Chapter 5

偏微分方程数值解

偏微分方程(PDE)分类 Let $u := u(x,t)$ defined on a domain Ω, where u satisfy

椭圆型

$$a(x)u_{xx} + b(x)u_x + c(x)u = f(x)$$

抛物型

$$u_t = (b(x,t)u_x)_x + c(x,t)u + d(x,t)$$

双曲型

$$u_{tt} - \nu^2 u_{xx} = f(x)$$

with certain **初值** and/or **边值** conditions.

5.1 椭圆边值问题

5.1.1 五点差分格式

记$u_{i,j}$表示网格点(i,j)上待求函数的近似值，那么

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} &= \frac{-u_{i-1,j}+2u_{i,j}-u_{i+1,j}}{h_x^2}+O(h_x^2)\\ \frac{\partial^2 u}{\partial y^2} &= \frac{-u_{i,j-1}+2u_{i,j}-u_{i,j+1}}{h_y^2}+O(h_y^2).\end{aligned}$$

因此在二维情形（设$h_x = h_y = h$，舍去高阶无穷小项后）可得

$$-\triangle u \approx \frac{1}{h^2}\begin{pmatrix} & -u_{i,j+1} & \\ -u_{i-1,j} & 4u_{i,j} & -u_{i+1,j} \\ & -u_{i,j-1} & \end{pmatrix} \tag{5.1}$$

稀疏Laplace算子-Matlab表示:上述稀疏Laplace算子在Matlab中的实现通常有两中不同的做法

- kron — 基于内部未知点($(n-1)\times(n-1)$个)；
- spLaplacian5.m — 基于全部点($(n+1)\times(n+1)$个)。

推荐采用后一种方案，代价是将边界条件也作为方程，优点是算子离散和边界条件的处理相对独立，因此数学上更直观。

例5.1.1. 考虑如下*Poisson*方程的*Dirichlet*边值问题

$$-\triangle u = f, \quad (x,y)\in[0,1]^2. \tag{5.2}$$

取解析函数

$$u(x,y) = \sin(\pi x)\sin(\pi y), \tag{5.3}$$

作为测试解，相应地取$f = 2\pi^2 u(x,y)$。

实现细节参考testPoisson.m以及相关.m文件。

5.1.2 非线性问题

考虑如下形式的"半"线性问题

$$-\triangle u + f(\mathbf{x}, u) = g, \quad \mathbf{x}\in\Omega\subset\mathbf{R}^2 \tag{5.4}$$

仍取前例中的解析函数作为测试解，此外令

$$f(\mathbf{x}, u) = u^3. \tag{5.5}$$

右端项g根据u和f的表达式可计算得到，参考fung.m

离散格式

可在所有内点$i,j = 1,\cdots,n-1$上建立方程

$$\frac{1}{h^2}\begin{pmatrix} & -u_{i,j+1} & \\ -u_{i-1,j} & 4u_{i,j} & -u_{i+1,j} \\ & -u_{i,j-1} & \end{pmatrix} + f(x_i, y_j, u_{i,j}) = g_{i,j}.$$

如果f中不包含一阶微分算子(反应-扩散问题)，那么f(线性化后)只对$u_{i,j}$有贡献，若考虑带一阶微分算子项的f,称为对流-扩散问题。不妨将上述代数方程简记为

$$A\mathbf{u} + f(\mathbf{u}) = \mathbf{g} \tag{5.6}$$

Newton迭代格式

令$F(\mathbf{u}) = A\mathbf{u} + f(\mathbf{u}) - \mathbf{g}$ 则有Newton迭代

$$\mathbf{u}^{new} = \mathbf{u}^{old} - F'(\mathbf{u}^{old})^{-1}F(\mathbf{u}^{old}) \tag{5.7}$$

其中$F'(\mathbf{u}) = A + f'(\mathbf{u})$. Matlab实现的时候会引进一些额外的变量以及向量化，请参考test_semi_newton.m

例5.1.2 (练习)**.**

- 修改算例一(用不同u)，记录$h = 10, 20, 40, 80, 160, 320$时数值解的$L_2$或$L_\infty$误差，计算收敛阶
- 修改半线性问题算例，计算$Newton$迭代法的收敛阶
- 尝试将上述方法扩展至x-和y-方向的区间和步长不一致的情形：$h_x \neq h_y$以及$(x, y) \in [a, b] \times [c, d]$
- 尝试变更方程编号的顺序（列优先或其他感兴趣的顺序）
- 进一步研究如何利用$Newton$迭代法求逆矩阵，以及其他可能加速求解线性方程足的方法

