Contents

Chapter 4

Numerical Solutions to Partial Differential Equations

4.1 Parabolic Equations for Initial Value Problems(IVPs)

4.1.1 Explicit(iterative) numerical scheme

Let us consider the simplest parabolic problem related with time t and one spatial dimension x

$$
\begin{aligned}
u_t = \nu u_{xx}, &\quad 0 < x < 1, \quad t > 0, && (4.1)\\
u(0,t) = u(1,t) = 0, &\quad t \geq 0, && (4.2)\\
u(x,0) = u^0(x), &\quad 0 \leq x \leq 1. && (4.3)
\end{aligned}
$$

From physical point of view, this equation modeling the no-source heat diffusion on interval $[0,1]$ with homogeneous media. In this simple case, homogeneous Dirichlet boundary condition is imposed. Mathematically, the solution for equation (4.1) could be obtained by separation of variable. Assuming the solution be in the form of $u(x,t) = f(x)g(x)$, it is true that

$$u(x,t) = \sum_{m=1}^{\infty} a_m e^{-(m\pi)^2 t} \sin m\pi x, \tag{4.4}$$

where a_m is the Fourier coefficients

$$a_m = 2\int_0^1 u^0(x) sinm\pi x dx.$$

Since there is a finite integer m, (4.4) is basically a good approximation to the analytic solution, however, this strategy is hard to applied in more general partial differential equations.

In many applications, it is sufficient to obtain the solution at discrete spatial point x_i and certain time step t_n. For the ease of representation, let h and τ be the spacing, then $x_j = jh, t_n = n\tau$. So that

$$
\begin{aligned}
\frac{\partial u}{\partial t}(x_j, t_n) &\approx \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\tau} := \frac{U_j^{n+1} - U_j^n}{\tau} \\
\frac{\partial^2 u}{\partial x^2}(x_j, t_n) &\approx \frac{u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)}{(h)^2} := \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(h)^2}
\end{aligned}
$$

With the above notations, equation (4.1) holds at (x_j, t_n), which means spatial point x_j at time step t_n

$$U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n), \tag{4.5}$$

where $\mu = \nu\frac{\tau}{h^2}$. One can obtain the approximated solution iteratively at the next time step t_{n+1} by knowing $U_j^n, \forall j$. In this sense, the iterative scheme (4.5) is referred as an **explicit Scheme**.

Given $\nu, f, [a, b]$ and N, T, τ;
$h = (b-a)/N$ and set $x_j = j * h, \forall j = 0, 1, \cdots, N$;
u = zeros(N+1,T+1) ;
for $n = 1, 2, \cdots, T$ **do**
  $u(0, n) = a(n\tau); u(N, n) = b(n\tau)$;
  for $j = 1, 2, \cdots, N-1$ **do**
    $U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n)$;
  end
end

例4.1.1. Please calculate by (4.5) with $\nu = 5, f(x, 0) = \cos\frac{\pi x}{2}, a(0, t) = 0, b(1, t) = 0$. Suggested computational parameters $N = 100, T = 1, \tau = 0.0015$.

4.1.2 Error estimation for explicit scheme

Does we do the right thing to solve the parabolic equation (4.1)?

定理4.1.1 (Consistency)**.** Let $L = \frac{\partial}{\partial t} - \nu\frac{\partial^2}{\partial x^2}, (\nu > 0)$ be the operator and $U_j^{n+1} = L_h U_j^n$ be the finite difference scheme, where L_h dependent on the time and space step τ and h. It is defined that the finite difference scheme is consistent with the original differential equation, if

$$T(x_j, t_n) = \left(L_h u(x_j, t_n) - u(x_j, t_{n+1})\right) \to 0, \qquad \tau, h \to 0.$$

截断误差(Truncation Error):

$$\begin{aligned} T(x,t) &= \frac{u(x, t+\tau) - u(x,t)}{\tau} - \nu\frac{(u(x+h,t) - 2u(x,t) + u(x-h,t))}{h^2} \\ &= (u_t(x,t) + \frac{\tau}{2}u_{tt}(x,t) + \ldots) - \nu(u_{xx} + \frac{h^2}{12}u_{xxxx} + \ldots) \\ &\approx \frac{\tau}{2}u_{tt}(x,t) - \frac{\nu h^2}{12}u_{xxxx} \end{aligned}$$

收敛性：Is $U_j^n \to u(x_j, t_n)$?

