Contents

Chapter 5

Numerical Solutions to Differential Equations

5.1 Ordinary Differential Equations

5.1.1 Initial Value Problem

Considering first-order Ordinary Differential Equations(ODEs)

$$\mathbf{y}' = \mathbf{y}'(t) := \begin{bmatrix} y_1'(t) \\ y_2'(t) \\ \vdots \\ y_n'(t) \end{bmatrix} = \begin{bmatrix} f_1(t,\mathbf{y}) \\ f_2(t,\mathbf{y}) \\ \cdots \\ f_n(t,\mathbf{y}) \end{bmatrix} := \mathbf{f}(t,\mathbf{y}), \tag{5.1}$$

where $\mathbf{y} := (y_1, y_2, \cdots, y_n)^T$ and $\mathbf{f} : \mathbb{R}^{n+1} \to \mathbb{R}$. When $n > 1$, it is a system of coupled ODEs.

例5.1.1. *An given n-th order ODE*

$$y^{(n)} = f(t, y, y', y'', \cdots, y^{(n-1)})$$

can be transformed into a first-order system

$$\mathbf{y}' = \mathbf{f}(t,\mathbf{y}).$$

The above ODEs (5.1) will admit a unique solution as soon as an initial condition

$$\mathbf{y}(t_0) = \mathbf{y}_0 \tag{5.2}$$

is given. In the literature, people referred (5.1)+(5.2) as the Initial Value Problems(IVPs) for ODEs. By integrating the ODE, its solution is given by the integral

$$\mathbf{y}(t) = \mathbf{y}_0 + \int_{t_0}^{t} \mathbf{f}(s)ds \tag{5.3}$$

定理5.1.1 (Existence and Uniqueness of the solution to IVPs)**.** *If* $\mathbf{f} : \mathbf{R}^{n+1} \to \mathbf{R}^n$ *is Lipschitz continuous on* D*, which means*

$$\|\mathbf{f}(t, \hat{\mathbf{y}}) - \mathbf{f}(t, \mathbf{y})\| \leq L\|\hat{\mathbf{y}} - \mathbf{y}\|,$$

then the solution to IVPs (5.1)+(5.2) has unique solution for any given $\mathbf{y}_0$ *defined on* D*.*

例5.1.2 (Newton's Second Law of Motion)**.** *As well known as the formula* $F = ma$*, force equals mass times acceleration. It is straightforward that* $a = s''(t)$*, where* t *means the time and* $s(t)$ *is the displacement at time* t*. Considering the trajectory of falling object under the force of Earth's gravity, which means* $F = -mg$*. When the initial position* $s(0)$ *and initial velocity* $v(0) = s'(0)$ *are given, we have its solution*

$$s(t) = -\frac{1}{2}gt^2 + s'(0)t + s(0).$$

Considering the linear and homogeneous system of ODEs in the form of

$$\mathbf{y}' = A\mathbf{y},$$

where A is an $n \times n$ constant coefficient matrix, which is assumed to be diagonalizable. The initial condition $\mathbf{y}(t_0) = \mathbf{y}_0$ is given, then it is easy to confirm that

$$\mathbf{y}(t) = \sum_{i=1}^{n} \alpha_i \mathbf{v}_i e^{\lambda_i t},$$

where $\{\lambda_i\}_{i=1}^n$ and $\{\mathbf{v}_i\}_{i=1}^n$ are eigenvalues and corresponding eigenvectors of A, and $\mathbf{y}_0 = \sum_{i=1}^{n} \alpha_i \mathbf{v}_i$.

Proposition 5.1.1 (Stability of Solutions)**.**

5.1.2 Numerical Methods for ODEs

Finite Difference Approximations

It is essential to explain the approximation of the first order and the second order derivatives.

1. 向前（向后）一阶差商

$$f'(x) \approx D_h^+ := \frac{f(x+h) - f(x)}{h}$$

2. 中心一阶差商

$$f'(x) \approx D_{2h} := \frac{f(x+h) - f(x-h)}{2h}$$

3. 单边差商

$$f'(x) \approx D_{2h}^+ := \frac{-3f(x)+4f(x+h)-f(xi+2h)}{2h}$$

请用Taylor公式验证上述格式的精度分别为$o(h)$以及$o(h^2)$.
中心二阶差商

$$f''(x) = (f(x+h)-2f(x) + f(x-h))/h^2$$

假设$D_h^2 f(x) = Af(x+h) + Bf(x) + Cf(x-h)$,则由Taylor展开：

$$\begin{cases} A+B+C = & 0; \\ h(A-C) = & 0; \\ \dfrac{h^2}{2}(A+C) = & 1. \end{cases}$$

此时的误差为$-\frac{h^2}{12}f^{(4)}(x)$(How to prove?)