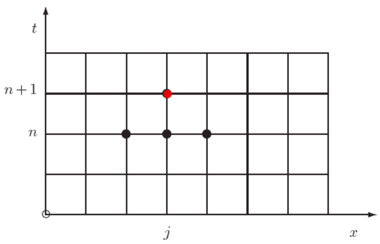
5.2 抛物型

一维(空间)模型 热传导过程的数学建模

$$u_t = \nu u_{xx}, \quad x \in (0,1), \quad t > 0 \tag{5.8}$$
$$u(x,0) = f(x), \quad x \in [0,1] \tag{5.9}$$
$$u(0,t) = a(t), \quad t \geq 0 \tag{5.10}$$
$$u(1,t) = b(t), \quad t \geq 0 \tag{5.11}$$

where $f(0) = a(0)$ and $f(1) = b(1)$.

显格式(Explicit Schemes) Let h and τ be the spacing, then $x_j = jh, t_n = n\tau$. So that



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

Then at (x_j, t_n) the 1D parabolic equation yields $\left(\mu = \nu \frac{\tau}{(h)^2}\right)$

$$U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n), \tag{5.12}$$

It is preferred 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

- 算例参数：$\nu = 5, f(x, 0) = \cos\frac{\pi x}{2}, a(0, t) = 0, b(1, t) = 0$
- 计算参数：$N = 100, T = 1, \tau = 0.0015$

相容性：Does it do the right thing?

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*

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

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 $(x^*, t^*) \in (0,1) \times (0,T)$,*

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

- **Approximation Error:** $e_j = U_j^n - u(x_j, t_n)$
- 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 yield $E^n \le \frac{1}{2}\tau\left(M_{tt} + \frac{1}{6\mu}M_{xxxx}\right)$ 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.

- The previous explicit scheme convergent if $\mu := \frac{\tau}{h^2} \le \frac{1}{2}$.

Fourier(误差)分析方法 Using **Fourier mode**

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

as the solution of the finite differentce scheme (5.12) it yields

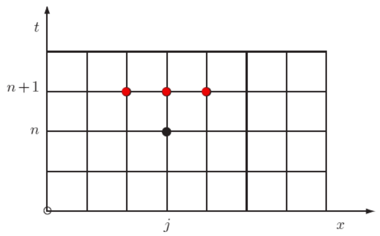
$$\begin{aligned}\lambda &:= \lambda(k) = 1 + \mu(e^{ikh} - 2 + e^{-ikh}) \\ &= 1 - 2\mu(1 - cos(kh)) \\ &= 1 - 4\mu sin^2 \frac{1}{2} kh\end{aligned}$$

- Since $U_j^{n+1} = \lambda U_j^n$, λ is referred as **amplification factor**
- 特殊频率$k = m\pi$处, $\mu > \frac{1}{2}$ makes $\lambda > 1$,导致发散
- **stable**: there exist a K independent of k, which makes

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

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

$$U_j^{n+1} = U_j^{n+1} + \mu(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) \tag{5.13}$$



The implicit scheme yields

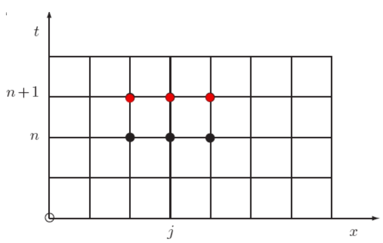
$$-\mu U_{j-1}^{n+1} + (1 + 2\mu)U_j^{n+1} - \mu U_{j+1}^{n+1} = U_j^n, \qquad \forall j = 1, 2, \ldots, (N - 1).$$

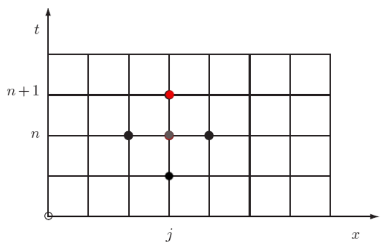
U_0^{n+1} and U_N^{n+1} are known with the boundary condition.

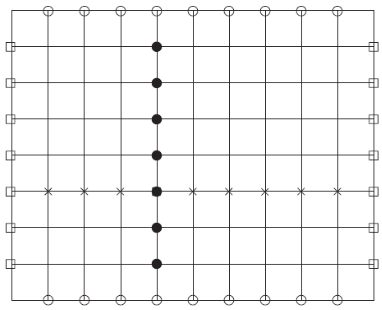
- **Thomas algorithm** is most efficient for tri-diagonal system
- using Fourier mode $U_j^n = (\lambda)^n e^{ik(jh)}$ yields

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

which says the implicit scheme is **unconditionally stable**







- However, the truncation error is same with the explicit one.

