $e^{2i\theta}=1$ meaning that the two eigenvalues are ±1 or $c=0$ or ± 2. Clearly, if $a\lambda<1$, c cannot be ± 2. Hence, the only possibility is $c=0$, in which case the matrix is the identity matrix so G^n is fine. Hence, by Theorem 3.7 in the book, this is fine.

Now, consider $a\lambda=1$, then c can be ± 2 if $\xi h=\pi$ or $-\pi$. In this case, the matrix is in fact unstable. This can be seen by taking special initial values $v_j^0=(-1)^j$ and $w_{j+1/2}^0=0$ to check.

2 Initial boundary value problem

In this section, we focus on treating the boundary conditions in initial boundary value problems.

2.1 Suitable boundary conditions

For the advection equation on $x \in (0,1)$, the initial boundary value problem is

$$\begin{aligned} &\partial_t u + a\partial_x u = 0, \quad a > 0 \\ &u(x,0) = g(x), \quad u(0,t) = \varphi(t), t > 0. \end{aligned}$$

Here, for $a > 0$, the information is propagated from left to right so the boundary condition must be given at $x = 0$. One cannot impose the boundary condition at $x = 1$ if one solves the equation forward.

On the contrary, if $a < 0$ and one solves the problem forward, the condition should be given at $x = 1$.

Consider the system of equations,

$$\boldsymbol{u}_t + A\boldsymbol{u}_x = 0, \tag{2}$$

Suppose

$$A = S\Lambda S^{-1}$$

be the eigendecompostion. Then, $\boldsymbol{w} = S^{-1}\boldsymbol{u}$ satisfies

$$\frac{\partial \boldsymbol{w}}{\partial t} + \Lambda \frac{\partial \boldsymbol{w}}{\partial x} = 0. \tag{3}$$

For the modes with negative values in Λ, one should impose the boundary value of w at $x = 1$. Those with positive eigenvalues should be imposed at $x = 0$. There is no need to put boundary condition for those with zero eigenvalue.

Remark 1. *1. In the book, there is a sign error. The book tried to say*

$$S^{-1}AS = \begin{bmatrix} -\Lambda^I & & \\ & -\Lambda^{II} & \\ & & -\Lambda^{III} \end{bmatrix}$$

2. *In general one does not have to put the boundary values for the eigenmodes. Suppose that there are p_1 eigenvalues with positive sign and p_3 eigenvalues with negative sign. Let*

$$S^{-1} = \begin{bmatrix} d_1^T \\ \cdots \\ d_p^T \end{bmatrix}.$$

Then, one can impose p_1 boundary conditions at $x = 0$. These conditions can be any linear combination $\alpha^T \boldsymbol{u}$ except that one cannot impose $d_i^T \boldsymbol{u}$ $(i > p_1)$. Similarly, you may impose p_3 conditions at $x = 1$ with any combination expect $d_i^T \boldsymbol{u}$ with $i < p - p_3$.

For the wave equation $u_{tt} = a^2 u_{xx}$, $x \in (0, 1)$. Besides the two initial conditions $u(x, 0), u_t(x, 0)$, since the spatitial derivatives are second order, there should be two boundary conditions. For example, one may impose $u(0, t)$ and $u(1, t)$, or the mixed boundary conditions there.

2.2 Approximation of BCs

In principle, the boundary conditions in the initial boundary value problems can be treated similarly as in the elliptic equations.

- For Dirichlet boundary conditions, one may simply impose $u_0^n \leftarrow u(0, t^n)$ for example.
- For the Neumann boundary condition or the mixed boundary condition, one may use the one-sided or the ghost point method to achieve this. For hyperbolic equations, treating the boundary conditions with first order accuracy sometimes is fine and will not pollute the second order accuracy in the middle.

One possible project: explore how the one-sided first order approximation affects the order of the solutions for elliptic equations, and for hyperbolic equations. Literature review and experiments are necessary.