定理4.1.2 (Convergent)**.** Using fixed initial and boundary values and $\mu = \tau/(h)^2$, and let $\tau \to 0, h \to 0$. If on any given position $(x^*, t^*) \in (0,1) \times (0, T)$,

$$U_j^n \to u(x_j, t_n), \forall x_j \to x^*, t_n \to t^*.$$

It is essential to calculate the **Approximation Error:** $e_j = U_j^n - u(x_j, t_n)$ to evaluate the quality of approximation. In this sense, the finite difference scheme $T(x,t)$ yields

$$e_{j+1} = (1-2\mu)e_j^n + \mu e_{j+1}^n + \mu e_{j-1}^n - T_j^n\tau,$$

which result in $E^n \le \frac{1}{2}\tau\big(M_{tt} + \frac{1}{6\mu}M_{xxxx}\big)$ if define $E^n = \max\{|e_j|, j = 0, 1, \cdots, n\}$ and M_{tt} and M_{xxxx} be the upper limit for u_{tt} and u_{xxxx} respectively.

Proposition 4.1.1 (Stability Condition)**.** The explicit scheme (4.5) is convergent if $\mu := \frac{\tau}{h^2} \le \frac{1}{2}$.

4.1.3 Implicit schemes

The stability condition $\mu = \frac{\tau}{h^2} \le \frac{1}{2}$ is too strict, which means too small time step $\tau \le \frac{1}{2}h^2$ when the grid space $h \to 0$. The following scheme is another good choice

$$U_j^{n+1} = U_j^{n+1} + \mu(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) \tag{4.6}$$

The implicit scheme yields

$$-\mu U_{j-1}^{n+1} + (1+2\mu)U_j^{n+1} - \mu U_{j+1}^{n+1} = U_j^n, \qquad \forall j = 1, 2, \ldots, (N-1).$$

U_0^{n+1} and U_N^{n+1} are known with the boundary condition. It requires to solve a linear equation system with a tri-diagonal coefficient matrix. **Thomas algorithm** is the natural choice.

例4.1.2 (Fourier mode error estimation)**.** Error analysis for explicit scheme (4.5) with Fourier mode

$$U_j^n = (\lambda)^n e^{ik(jh)}.$$

It yields

$$\begin{aligned}
\lambda &:= \lambda(k) = 1 + \mu(e^{ikh} - 2 + e^{-ikh}) \\
&= 1 - 2\mu(1 - cos(kh)) \\
&= 1 - 4\mu sin^2\frac{1}{2}kh
\end{aligned}$$

Since $U_j^{n+1} = \lambda U_j^n$, λ is referred as **amplification factor**. In the mode $k = m\pi$, $\mu > \frac{1}{2}$ makes $\lambda > 1$, which make the iterative scheme (4.5) divergent! However in the case of convergence, there exist a K independent of k, which makes

$$|[\lambda(k)]^n| \le K, \qquad \forall k, n\tau \le T.$$

By applying the analysis on Fourier mode $U_j^n = (\lambda)^n e^{ik(jh)}$, it is trivial to verify the stability of the implicit scheme. We have

$$\lambda = \frac{1}{1 + 4\mu\sin^2\frac{1}{2}kh} < 1,$$

which imply that the implicit scheme (4.6) is **unconditionally stable**. This mean that the time-step length could be much larger than the explicit scheme, however, its truncation error is still the same with explicit scheme,

4.1.4 Mixed method: θ-scheme

It is straightforward to consider a mixed/weighted version between the explicit one and the implicit one, in order to take full advantages in their own property. A general formulation looks like

$$U_j^{n+1} - Y_j^n = \mu\big[\theta\delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n\big], \qquad \forall j = 1, 2, \ldots, J-1$$

As for any $\theta \ne 0$, straightforward simplification results into a tri-diagonal linear system

$$-\theta\mu U_{j-1}^{n+1} + (1+2\theta\mu)U_j^{n+1} - \theta\mu U_{j+1}^{n+1} = \big[1 + (1-\theta)\mu\delta_x^2\big]U_j^n \tag{4.7}$$

例4.1.3 (Crand-Nickson)**.** There are many other stencils to solve the heat equation, which is mentioned in the text book of Richtmyer and Morton(1967). However, a most popularly stencil is the case of $\theta = \frac{1}{2}$, which is proposed in 1947 and is named after the authors.

The stability region are interested for θ-scheme. Considering the Fourier mode $U_j^n = \lambda^n e^{ik(j\triangle x)}$ as a solution of scheme (4.7).It finally leads to

$$\mu(1-2\theta) > \frac{1}{2}.$$

According to the above criteria, the θ-scheme for (4.7) is stable if $\mu \leq \frac{1}{2}\big(1-2\theta\big)^{-1}$ in the case of $0 \leq \theta < \frac{1}{2}$, and is stable for any given μ in the case of $\frac{1}{2} \leq \theta \leq 1$.