Euler's Method

考虑一维一阶常微分初值问题：

$$\frac{dy}{dx} = f(x,y), x \in [a,b]$$

$$y(a) = y_0,$$

基本思想：从初值出发，每一步都沿切线方向积分一步：

$$y(x_k) = y(x_{k-1}) + (x_k - x_{k-1})y'(x_{k-1}) = y(x_{k-1}) + h_k f(x_{k-1}, y)$$

其中，第k步的误差，即截断误差可以定义为：

$$R_k = \int_{x_{k-1}}^{x_k} f(s, y(s))ds - h_k f(x_{k-1}, y(x_{k-1})).$$

这里，记$h_k := (x_k - x_{k-1})$是步长.

例5.1.3 (Euler). *Considering the following initial problem:*

$$y' = y, y(0) = 1.$$

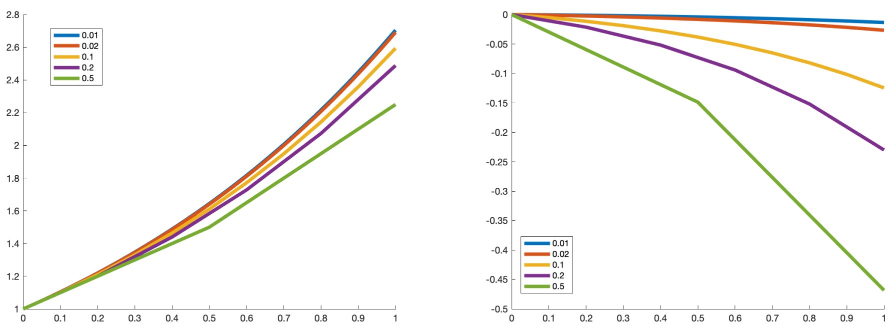


Figure 5.1: (Left)The Euler solution, (Right) Errors

整体误差和局部误差 整体误差不是简单的局部误差的和，注意：发散情形：局部误差会被放大，其和大于整体误差; 收敛情形：整体误差小于局部误差的和。

隐式欧拉

$$y(x_k) = y(x_{k-1}) + (x_k - x_{k-1})y'(x_k)$$

无条件稳定(对h无限制)，精度只有一阶:

$$\left|\frac{1}{1-h\lambda}\right| = 1 + h\lambda + (h\lambda)^2 + \cdots < 1$$

梯形/中点法

$$y(x_k) = y(x_{k-1}) + (x_k - x_{k-1})(y'(x_{k-1}) + y'(x_k))/2$$

(部分情形)无条件稳定，二阶收敛(与$e^{h\lambda}$的展开式比较)：

$$\left|\frac{1+h\lambda/2}{1-h\lambda/2}\right| = 1 + h\lambda + \frac{(h\lambda)^2}{2} + \frac{(h\lambda)^3}{4} + \cdots < 1$$

Definition 5.1.1 (相容性)**.** 如果单步法的增量函数φ满足：

$$\varphi(x, y, 0) = f(x, y)$$

则称单步法与微分方程是相容的。

Definition 5.1.2 (稳定性)**.** 如果φ对于任意$(x, y) \in \Omega$以及小于某个步长h时关于y满足$Lipschitz$条件，则单步方法是稳定的。

Definition 5.1.3 (收敛性)**.** 由增量函数$\varphi(x, y, h)$所确定的单步法是收敛的，若

$$\lim_{h\to 0} y_m = y(x), x = x_m$$

若φ关于x、h满足$Lipschitz$条件，则收敛性与相容性等价

Runge-Kutta方法

记$a_{i,j}, c_i(i-2, 3, \ldots, s; j < i)$和$b_i(i = 1, 2, \ldots, s)$是一些待定的实数权值。则s级显Runge-Kutta方法：

$$y_{m+1} = y_m + h(b_1k_1 + \cdots + b_sk_s),$$

其中，

$$\begin{aligned}
k_1 &= f(x_m, y_m), \\
k_2 &= f(x_m + c_2h, y_m + ha_{2,1}k_1), \\
k_3 &= f(x_m + c_3h, y_m + h(a_{3,1}k_1 + a_{3,2}k_2)), \\
&\cdots\cdots \\
k_s &= f(x_m + c_sh, y_m + h(a_{s,1}k_1 + \cdots + a_{s,s-1}k_s - 1))
\end{aligned}$$

可以按Taylor公式确定系数。由于定解条件少于参数个数，因此这里公式中的参数的值不唯一，常用的有Heun公式、Gill公式等。此外，我们也既避免计算y的高阶导数，也保证差分的高精度。

The most famous numerical methods for ordinary differential equation is the forth order Runge-Kutta formula, which is

$$y_{k+1} = y_k + \frac{h_k}{6}\big(k_1 + 2k_2 + 2k_3 + k_4\big), \tag{5.4}$$

with the definition of momentum

$$\begin{aligned} k_1 &= f(t_k, y_k), \\ k_2 &= f(t_k + \frac{1}{2}h_k, y_k + \frac{1}{2}h_k k_1), \\ k_3 &= f(t_k + \frac{1}{2}h_k, y_k + \frac{1}{2}h_k k_2), \\ k_4 &= f(t_k + h_k, y_k + h_k k_3), \end{aligned}$$