其他隐格式

- Crand-Nickson(Left, $\lambda < -1$): $\mu(1-2\theta) > \frac{1}{2}$
- Leap Frog(Right): $\lambda^2 + 8\lambda\mu\sin^2\frac{1}{2}kh - 1 = 0$

更一般的边界条件

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

- First order: $\frac{U_1^n - U_0^n}{h} = \alpha^n U_0^n + g^n$
- Second order: $\frac{2U_0^n - 3U_1^n + U_2^n}{h} = \alpha^n U_0^n + g^n$

非线性

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

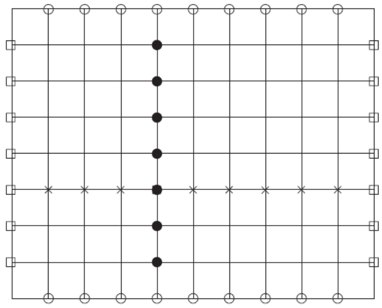
The linearization is necessary at each time step

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

- 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 $b(u)$

空间变量多元情形 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 $\triangle y$

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

- Explicit scheme

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

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

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

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.

At last, split into two steps as

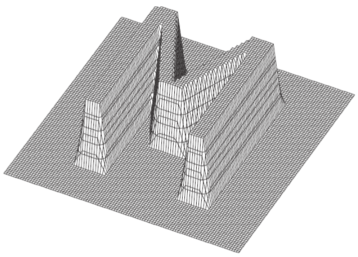
$$\begin{aligned}(1 - \frac{1}{2}\mu_x\delta_x^2)U^{n+\frac{1}{2}} &= (1 + \frac{1}{2}\mu_y\delta_y^2)U^n \\ (1 - \frac{1}{2}\mu_y\delta_y^2)U^{n+1} &= (1 + \frac{1}{2}\mu_x\delta_x^2)U^{n+\frac{1}{2}}\end{aligned}$$

延伸：算子分裂法

一个算例

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

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



- set $f(x, y)$ as any function you like, for e.g.,
- try different $\triangle x$ and $\triangle y$, for e.g. $\frac{1}{100}, \frac{1}{200}, \frac{1}{400}$
- try the implicit scheme and the ADI iterative method

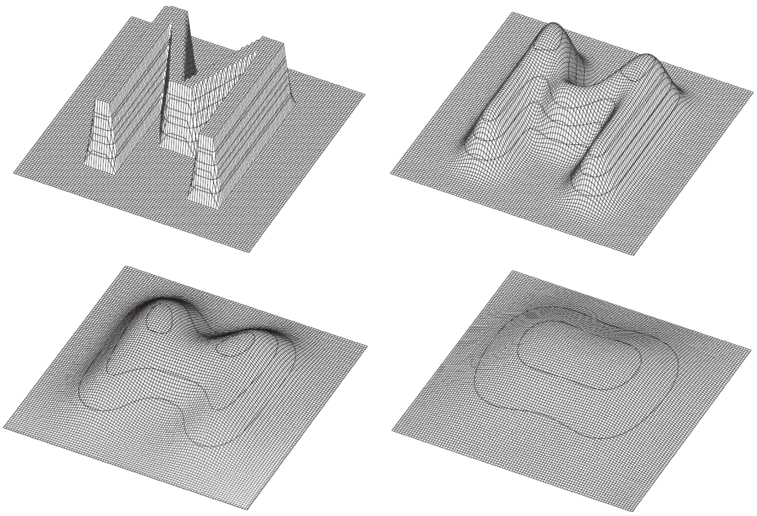


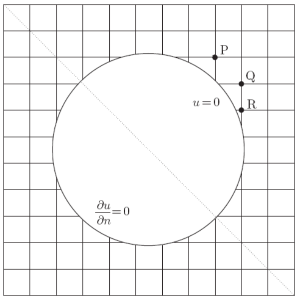
Figure 5.1: Numerical solution at $t = 0$(Upper Left), $t = 0.001$(Upper right), $t = 0.004$(Lower Left) and $t = 0.01$(Lower Right)

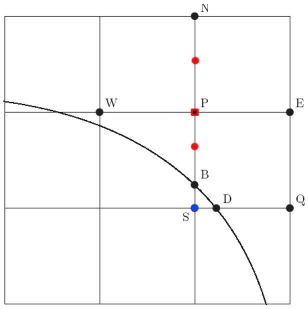
非规则区域的边界处理

1. Set up equation at P with non-uniform finite difference scheme
2. Firstly **Extrapolating**(外插) at S with B,N and P, and take S and the new boundary point, for e.g. with second order,

$$U_S = \frac{\alpha(1-\alpha)u_N + 2u_B - 2(1-\alpha^2)u_P}{\alpha(\alpha+1)},$$

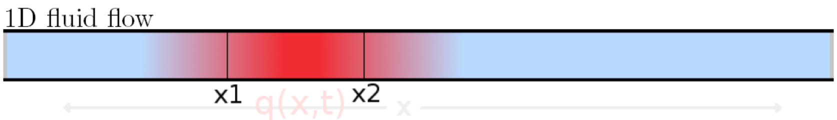
where $|PB| = \alpha|PS| := \alpha\triangle y$





5.3 双曲型

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

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

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.