定理4.1.3 (Maximum value principle)**.** Assuming that $0 \leq \theta \leq 1$ and $\mu(1-\theta) \leq \frac{1}{2}$ hold for the parameters of the θ-method, then $\{u_j^n\}$, the solution of (4.7), satisfying

$$U_{min} \leq U_j^n \leq U_{max}, \tag{4.8}$$

where U_min and U_max are the minimum and maximum value among all initial position and boundary position.

General boundary conditions can also be treated in discrete. As for the Robin type

$$\frac{\partial u}{\partial x} = \alpha(t)u + g(t), \alpha(t) > 0, x = 0,$$

A first order scheme $\frac{U_1^n - U_0^n}{h} = \alpha^n U_0^n + g^n$ is sufficient in most of the applications. Second order scheme $\frac{2U_0^n - 3U_1^n + U_2^n}{h} = \alpha^n U_0^n + g^n$ is also constantly used for better resolutions.

As for the nonlinear case, such as

$$u_t = b(u)u_{xx}, \forall x \in (0,1)$$

The linearization is necessary at each time step

$$U_j^{n+1} = U_j^n + \mu b(U_j^n)(U_{j+1}^n - 2U_j^n + U_{j-1}^n)$$

The error analysis at each step is similar with the linear case.It is very hard to obtain a general global error analysis, which is dependent heaily on $b(u)$.

In practical applications, multiple spatial dimension are constantly concerned. Let Ω be a rectangular domain $(0,X) \times (0,Y)$

Find a function $u(x,y,t)$ defined on Ω

$$\begin{aligned} u_t(x,y,t) &= b(u_{xx}(x,y,t) + u_{yy}(x,y,t)), \qquad (b > 0) \\ &:= b\triangle u(x,y,t) := b\nabla^2 u(x,y,t), \end{aligned}$$

with proper Dirichlet boundary condition and initial value $u(x,y,0)$

Explicit V.S. Implicit time step $\triangle t$, grid space $\triangle x$ and $\triangle y$

$$U_{r,s}^n \approx u(x_r, y_s, t_n), \qquad \forall r = 0, \cdots, Nx, s = 0, \cdots, Ny.$$

Explicit scheme

$$\frac{1}{\triangle t}\big(U_{r,s}^{n+1} - U_{r,s}^n\big) = \frac{b}{(\triangle x)^2}\big(U_{r+1,s}^n - 2U_{r,s}^n + U_{r-1,s}^n\big) - \frac{b}{(\triangle y)^2}\big(U_{r,s+1}^n - 2U_{r,s}^n + U_{r,s-1}^n\big)$$

Implicit scheme(**Jacobi** and **Gauss Sediel** solver)

$$\frac{1}{\triangle t}(U_{r,s}^{n+1} - U_{r,s}^{n}) = \frac{b}{(\triangle x)^2}(U_{r+1,s}^{n+1} - 2U_{r,s}^{n+1} + U_{r-1,s}^{n+1}) - \frac{1}{(\triangle y)^2}(U_{r,s+1}^{n+1} - 2U_{r,s}^{n+1} + U_{r,s-1}^{n+1})$$

To solve the multiple-dimensional problem in an efficient manner, the Alternative Direction Interaction(ADI) method is proposed by Peaceman D.W. and Rachford H.H. Jr in 1955. It is convenient to take the two dimensional as illustration. Consider the Crank-Nicolson scheme

$$(1 - \frac{1}{2}\mu_x\delta_x^2 - \frac{1}{2}\mu_y\delta_y^2)U^{n+1} = (1 + \frac{1}{2}\mu_x\delta_x^2 + \frac{1}{2}\mu_y\delta_y^2)U^n,$$

a slight modification is made by approximation

$$(1 - \frac{1}{2}\mu_x\delta_x^2)(1 - \frac{1}{2}\mu_y\delta_y^2)U^{n+1} = (1 + \frac{1}{2}\mu_x\delta_x^2)(1 + \frac{1}{2}\mu_y\delta_y^2)U^n$$

which leads to a two step method

$$\begin{aligned} (1 - \frac{1}{2}\mu_x\delta_x^2)U^{n+\frac{1}{2}} &= (1 + \frac{1}{2}\mu_y\delta_y^2)U^n \\ (1 - \frac{1}{2}\mu_y\delta_y^2)U^{n+1} &= (1 + \frac{1}{2}\mu_x\delta_x^2)U^{n+\frac{1}{2}}. \end{aligned}$$

It is essentially an type of operator splitting technique.