例5.1.4 (explicit Runge-Kutta method(example 9.12)). *Solve the following ODE numerical via Runge-Kutta method:*

$$y' = -2ty^2, y(0) = 1$$

Starting from $t_0 = 0$ *to* $t_1 = 0.25$ *with time-step length* $h = 0.25$*, then we have* $k_1 = f(t_0, y_0) = 0, k_2 = f(t_0 + h, y_0 + hk) = -0.5$. *...*
It is not difficult to known that the analytic solution for the current problem is $y(t) = \frac{1}{1+t^2}$*, so that one can evaluate at the specific time, for example* $y(0.25) = 0.9412, y(0.5) = 0.8$*, for the purpose of calculating numerical errors. We plot the numerical solution as well as it's error in Fig.5.1.4*

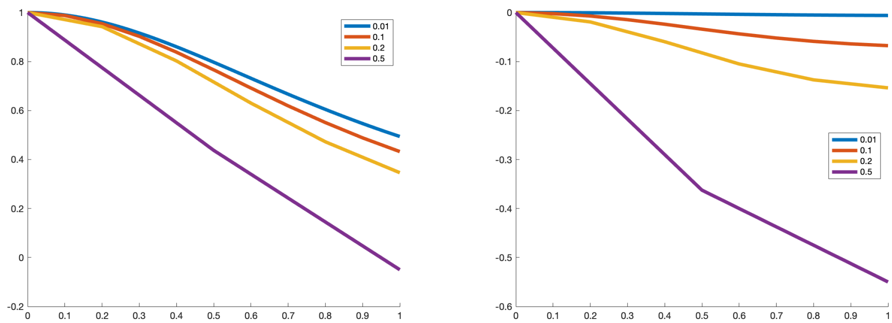


Figure 5.2: (Left)The Runge-Kutta solution with Heun formula, (Right) Errors

5.1.3 Stablity Improvements

implicit scheme

Let us present a numerical example as the exercise

例5.1.5 (implicit Runge-Kutta method). *Using Hammer method to solve the following ODE:*

$$y' = -2xy^2, y(0) = 1$$

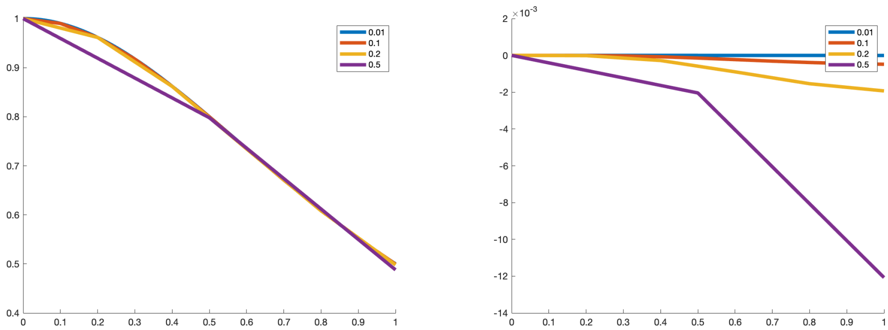


Figure 5.3: (Left)The Runge-Kutta solution with Hammer formula, (Right) Errors

如果k_i的计算中用到了所有的k值，即：

$$y_{m+1} = y_m + h(b_1 k_1 + \cdots + b_s k_s),$$

其中k_i满足：

$$k_i = f(x_m + c_i h, y_m + h(a_{i,1} k_1 + \cdots + a_{i,s} k_s))$$

常用的隐式方法有：隐式中点公式，Hammer 和Hollingsworth公式，Kuntzmann和Butcher公式等。

线性多步法

It is worth to mention that 形如的方法都属于单步法:

$$y_{m+1} = y_m + h\varphi(x_m, y_m, h),$$

其中φ被称为单步法的增量函数。单步法的截断误差可表示为

$$R_m = y_{m+1} - y_m - h\varphi$$

As the improvements, the multi-step schemes yield larger stable region as well as better precision. Considering problem $y' = f(x, y)$, where $y_m = y(x_m), f_m = f(x_m, y_m)$. We have

$$y_{m+1} = \sum_{i=1}^{k} \alpha_i y_{m-i+1} + h\Phi(x_{m+1}, x_m, \ldots, x_{m-k+1}, y'_{m+1}, \ldots, y'_{m-k+1}; h),$$

where $k \in N^+$, $\{\alpha_i\}$ is given real number and h is the time-step length. Then the truncation error is

$$R(x_m, y_m, h) = y_{m+1} - \sum_{i=1}^{k} \alpha_i y_{m-i+1} - h\Phi$$

p阶：使误差等于$O(h^{p+1})$成立的最大整数！

多步法的典型构造方法是多样的。Adams外插法是一种显式方法。相应的有Adams内插法是一种隐式方法。待定系数法求p阶m步线性多步法

例5.1.6 (Linear multi-step method). *Using linear multi-step method to solve the following ODE:*

$$y' = -2xy^2, y(0) = 1$$

例 9.13 多步法的推导 为说明多步法的其他推导方法，我们导出形如

$$y_{k+1}=\alpha_1 y_k+h(\beta_1 y'_k+\beta_2 y'_{k-1})$$

的显式两步法，其中 α_1、β_1 和 β_2 是待定参数. 为使符号简化，只考虑一维情形，结果可推广到方程组的向量情形. 用待定系数法，令公式对前三个单项式精确成立. 若 $y(t)=1$，则 $y'(t)=0$，得到方程