Numerical boundary condition

Here, we use an example to illustrate the issue of numerical boundary. Consider the advection equation for $x \in (0,1)$:

$$\partial_t u - \partial_x u = 0.$$

Since $a = -1 < 0$, the boundary condition should be imposed at $x = 1$. Hence, a possible set of conditions is

$$u(x,0) = g(x), \quad u(1,t) = \varphi(t).$$

For PDEs, such initial condition and the boundary condition are enough to determine the solution. For numerical scheme, like the leapfrog

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\tau} - \frac{u_{j+1}^n - u_{j-1}^n}{2h} = 0 \Rightarrow u_j^{n+1} = u_j^{n-1} + \lambda(u_{j+1}^n - u_{j-1}^n).$$

Clearly, in the numerical scheme, one needs u_0^n and u_M^n for every step. u_M^n is given by the boundary condition, but u_0^n is unknown. We must have an equation for u_0^n to solve this numerical scheme. Such an imposed equation is called the **numerical boundary condition**.

Remark 2. *For general systems, one cannot impose the boundary value at $x = 0$ for the modes with nonpositive eigenvalues ($\lambda_i \leq 0$). In PDE level, the boundary values of these modes should be determined by the initial values (Any other combinations are permitted.) Hence, to evolve the numerical equations, one should impose the numerical boundary conditions for these modes.*

According to the nature of hyperbolic equations, these numericial boundary condition should be consistent with the information propagated along the characteristics. You cannot impose them arbitrarily. If imposed improperly, the solution will not be stable.

For example, the naive numerical boundary condition obtained by the extrapolation

$$u_0^n = 2u_1^n - u_2^n$$

is not stable. In fact, this gives the induction relation

$$u_1^{n+1} = u_1^{n-1} + 2\lambda(u_2^n - u_1^n).$$

Consider the special initial data $u_j^0 = \delta_{j1}$. You may do induction to find the solution and find that the solution blows up.

To treat the numerical boundary condition, we may make use of the integration approach as in the finite volume method, and make use of the characteristics. For example, taking the cell $[x_0, x_1] \times [t_{n-1}, t_n]$:

$$\iint_{[x_0,x_1]\times[t_{n-1},t_n]} \partial_t u dx dt = \iint_{[x_0,x_1]\times[t_{n-1},t_n]} \partial_x u dx dt$$

Then,

$$\int_{x_0}^{x_1} (u(x, t_n) - u(x, t_{n-1}))dx = \int_{t_{n-1}}^{t_n} (u(x_1, t) - u(x_0, t))dt.$$

Considering the direction of the characteristics, we may use the $x = 0$ and $t = t_{n-1}$ lines to approximate the integrals:

$$h[u(x_0, t_n) - u(x_0, t_{n-1})] \approx \tau[u(x_1, t_{n-1}) - u(x_0, t_{n-1})]$$

This is then

$$u_0^{n+1} = u_0^n + \lambda(u_1^n - u_0^n).$$

This is a stable numerical boundary condition. As can be seen, this is just the upwind scheme. There could be higher order approximations. However, for such hyperbolic problems, treating this numerical boundary with first order accuracy will not pollute the accuracy in the middle.

3 Comments on other cases

Those who want to know more about solving hyperbolic equtions could read the book “Finite volume methods for hyperbolic problems” by Randall J. Leveque. This book is very complete in describing all types of methods for multidimensional and nonlinear problems, together with many applications like shallow water waves, the Euler equations etc.

3.1 Multidimensional problems

For multidimensional problems

$$\partial_t u + \vec{a} \cdot \nabla u = 0,$$

where $u = u(x, y)$ and $\vec{a} \cdot \nabla u = a\partial_x u + b\partial_y u$. Direct generalization of the schemes like upwind, L-F and Lax Wendroff are possible, though some scheme, like the Lax-Wendroff could be complicated (see section 19.1.2 in the book "Finite volume methods for hyperbolic problems" by Leveque).