例4.1.4.

$$u_t = u_{xx} + u_{yy}, \qquad (x, y) \in (0, 1) \times (0, 1)$$

with given initial function $u(x, y, 0) = u^0(x, y)$ and fixed value 0 on all the four boundaries.

The initial value $u^0(x, y)$ can be arbitrary function, such as the first plot in Fig.4.1 One can also try different $\triangle x$ and $\triangle y$, for e.g. $\frac{1}{100}, \frac{1}{200}, \frac{1}{400}$. On the other hand, implicit scheme and the ADI iterative method can also be applied. We plot the the solution at four different time steps

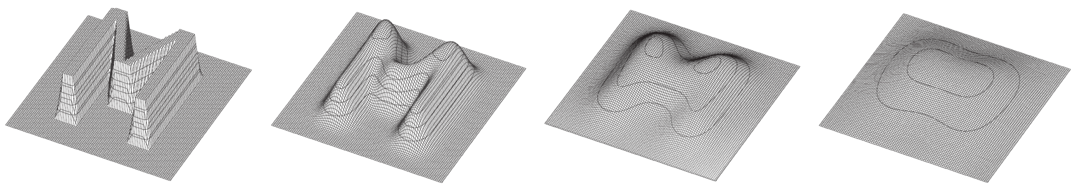


Figure 4.1: From left to right: the numerical solution at $t = 0, 0.001, 0.004$ and $t = 0.01$

4.2 Hyperbolic Equation-based Initial Value Problems(IVPs)

Let us introduce the basic idea of numerical methods for hyperbolic equation-based IVPs. One dimensional linear convection equation is convenient for this purpose

$$\begin{cases} \frac{\partial u}{\partial t} + a(x,t)\frac{\partial u}{\partial x} = 0, & \forall t, x, \\ u(x, 0) = u^0(x), & \forall x. \end{cases} \tag{4.9}$$

It is trivial to verify that u is a series of constants along the family of characteristic curves $x(t)$ satisfying
$$\frac{dx}{dt} = a(x,t).$$
Supposing that $a(x,t)$ is Lipschitz continuous with respective to x and continuous with respective to t, there will be no intersection between different $x(t)$. In this sense, the so-call *method of characters* gives the analytic solution
$$u(x,t) = u_0(x - a(x,t)t) := u_0(x - at).$$

4.2.1 Upwind scheme

It is necessary to develop numerical methods to evaluate the solution on fixed grid, since most of other cases could not be solved with the above strategy. Let U_j^n be the solution on point x_j at time step t_n, which is constantly denoted as the grid point (x_j, t_n). It is worth to mention that the very first concept is proposed in a famous paper on finite difference methods by Courant, Friedrichs and Lewy in 1928.

By doing finite difference approximations to the derivatives in (4.9), which yields finite difference equaiton
$$\frac{U_j^{n+1} - U_j^n}{\triangle t} + a\frac{U_j^n - U_{j-1}^n}{\triangle x} = 0.$$
A simplification results into a iterative scheme
$$U_j^{n+1} = U_j^n - \frac{a\triangle t}{\triangle x}\big(U_j^n - U_{j-1}^n\big) := (1-\nu)U_j^n + \nu U_{j-1}^n, \tag{4.10}$$
where $\nu = \frac{a\triangle t}{\triangle x}$. From algebraic point of view, iterative scheme (4.10) is fundamentally a combination of certain neighbored grid point. As well as in the parabolic equation, it is referred as an explicit scheme to solve the linear convection equation. It is essential to mention that a necessary condition for the convergence of (4.10) is $\nu \leq 1$.

For the ease of analysis, it is preferred to define $\nu = |a|\triangle t/\triangle x$ as the *CFL*-number. Since we do not known the direction of characteristic curve at (x_j, t_n), which is determined by the sign of a. A classical compact and stable finite difference scheme is the *upwind scheme*
$$U_j^{n+1} = \begin{cases} U_j^n - \nu\big(U_{j+1}^n - U_j^n\big) = (1+\nu)U_j^n - \nu U_{j+1}^n, & a < 0, \\ U_j^n - \nu\big(U_j^n - U_{j-1}^n\big) = (1-\nu)U_j^n + \nu U_{j-1}^n, & a > 0, \end{cases} \tag{4.11}$$

4.2.2 Lax-Wendroff Scheme

The phase error of the upwind scheme is in fact smaller than high order schemes, however, the disappation error are too sevier to prevent it from practical using. Remind that larger stencil will leads to better approximation in the interpolation theory, it is natural to reconstruct a better approximation U using quadratic interpolation.