$$1=\alpha_1\cdot 1+h(\beta_1\cdot 0+\beta_2\cdot 0).$$

若 $y(t)=t$，则 $y'(t)=1$，得到方程

$$t_{k+1}=\alpha_1 t_k+h(\beta_1\cdot 1+\beta_2\cdot 1).$$

若 $y(t)=t^2$，则 $y'(t)=2t$，得到方程

$$t_{k+1}^2=\alpha_1 t_k^2+h(\beta_1\cdot 2t_k+\beta_2\cdot 2t_{k-1}).$$

由于这三个方程对任何 t_i 都成立，不妨取 $t_{k-1}=0$，$h=1$（因而 $t_k=1$，$t_{k+1}=2$），求解相应的 3×3 线性方程组，得 $\alpha_1=1$，$\beta_1=\frac{3}{2}$，$\beta_2=-\frac{1}{2}$. 这样，两步显式法为

$$y_{k+1}=y_k+\frac{h}{2}(3y'_k-y'_{k-1}),$$

由约束条件，它是二阶的. 类似地，还可以推导形如

$$y_{k+1}=\alpha_1 y_k+h(\beta_0 y'_{k+1}+\beta_1 y'_k)$$

的隐式两步法. 同样，用待定系数法，令公式对前三个单项式精确成立，得到三个方程

$$\begin{cases}1=\alpha_1\cdot 1+h(\beta_0\cdot 0+\beta_1\cdot 0),\\ t_{k+1}=\alpha_1\cdot t_k+h(\beta_0\cdot 1+\beta_1\cdot 1),\\ t_{k+1}^2=\alpha_1\cdot t_k^2+h(\beta_0\cdot 2t_{k+1}+\beta_1\cdot 2t_k).\end{cases}$$

为简化，取 $t_k=0$、$h=1$（从而 $t_{k+1}=1$），求解相应的 3×3 线性方程组，得 $\alpha_1=1$、$\beta_1=\frac{1}{2}$、$\beta_2=\frac{1}{2}$. 这样，隐式两步法为

$$y_{k+1}=y_k+\frac{h}{2}(y'_{k+1}+y'_k).$$

可以看出，这就是梯形方法，由约束条件知道，它是二阶的. 用同样的方法，还可以得到更高阶的方法，只需令公式对前若干个单项式精确成立，单项式的个数要与公式中待定参数的个数相同，然后求解相应的线性方程组，得到参数的值即可. ■

例 9.14 预估-校正方法 为说明预估-校正方法，我们用例 9.13 中得到的两步法来解例 9.11 和例 9.12 中的一维非线性常微分方程

$$y'=-2ty^2,$$

初值为 $y(0)=1$. 由于二阶显式格式需要两个初值，所以除了 $t_0=0$ 时的初值 $y_0=1$ 外，还要使用例 9.12 中用单步 Heun 法得到的 $t_1=0.25$ 时的值 $y_1=0.9375$. 从 $t_1=0.25$ 到 $t_2=0.5$，取步长 $h=0.25$，使用二阶显式方法，得到预估值

$$\hat{y}_2=y_1+\frac{h}{2}(3y'_1-y'_0)=0.9375+0.125(-1.3184+0)=0.7727.$$

计算 f 在预估值 $\hat{y}_2$ 处的值，得到相应的导数值 $\hat{y}'_2=-0.5971$. 在相应的隐式方法中（在这里为梯形公式）将这些预估值代入，得到解的校正值

$$y_2=y_1+\frac{h}{2}(\hat{y}'_2+y'_1)=0.9375+0.125(-0.5971-0.4395)=0.8079.$$

用这个新的 y_2 再计算 f 的值，得到改进值 $y'_2=-0.6528$，以便在下一步计算时使用. 到这里，完成了 PECE 程序的一步. 如果需要的话，还可以反复校正，直到收敛. 这个问题的精确解为 $y(t)=1/(1+t^2)$，因而在积分点上的真值为 $y(0.25)=0.9412$、$y(0.5)=0.8$. ■

最常用的成对多步方法之一是显式四阶 Adams-Bashforth 预估格式

$$\boldsymbol{y}_{k+1}=\boldsymbol{y}_k+\frac{h}{24}(55\boldsymbol{y}'_k-59\boldsymbol{y}'_{k-1}+37\boldsymbol{y}'_{k-2}-9\boldsymbol{y}'_{k-3})$$

和隐式四阶 Adams-Moulton 校正格式

$$\boldsymbol{y}_{k+1}=\boldsymbol{y}_k+\frac{h}{24}(9\boldsymbol{y}'_{k+1}+19\boldsymbol{y}'_k-5\boldsymbol{y}'_{k-1}+\boldsymbol{y}'_{k-2}).$$