The upwind methods for higher dimensional problems in the finite volume framework could be replaced by a more general method, the Godunov's method.

The generalization of Lax-Friedrichs in FDM could straightforward

$$\frac{u_{jm}^{n+1} - \frac{1}{4}(u_{j,m+1}^n + u_{j,m-1}^n + u_{j+1,m}^n + u_{j-1,m}^n)}{\tau} + a\frac{u_{j+1,m}^n - u_{j-1,m}^n}{2h} + b\frac{u_{j,m+1}^n - u_{j,m-1}^n}{2h} = 0.$$

The stability condition becomes worse. Often, in d-dimensional problem, it becomes $d|a|\lambda \le 1$ if $\vec{a} = (a, a, \cdots, a)$.

Here, we will mention two approaches for designing FDM for multi-dimensional problems. [As mentioned, the finite volume method (FVM) is a more flexible framework for the general hyperbolic problems. You may use these ideas as well to design the general FVM schemes.]

1. Dimension splitting. The locally one dimensional schemes (局部一维格式)

   The idea of such method is based on the so-called time-splitting method, or fractional step methods.

   The idea is to split $\partial_t u + au_x + bu_y = 0$ into two substeps from t_n to t_{n+1}:

$$\partial_t u^* + a\partial_x u = 0,$$
$$\partial_t u + b\partial_y u = 0$$

Each substep can be solved as a one-dimensional problem. We will mention this strategy in more detail for mixed type problems later. The issue of such strategy is that the boundary condition of u^* should be addressed carefully.

2. To address the stability issue, one may use the implicit schemes. However, multi-dimensional implicit schemes are often not easy to invert as the matrices are not tri-diagonal (三对角).

   To resolve this problem, one could use the alternating dimenisonal implicit scheme (交替方向隐式格式). We will discuss this in more detail for parabolic equations. Here, we ignore them.

3.2 Nonlinear problems

The nonlinear hyperbolic problems are very different from the linear problems. In linear problems, the characteristics will not intersect.

$$\partial_t u + \vec{a}(x,t) \cdot \nabla u = 0.$$

The characteristics given by

$$\dot{x} = \vec{a}(x(t), t)$$

will not intersect by the existence and uniqueness theorem in ODE theory. Hence, the solution at every point is well-defined.

However, for nonlinear problems, the characteristics could intersect. The simplest example is the Burger's equation

$$\partial_t u + u u_x = 0.$$

The characteristics determined by

$$\dot{x} = u(x(t), t)$$

could intersect! The reason is that along the this line, u is constant so that $x = x(t)$ is a straight line. Different initial values could make them intersect.

This means that u will stop to be differentiable (otherwise the existence and uniqueness theorem will ensure the nonintersection). For solutions with discontinuity, we must introduce the concept of **weak solutions**.

Among all the *weak solutions*, we aim to find the **entropy solutions**. The entropy solutions at the discontinuity will have the so-called rarefactions and shocks. For the discretization, it is better to have the conservative form

$$\partial_t u + \frac{1}{2}(u^2)_x = 0.$$

The conservative form is more stuiable for entropy solutions and to capture the shocks physically. This can be discretized using the finite volume approach. For example, the upwind scheme is

$$u_j^{n+1} = \begin{cases} u_j^n - \lambda(\frac{1}{2}(u_j^n)^2 - \frac{1}{2}(u_{j-1}^n)^2), & f'(u_j^n) \geq 0 \\ u_j^n - \lambda(\frac{1}{2}(u_{j+1}^n)^2 - \frac{1}{2}(u_j^n)^2), & f'(u_j^n) < 0 \end{cases}$$

The upwind scheme is better be replaced by the Gudonov's method. In the case of rarefaction, one needs to use a certain value between u_j and u_{j-1}.