The Lax-Wendroff scheme has been the most intrisic scheme since it is proposed in 1960. Let us skip the details and only gives its formulation
$$U_j^{n+1} = \frac{1}{2}\nu(1+\nu)U_{j-1}^n + (1-\nu^2)U_j^n - \frac{1}{2}\nu(1-\nu)U_{j+1}^n. \tag{4.12}$$

The most significant advantage is its convenience in generalization to solving hyperbolic systems, and let us illustrated in the chapter of the finite element methods. Here we are intend to emphasis the stability of the scheme, which is independent on the sign of its Fourier modes Fourier mode analysis gives its amplification factor being

$$|\lambda(k)|^2 = 1 - 4\nu^2(1-\nu^2)\sin^4\frac{k}{2}\triangle x.$$

It shows that the Lax-Wendroff scheme is stable if $\nu \le 1$.

例4.2.1. Solve the linear convection equation with upwind scheme and Laxwendroff scheme. Please show the numerical results under different initial conditions, including the impulse function and a smooth one

$$u(x,0) = \exp -10(4x-1)^2,$$

4.2.3 Leap-Frog scheme

In this scheme, three different time-levels are concerned, and it is another important scheme other than the Lax-Wendroff scheme.

$$\frac{U_j^{n+1} - U_j^{n-1}}{2\triangle t} + a\frac{U_j^{n+1} - U_{j-1}^n}{2\triangle x} = 0.$$

A simplification results into a iterative scheme

$$U_j^{n+1} = U_j^{n-1} - \nu\big(U_{j+1}^n - U_{j-1}^n\big), \tag{4.13}$$

where $\nu = a\triangle t/\triangle x$ is the same as usual.

Hyperbolic equation system.

例4.2.2. Solve the second order partial differential equation $u_{tt} = a^2 u_{xx}$, with discontinuous and smooth initial conditions, as the same as given in the previous example.

Solution: Firstly, convert the second order equation into a first order system

$$\begin{aligned} v_t + aw_x &= 0, \\ w_t + av_x &= 0. \end{aligned}$$

As for a two-component linear system, a stagger-grid/two-step scheme is preferred for practical reason

$$\begin{aligned} V_j^{n+1/2} &= V_j^{n-1/2} - \nu\big(W_{j+1/2}^n - W_{j-1/2}^n\big), \\ W_{j+1/2}^{n+1} &= W_{j+1/2}^n - \nu\big(V_{j+1}^{n+1/2} - V_j^{n+1/2}\big). \end{aligned} \tag{4.14}$$

4.2.4 Numerical analysis for the methods

Different with those for solving parabolic equations, explicit numerical schemes are widely interested for hyperbolic equations.

Convergence

We say that the numerical solution for a hyperbolic equation is convergent in the meaning of $\triangle x \to 0$ and $\triangle t \to 0$, it requires

The method be *consistent*, which promises the local truncation error goes to 0 as $\triangle t \to 0$. The method be *stable*, which means any small error in each timestep is under control(will not grow too fast)

Consistency

Denote the numerical method as $A^{n+1} = \mathcal{N}(Q^n)$ and the exact value as q^n and q^{n+1}. Then the local truncation error is defined as

$$\tau = \frac{\mathcal{N}(q^n) - q^{n+1}}{\triangle t}$$

We say that the method is *consistent* if τ vanished as $\triangle t \to 0$ for all smooth $q(x,t)$ satisfying the differential equation. It is usually stratightforward when Taylor expasions are used.

Stability

Courant-Friedrichs-Levy condition: the numerical domain of dependence contains the true domain of dependence domain of the PDE, at least in the limit as $\triangle t, \triangle x \to 0$

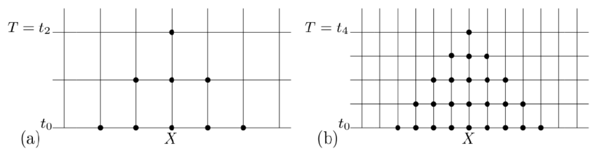


Fig. 4.3. (a) Numerical domain of dependence of a grid point when using a three-point explicit finite difference method, with mesh spacing Δx^a. (b) On a finer grid with mesh spacing $\Delta x^b = \frac{1}{2}\Delta x^a$.

For a hyperbolic system with characterestic wave speeds λ^p,

$$\frac{\triangle x}{\triangle t} \geq \max_p |\lambda^p|, \qquad p = 1, \cdots, m.$$

This condition is necessary but not sufficient !