Stiffness

ODE的Jacobi矩阵特征值相互差别极大，则称它是刚性的！

例 9.10 刚性 为说明刚性常微分方程的数值求解，考虑初值条件为 $y(0)=1$ 的初值问题

$$y' = -100y + 100t + 101.$$

这个常微分方程的通解为 $y(t)=1+t+ce^{-100t}$，满足初始条件的特解为 $y(t)=1+t$(即 $c=0$). 由于解是线性的，所以这个问题的欧拉方法理论上是精确的. 为了说明截断误差或舍入误差的影响，给初始值一个轻微的扰动. 取步长 $h=0.1$，对给定的初值，结果为

t	**0.0**	**0.1**	**0.2**	**0.3**	**0.4**
精确解	1.00	1.10	1.20	1.30	1.40
欧拉解	0.99	1.19	0.39	8.59	−64.2
欧拉解	1.01	1.01	2.01	−5.99	67.0

5.2 Parabolic Partial Differential Equations

5.2.1 Explicit(iterative) numerical scheme

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

$$u_t = \nu u_{xx}, \quad 0 < x < 1, \quad t > 0, \tag{5.5}$$

$$u(0,t) = u(1,t) = 0, \quad t \geq 0, \tag{5.6}$$

$$u(x,0) = u^0(x), \quad 0 \leq x \leq 1. \tag{5.7}$$

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 (5.5) 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

$$u(x,t) = \sum_{m=1}^{\infty} a_m e^{-(m\pi)^2 t} \sin m\pi x, \tag{5.8}$$

where a_m is the Fourier coefficients

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

Since there is a finite integer m, (5.8) 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 (5.5) holds at (x_j, t_n), which means spatial point x_j at time step t_n

$$U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n), \tag{5.9}$$

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 (5.9) is referred to 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5.2.1. *Please calculate by (5.9) with* $\nu = 5, f(x, 0) = \cos\frac{\pi x}{2}, a(0, t) = 0, b(1, t) = 0$. *Suggested computational parameters* $N = 100, T = 1, \tau = 0.0015$.

5.2.2 Error Analysis

Does we do the right thing to solve the parabolic equation (5.5)?

定理5.2.1 (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*

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

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5.2.2 (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 $E^n \leq \frac{1}{2}\tau\big(M_{tt} + \frac{1}{6\mu}M_{xxxx}\big)$ 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 5.2.1 (Stable condition for scheme(5.9))**.** *The previous explicit scheme convergent if* $\mu := \frac{\tau}{h^2} \leq \frac{1}{2}$.

Analysis by **Fourier mode**

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

for the solution of finite differentce scheme (5.9) 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 (5.9) divergent! However in the case of convergence, there exist a K independent of k, which makes

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

5.2.3 Implicit schemes

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

$$U_j^{n+1} = U_j^{n+1} + \mu(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) \tag{5.10}$$

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.

- **Thomas algorithm** is most efficient for tri-diagonal system
- using Fourier mode $U_j^n = (\lambda)^n e^{ik(jh)}$ yields

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

  which says the implicit scheme is **unconditionally stable**
- However, the truncation error is same with the explicit one.

Crand-Nickson scheme ($\lambda < -1$): $\mu(1-2\theta) > \frac{1}{2}$ and Leap Frog scheme: $\lambda^2 + 8\lambda\mu\sin^2\frac{1}{2}kh - 1 = 0$ are two constantly used implicit schemes.

定理5.2.3 (Maximum value principle)**.**

$$U_{min} \leq U_j^n \leq U_{max}$$

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 $b(u)$.

5.2.4 Multiple Spatial Dimension

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

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

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

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

交替方向(隐) Alternative Direction Interaction(ADI) Two dimensional Crank-Nicolson scheme

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

with a slight modification

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

- Peaceman D.W. and Rachford H.H. Jr(1955), The numerical solution of parabolic and elliptic differential equations, J. Soc. Indust. Appl. Math. 3, 28-41.

Finally, split into two steps as

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

例5.2.2.

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

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.5.4 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

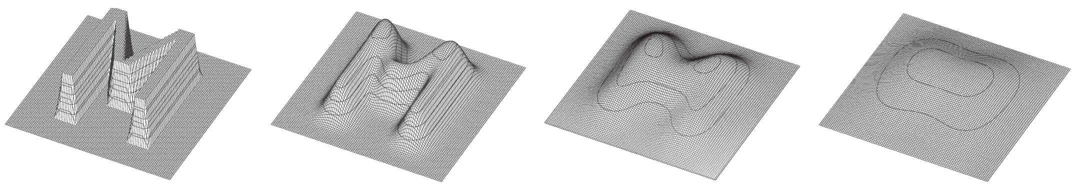
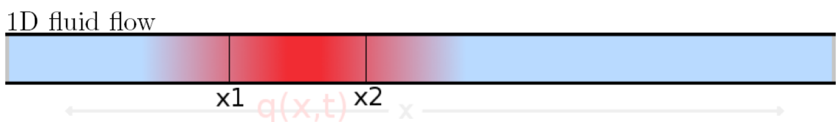


Figure 5.4: From left to right: the numerical solution at $t = 0, 0.001, 0.004$ and $t = 0.01$

5.3 Hyperbolic Partial Differential Equations

输运项(流通量)概念 以如下一维情形为例



$$\int_{x_1}^{x_2} q(x,t)dx = \text{mass of tracer between } x_1 \text{ and } x_2.$$

$$\frac{d}{dt}\int_{x_1}^{x_2} q(x,t)dx = F_1(t) - F_2(t),$$

where F_i is the flux of mass from right to left at x_i.