4 1D heat equation / diffusion equation, and some typical two level schemes

Consider the 1D heat equation/ diffusion equation:

$$u_t = (a(x)u_x)_x + f(x), a > 0.$$
$$u(x, 0) = \eta(x),\ u(0, t) = g_0(t),\ u(1, t) = g_1(t).$$

(If $\kappa < 0$, the equation is ill-posed.)

We first of all discuss the constant coefficient case for $x \in \mathbb{R}$ (the forcing term f does not affect much):

$$\partial_t u = a\partial_{xx} u, \quad x \in \mathbb{R}.$$

The dispersion relation of the heat equation is

$$\omega(\xi) = -ia\xi^2.$$

This means that all modes will decay. The long wavelengh modes (small ξ) decay slowly while the short wavelength modes decay fast.

4.1 Typical two-level schemes

We have introduced the scheme where the centered difference is used in space and forward Euler is used in time:

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

We have shown that the local truncation error is $O(\tau+h^2)$. We have already seen that it is convergent provided that $a\mu=a\frac{\tau}{h^2}\le\frac{1}{2}$ in ℓ^∞ norm. Moreover, using the theory of stability region or von Neumann analysis, it is also ℓ^2 stable if $a\frac{\tau}{h^2}\le 1/2$.

Clearly, one needs

$$\tau\sim h^2.$$

This is a restriction for the time step size. For hyperbolic equtions, we know that this restriction for forward Euler is due to that the eigenvalues of hyperbolic equations are imaginary. How about the diffusion equation? Can we choose other explicit scheme to relax this?

In fact, after we discretize in space using the centered difference, the highest frequency (short wavelength) will roughly be $1/h^2$. The eigenvalues are all **real** and nonpositive! Hence, the numerical methods containing negative real axis is fine. The reason here is that the eigenvalues ineed has a large range $0\sim 1/h^2$. Often, we care about the modes with eigenvalues $O(1)\sim O(1/h)$ since we use step size h to resolve the spatial variations. We do not care those modes that have big eigenvalues, but they bring restrictions on the step size for stability. This is the typical issue in the **stiff problems**. The restriction is exactly because the problem is stiff and we use the explicit method.

Hence, it is better that we adopt some implicit schemes. Consider a more general θ-method for time discretization,

$$u^{n+1} = u^n + \tau(\theta f(t^n, u^n) + (1-\theta)f(t^{n+1}, u^{n+1})).$$

Applying this to the diffusion equation, we have the **weighted implicit scheme** (加权隐式格式):

$$\frac{u_j^{n+1} - u_j^n}{\tau} - a\left[\theta\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} + (1-\theta)\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{h^2}\right] = 0.$$

As we know, the backward Euler ($\theta = 1$) and the trapezoidal method $\theta = 1/2$ are A-stable ODE methods. Then, one can expect that the scheme with backward Euler

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

and the **Crank-Nicolson** method

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

should be **unconditionally stable**.

In fact, with the Fourier analysis, the growth matrix is

$$G(\xi; \tau, h) = \frac{1 - 4(1-\theta)a\mu\sin^2(\xi h/2)}{1 + 4\theta a\mu\sin^2(\xi h/2)}.$$

One may find for $|G| \le 1$, the stability condition is

$$2a\mu(1 - 2\theta) \le 1.$$

Then, for $\theta \ge 1/2$, it is unconditionally stable.

Below, we briefly discuss the case $\theta = 1$ and $\theta = 1/2$:

- If we do Taylor expansion at $(x_{j+1/2}, t^{n+1/2})$, we can show that the local truncation error for Cranck-Nicolson is $O(\tau^2 + h^2)$. Hence it is of second order accuracy in both time and space.

- They are unconditionally stable.

- The matrices are tridiagonal and easy to be inverted to find u^{n+1}.

- The trapezoidal is not L-stable. The short wavelength modes will not decay that fast. Hence, if you desire those modes to decay fast, you probably want the backward Euler. Otherwise, the Crank-Nicolson is good.