定理4.2.1 (Lax等价性原理)**.** content

定理4.2.2 (Von Neumann定理)**.** content

4.3 Finite Volume Methods(FVMs) for Conservation Law

The finite volume method (FVM) is a constantly used discretization strategy for hyperbolic type partial differential equations, especially in the application of conservation law and other models arising from computational fluid dynamics.

FVMs seem to be perfectly suited to the conservation or divergence form of partial differential equations since they appear automatically in conservation form. Most of the numerical methods for conservation law can be category into FVMs. Let us take the following general form

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = 0, \tag{4.15}$$

where $\mathbf{u} = \mathbf{u}(x,t)$ is the unknown vector-valued function and $\mathbf{f}(\mathbf{u})$ is referred as the *flux function*. It is convenient to define $\mathbf{F}(x,t) := \mathbf{f}(\mathbf{u})(x,t)$, and we shall omit the dependency on variable x and t if there is no confusing will arise, say, $\mathbf{F} = \mathbf{f}(\mathbf{u})$ as the flux function.

4.3.1 Finite Volume Formulas

The fundamental idea for Finite Volume Method(FVM) is to divide the domain into grid cells and then approximate the total integral of the flux over each grid cell. Denote cells $C_i = (x_{i-1/2}, x_{i+1/2})$ and mean values on cells

$$U_i^n \approx \frac{1}{|C_i|}\int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t_n)dx.$$

In this sense, FVM update the value of U_i^{n+1} based on the fluxes F^n between the cells, which is shown in Fig.4.3.1.

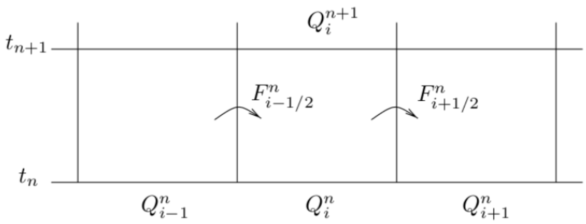


Figure 4.2: The concept of finite volume approximation.

Let us consider the FVM scheme for 1D conservation law. Remember that the FV approximation is performed in a cell-wise manner, then on any given cell C_i:=$[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$, one can integrate CLAW (4.15) on cell, it yields

$$\frac{d}{dt}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \mathbf{u}(x,t)dx = \mathbf{f}(\mathbf{u}(x_{i-\frac{1}{2}},t)) - \mathbf{f}(\mathbf{u}(x_{i+\frac{1}{2}},t)).$$

时间方向从t_n到t_{n+1}积分后同除以$\triangle x$：

$$\frac{1}{\triangle x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \mathbf{u}(x,t_{n+1})dx = \frac{1}{\triangle x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \mathbf{u}(x,t_n)dx - \frac{\triangle t}{\triangle x}\left[\int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{u}(x_{i-\frac{1}{2}},t))dt - \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{u}(x_{i+\frac{1}{2}},t))dt.\right]$$

According to the definition of mean values on cell $\mathbf{U}$ and flux funciton $\mathbf{F}$, we reach to

$$U_i^{n+1} = U_i^n - \frac{\triangle t}{\triangle x}\left(F^n_{i+\frac{1}{2}} - F^n_{i-\frac{1}{2}}\right), \tag{4.16}$$

where $\mathbf{F}_{i-\frac{1}{2}} \approx \frac{1}{\triangle t}\int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{u}(x_{i-1/2},t))dt$.

For the purpose of evaluate (4.16) repeatedly, we need to do the integration in $\mathbf{F}_{i-\frac{1}{2}}$ (as well as $\mathbf{F}_{i+\frac{1}{2}}$) numerically. However, more grid point should be added if numerical quadrature is applied. To do it efficiently, only the value of U_{i-1} and U_i by

$$\mathbf{F}^n_{i-1/2} = \mathcal{F}(U_{i-1}, U_i), \tag{4.17}$$

where $\mathcal{F}$ is referred as *numerical flux function.* Finally, the numerical methods reads

$$U_i^{n+1} = U_i^n - \frac{\triangle t}{\triangle x}\left(\mathcal{F}(U^n_{i-1}, U^n_i) - \mathcal{F}(U^n_i, U^n_{i+1})\right). \tag{4.18}$$

Practically, there some different choice for the numerical flux, $\mathcal{F}(U_{i-1}^n, U_{i+1}^n) = \frac{1}{2}\left[f(u_{i-1}^n) + f(u_i^n)\right]$ is an unstable one, which simply take the mean flux function value at the boundary of the cell. A stable version looks into the direction from which the flow come from(upwind), for e.g. $u_t + \lambda u_x = 0$ with $\lambda > 0$. It yields the so-called Godunov Scheme

$$U_i^{n+1} = U_i^n - \lambda \frac{\triangle t}{\triangle x}(U_i^n - U_{i-1}^n). \tag{4.19}$$