守恒(Conservation)的积分形式
微分形式：守恒律

For general autonomous flux $F = f(q)$, we have

$$\frac{d}{dt}\int_{x_1}^{x_2} q(x,t)\,\mathrm{d}x = f(q(x_1,t)) - f(q(x_2,t)).$$

For f sufficiently smooth, we have:

$$\frac{d}{dt}\int_{x_1}^{x_2} q(x,t)\,\mathrm{d}x = -\int_{x_1}^{x_2} \frac{\partial}{\partial x} f(q(x,t))\,\mathrm{d}x,$$

which we can write as

$$\int_{x_1}^{x_2} \left[\frac{\partial}{\partial t} q(x,t) + \frac{\partial}{\partial x} f(q(x,t))\right] \mathrm{d}x = 0.$$

A 1D *quasilinear* system

$$q_t + A(q,x,t) q_x = 0$$

is *hyperbolic* at (q,x,t) if $A(q,x,t)$ is diagonalizable with real eigenvalues.

The 1D nonlinear conservation law

$$q_t + f(q)_x = 0$$

is hyperbolic if the Jacobian matrix $\frac{\partial f}{\partial q}$ is diagonalizable with real eigenvalues for each physically relevant q.

Shengtai Li, An HLLC Riemann solver for magneto-hydrodynamics, J. Comp. Phys., 203, 344-357, 2005.

1. 线性化 例: the advection equation

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

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

2. Riemann Problem/Solver

The hyperbolic equation with initial data

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

Consider the linear hyperbolic IVP

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

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

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

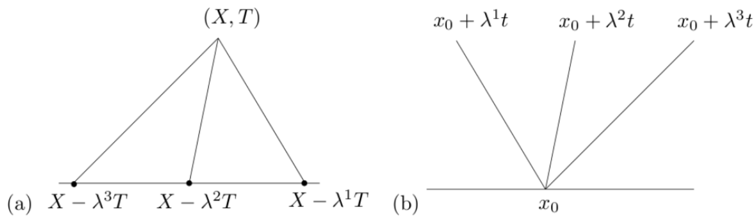


Fig. 3.2. For a typical hyperbolic system of three equations with $\lambda^1 < 0 < \lambda^2 < \lambda^3$, (a) shows the domain of dependence of the point (X, T), and (b) shows the range of influence of the point x_0.

(R. Leveque, 2002)

is known as the Riemann problem.

For the linear constant-coefficient system, the solution is

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

5.3.1 Finite Volume Method

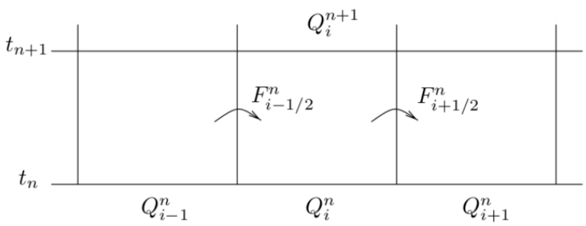
Denote cells $C_i = (x_{i-1/2}, x_{i+1/2})$ and mean values on cells

$$Q_i^n \approx \frac{1}{|C_i|}\int_{C_i} q(x,t_n)dx.$$

FVM update Q_i^{n+1} based on the fluxes F^n between the cells
FVM scheme for 1D conservation law 积分形式的守恒律(Remember that C_i:=$[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$)：

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

时间方向从t_n到t_{n+1}积分后同除以$\triangle x$： 根据平均流量Q和流通量F的定义：



$$\frac{1}{\Delta x}\int_{C_i} q(x,t_{n+1})\,\mathrm{d}x = \frac{1}{\Delta x}\int_{C_i} q(x,t_n)\,\mathrm{d}x - \frac{1}{\Delta x}\left[\int_{t_n}^{t_{n+1}} f(q(x_{i+1/2},t))\,\mathrm{d}t - \int_{t_n}^{t_{n+1}} f(q(x_{i-1/2},t))\,\mathrm{d}t\right].$$

$$Q_i^{n+1} = Q_i^n - \frac{\triangle t}{\triangle x}\left(F_{i+\frac{1}{2}}^n - F_{i-\frac{1}{2}}^n\right),$$

这里$F_{i-\frac{1}{2}} \approx \frac{1}{\triangle t}\int_{t_n}^{t_{n+1}} f(q(x_{i-1/2},t))dt$.

数值流通量(Numerical flux)

For a hyperbolic problem, information propagates at a finite speed. So it is reasonable to assume that we can obtain $F_{i-1/2}^n$ using only the values Q_{i-1}^n and Q_i^n:

$$F_{i-1/2}^n = \mathcal{F}(Q_{i-1}^n, Q_i^n)$$

where $\mathcal{F}$ is some *numerical flux function*. Then our numerical method becomes

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

FVM的收敛性(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)

相容性(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.

稳定性(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 $\triangle t, \triangle x \to 0$

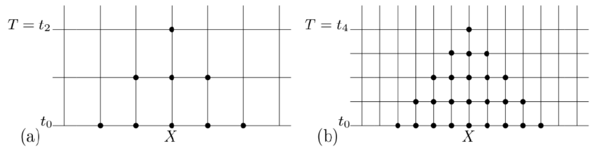


Fig. 4.3. (a) Numerical domain of dependence of a grid point when using a three-point explicit finite difference method, with mesh spacing Δx^a. (b) On a finer grid with mesh spacing $\Delta x^b = \frac{1}{2}\Delta x^a$.

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 !

通量(Flux)函数

To do the calculation,

$$Q_i^{n+1} = Q_i^n - \frac{\triangle t}{\triangle x}\big(F^n_{i+\frac{1}{2}} - F^n_{i-\frac{1}{2}}\big),$$

the key step is to compute the numerical flux term

- ¡2-¿ unstable: $\mathcal{F}(Q^n_{i-1}, Q^n_{i+1}) = \frac{1}{2}\big[f(Q^n_{i-1}) + f(Q^n_i)\big]$
- ¡3-¿ stable: looking into the direction from which the flow come from(upwind), for e.g. $q_t + \lambda q_x = 0$ with $\lambda > 0$, yields

$$Q_i^{n+1} = Q_i^n - \lambda\frac{\triangle t}{\triangle x}(Q_i^n - Q_{i-1}^n) \tag{5.11}$$

Roe 的方案 Recall the numerical method for Conservation Law

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

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

$$F^n_{i-\frac{1}{2}} = \frac{1}{2}\big[f(Q_{i-1}) + f(Q_i)\big] - \frac{1}{2}|A|\big[Q_{i-1} + Q_i\big]$$

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.

Recall the solution to the Riemann problem form a linear system

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

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

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

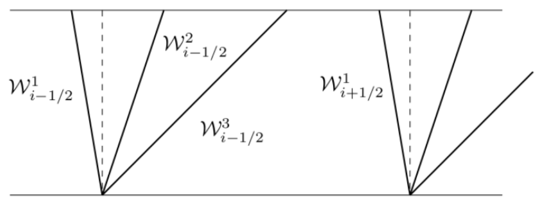


Fig. 4.7. An illustration of the process of Algorithm 4.1 for the case of a linear system of three equations. The Riemann problem is solved at each cell interface, and the wave structure is used to determine the exact solution time Δt later. The wave $\mathcal{W}^2_{i-1/2}$, for example, has moved a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

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

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

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.

Total Variation Diminision(TVD) 方案 Recall the numerical method for Conservation Law

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

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

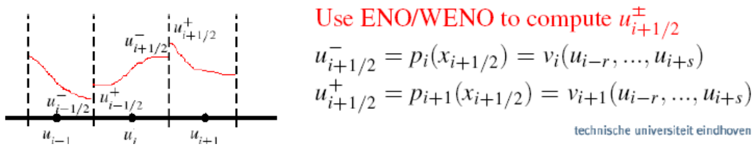
TVD: It is required that the numerical flux function $h(\cdot,\cdot)$ is monotone(Lipschitz continuous, monotone, $h(a, a) = a$)

Example

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

where $\alpha = \max\limits_{u} |f'(u)|$

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



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

1. ¡2-¿ 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

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

2. ¡3-¿ Evaluate u at each cell interface($u^{-}_{i+1/2}$ and $u^{+}_{i+1/2}$)

5.3.2 谱方法(Spectral methods)

Lloyd N. Trefethen:

Spectral methods are one of the "big three" technologies for the numerical solution of PDEs, which came into their own roughly in successive decades:

- 1950s: 有限差分方法
- 1960s: 有限元方法
- 1970s: 谱方法

Fast PDE Solver: $u_t + c(x)u_x = 0$

Remark: The examples and figures are from: Trefethen, spectral method in matlab.

4.Maxwell's Equation The governing equations for Electrodynamics are Understanding FDTD: http://www.eecs.wsu.edu/~schneidj/ufdtd/

Yee's grid The main concept of the Finite Difference Time Domain(FDTD) method is to define different component of the Electric field $\mathbf{E} := (\mathbf{E_x}, \mathbf{E_y}, \mathbf{E_z})$ and the magnetic field $\mathbf{H} := (H_x, H_y, H_z)$ at different surface of the rectangular grid, which is very convenient when discretizing the $\nabla\times$ operator using finite difference method.

Perfect Match Layer(PML) A widely used boundary condition in practical calculation for wave scattering problem in the recent twenty years.