例4.3.1 (此处应有一例)**.** content

4.3.2 Riemann Solver

线性化 例: the advection equation

Consider the linear hyperbolic IVP

$$\begin{cases} q_t + Aq_x = 0, \\ \quad q(x,0) = q_0(x) \end{cases}$$

Then we can write $A = R\Lambda R^{-1}$, where $R \in \mathbb{R}^{m\times m}$ is the matrix of eigenvectors and $\Lambda \in \mathbb{R}^{m\times m}$ is the matrix of eigenvalues. Making the substitution $q = Rw$, we get the decoupled system

$$w_t^p + \lambda^p w_x^p = 0, \quad p = 1 \ldots m.$$

$$\begin{cases} \omega_t + \lambda\omega_x = 0, \\ \omega(x,0) = \omega_0(x) \end{cases}$$

solved with the method of characteristics $\omega(x,t) = \omega_0(x - \lambda t)$.
Boundary condition for IBVP($a \le x \le b$)?

依赖域(Domain of dependence) .... 左图

影响域(Range of Influence) .... 右图

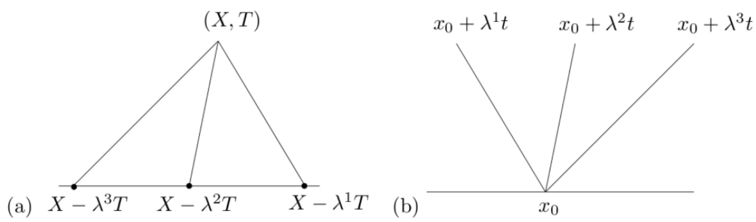


Fig. 3.2. For a typical hyperbolic system of three equations with $\lambda^1 < 0 < \lambda^2 < \lambda^3$, (a) shows the domain of dependence of the point (X, T), and (b) shows the range of influence of the point x_0.

(R. Leveque, 2002)

The hyperbolic equation with initial data

$$q_0(x) = \begin{cases} q_l & x < 0 \\ q_r & x > 0 \end{cases}$$

is known as the Riemann problem.

For the linear constant-coefficient system, the solution is

$$\begin{aligned} q(x,t) &= q_l + \sum_{p:\lambda^p < x/t} \left[l^p(q_r - q_l)\right] r^p \\ &= q_r - \sum_{p:\lambda^p \geq x/t} \left[l^p(q_r - q_l)\right] r^p \end{aligned}$$

Roe 的方案 Recall the numerical method for Conservation Law

$$Q_i^{n+1} = Q_i^n - \frac{\triangle t}{\triangle x}\left[\mathcal{F}(Q_i^n, Q_{i+1}^n) - \mathcal{F}(Q_i^n, Q_{i+1}^n)\right],$$

A linearized choice of the numerical flux based on the Godunov's method for the nonlinear problems. Define $|A| = R|\Sigma|R^{-1}$, where $|\Sigma| = diag(|\lambda^p|)$, then we can derive the Roe's flux as

$$F_{i-\frac{1}{2}}^n = \frac{1}{2}\left[f(Q_{i-1}) + f(Q_i)\right] - \frac{1}{2}|A|\left[Q_{i-1} + Q_i\right]$$

Remark:In this sense, R is properly chosen, such that A is a good enough approximation to nonlinear functional $\mathcal{F}$.

Godunov 的方案 **Remark**: Evolve step (2) requires solving the Riemann problem.

The following *REA algorithm* was proposed by Godunov (1959):

1. **Reconstruct** a piecewise polynomial function $\tilde{q}^n(x, t_n)$ from the cell averages Q_i^n. In the simplest case, $\tilde{q}^n(x, t_n)$ is piecewise constant on each grid cell:

$$\tilde{q}^n(x, t_n) = Q_i^n, \qquad \text{for all } x \in C_i.$$

2. **Evolve** the hyperbolic equation with this initial data to obtain $\tilde{q}^n(x, t_{n+1})$.
3. **Average** this function over each grid cell to obtain new cell averages

$$Q_i^{n+1} = \frac{1}{\Delta x}\int_{C_i} \tilde{q}^n(x, t_{n+1})\, \mathrm{d}x.$$

Recall the solution to the Riemann problem form a linear system

$$Q_i - Q_{i-1} = \sum_{p=1}^{m}\left[l^p\left(Q_{i+1} - Q_i\right)\right] r^p = \sum_{p=1}^{m} \mathcal{W}_{i-\frac{1}{2}}^p$$

If $\triangle t$ is small enough, waves from adjacent cells do not interact!

Godunov's method for General Conservation Laws 最后通过如下“迎风”组合获得流通量表达式

$$F_{i-\frac{1}{2}}^n = f(Q_{i-1}) + \sum_{p=1}^{m} (\lambda^p)^- \mathcal{W}_{i-\frac{1}{2}}^p,$$

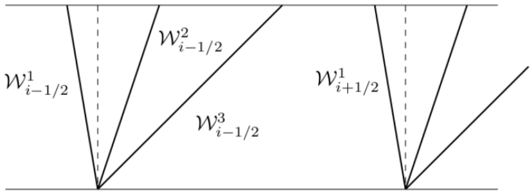


Fig. 4.7. An illustration of the process of Algorithm 4.1 for the case of a linear system of three equations. The Riemann problem is solved at each cell interface, and the wave structure is used to determine the exact solution time Δt later. The wave $\mathcal{W}^2_{i-1/2}$, for example, has moved a distance $\lambda^2\Delta t$ into the cell.

or

$$F^n_{i-\frac{1}{2}} = f(Q_i) + \sum_{p=1}^{m}(\lambda^p)^+\mathcal{W}^p_{i-\frac{1}{2}},$$

where $\lambda^+ = \max(\lambda, 0)$ and $\lambda^- = \min(\lambda, 0)$ is an upwind choice.

4.3.3 Total Variation Diminision(TVD)

Recall the numerical method for Conservation Law

$$Q^{n+1}_i = Q^n_i - \frac{\triangle t}{\triangle x}\left[\mathcal{F}(Q^n_i, Q^n_{i+1}) - \mathcal{F}(Q^n_i, Q^n_{i+1})\right],$$

where $\mathcal{F}(Q^n_i, Q^n_{i+1}) \approx F^n_{i+\frac{1}{2}} = h(Q^-_{i+\frac{1}{2}}, Q^+_{i+\frac{1}{2}})$.

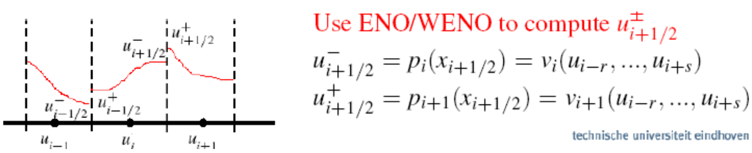
TVD: It is required that the numerical flux function $h(\cdot,\cdot)$ is monotone(Lipschitz continuous, monotone, $h(a, a) = a$)

Example

$$h(a, b) = 0.5(f(a) + f(b) - \alpha(b - a)),$$

where $\alpha = \max_u |f'(u)|$

(Weighted) Essentially Non-Oscillatory$\big($(W)ENO$\big)$ 方案 The main concept of (W)ENO is where



$\{u_i\}^n_{i=0}$ are the given **cell average** of a function $q(x)$.

Construct polynomials $p_i(x)$ of degree $k-1$, for each cell C_i, such that it is a k-th order accurate approximation to the function $q(x)$, which means

$$p_i(x) = q(x) + \mathcal{O}(\triangle^k) \qquad \forall x \in C_i, i = 0, 1, \cdots, N.$$

Finally, one can evaluate u at each cell interface($u^-_{i+1/2}$ and $u^+_{i+1/2}$).

例4.3.2 (此处应再有一例). content

4.3.4 Multiple Dimension Problems

软件包与参考教材

- K. W. Morton and D.F. Mayers: Numerical Solution of Partial Differential Equations（李治平 等 中译）
- 陆金甫, 关治: 偏微分方程数值解法
- Lloyd N. Trefethen: Finite Difference and Spectral Methods for Ordinary and Partial Differential Equations, 1996.
- A. Taflove and S. C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method, 3rd ed.

Exercise

1. Convection-Diffusion equation

$$e\frac{\partial u}{\partial t} = \nabla \cdot (b\nabla u - \mathbf{a}u) + cu + d,$$

   with proper parameter, boundary and initial conditions

2. Further numerically study of the quenching phenomenon (quenching1d.pdf)

3. Analyze of a two dimensional finite difference scheme (FDscheme2D.pdf)

4. **E. F. Toro**, Riemann Solvers and Numerical Methods for Fluid Dynamics, 3rd, Springer-Verlag.

5. **Ferziger Peric**: Computational Methods for Fluid Dynamics, 3rd eds.