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

```
% p6.m - variable coefficient wave equation

% Grid, variable coefficient, and initial data:
  N = 128; h = 2*pi/N; x = h*(1:N); t = 0; dt = h/4;
  c = .2 + sin(x-1).^2;
  v = exp(-100*(x-1).^2); vold = exp(-100*(x-.2*dt-1).^2);

% Time-stepping by leap frog formula:
  tmax = 8; tplot = .15; clf, drawnow
  plotgap = round(tplot/dt); dt = tplot/plotgap;
  nplots = round(tmax/tplot);
  data = [v; zeros(nplots,N)]; tdata = t;
  for i = 1:nplots
    for n = 1:plotgap
      t = t+dt;
      v_hat = fft(v);
      w_hat = 1i*[0:N/2-1 0 -N/2+1:-1] .* v_hat;
      w = real(ifft(w_hat));
      vnew = vold - 2*dt*c.*w; vold = v; v = vnew;
    end
    data(i+1,:) = v; tdata = [tdata; t];
  end
  waterfall(x,tdata,data), view(10,70), colormap([0 0 0])
  axis([0 2*pi 0 tmax 0 5]), ylabel t, zlabel u, grid off
```

- 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

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

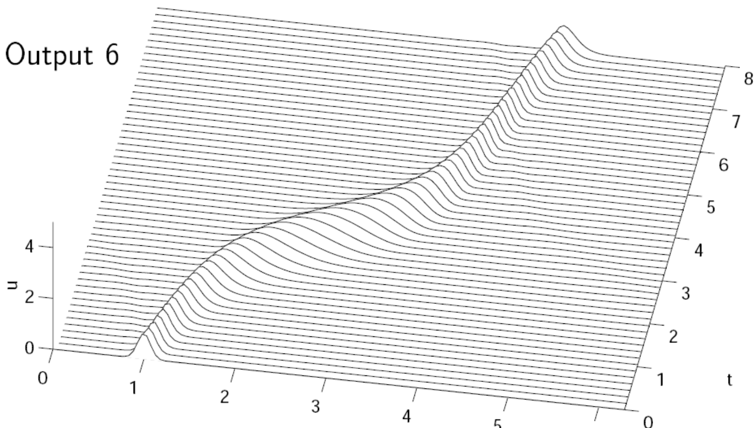
   with proper parameter, boundary and initial conditions

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

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

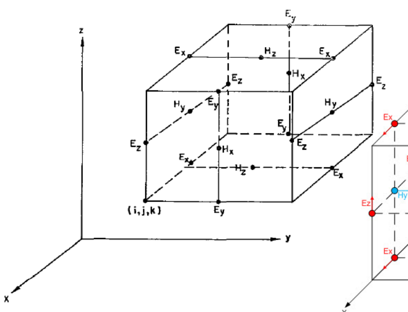
4. **E. F. Toro**, Riemann Solvers and Numerical Methods for Fluid Dynamics, 3rd, Springer-Verlag.

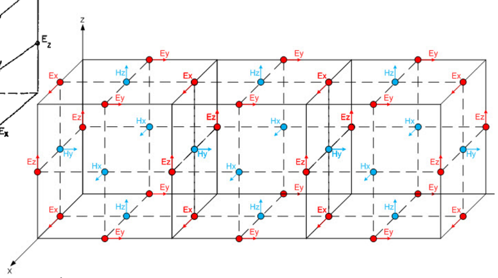
5. **Ferziger Peric**: Computational Methods for Fluid Dynamics, 3rd eds.



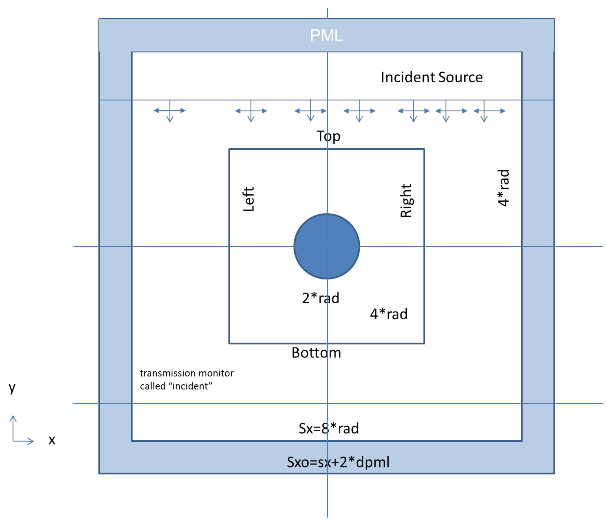
Output 6: Solution of (3.13).

$$
\begin{aligned}
\nabla \cdot \mathbf{D} &= \rho_v, \\
\nabla \cdot \mathbf{B} &= 0, \\
\nabla \times \mathbf{E} &= -\frac{\partial \mathrm{B}}{\partial t}, \\
\nabla \times \mathbf{H} &= \mathbf{J} + \frac{\partial \mathrm{D}}{\partial t}.
\end{aligned}
$$





g. 1. Positions of various field components. The E-components are in the middle of the edges and the H-components are in the center of the faces.


PML
Incident Source
Top
Left
Right
4*rad
2*rad
4*rad
Bottom
transmission monitor
called "incident"
y
x
Sx=8*rad
Sxo=sx+2*dpml