2. Riemann Problem/Solver

The hyperbolic equation with initial data

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

is known as the Riemann problem.

For the linear constant-coefficient system, the solution is

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

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

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

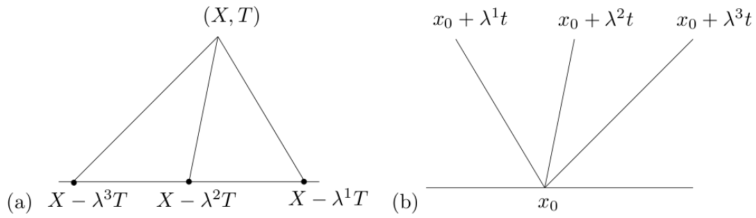


Fig. 3.2. For a typical hyperbolic system of three equations with $\lambda^1 < 0 < \lambda^2 < \lambda^3$, (a) shows the domain of dependence of the point (X, T), and (b) shows the range of influence of the point x_0.

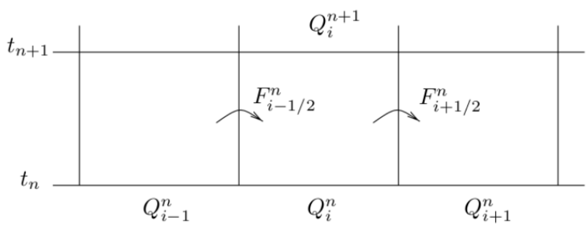
(R. Leveque, 2002)

5.3.1 2.有限体积法(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：

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

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

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 $\triangle t, \triangle x \to 0$
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 !

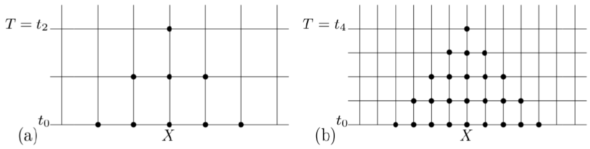


Fig. 4.3. (a) Numerical domain of dependence of a grid point when using a three-point explicit finite difference method, with mesh spacing Δx^a. (b) On a finer grid with mesh spacing $\Delta x^b = \frac{1}{2}\Delta x^a$.

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

$$Q_i^{n+1} = Q_i^n - \lambda\frac{\triangle t}{\triangle x}(Q_i^n - Q^n_{i-1}) \tag{5.14}$$

Roe 的方案 Recall the numerical method for Conservation Law

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

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

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

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

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

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:
$$\tilde{q}^n(x, t_n) = Q_i^n, \quad \text{for all } x \in C_i.$$
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
$$Q_i^{n+1} = \frac{1}{\Delta x}\int_{C_i} \tilde{q}^n(x, t_{n+1})\,\mathrm{d}x.$$

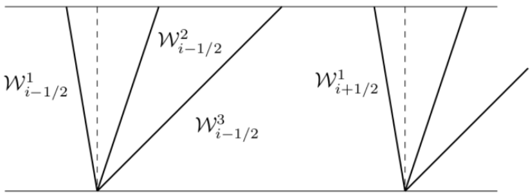


Fig. 4.7. An illustration of the process of Algorithm 4.1 for the case of a linear system of three equations. The Riemann problem is solved at each cell interface, and the wave structure is used to determine the exact solution time Δt later. The wave $\mathcal{W}^2_{i-1/2}$, for example, has moved a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

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

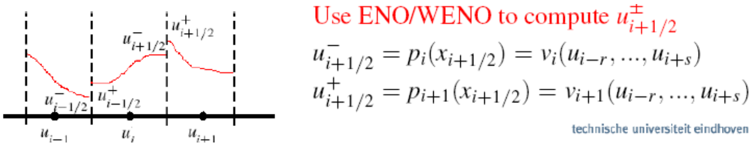
Total Variation Diminision(TVD) 方案 Recall the numerical method for Conservation Law
$$Q_i^{n+1} = Q_i^n - \frac{\triangle t}{\triangle x}\big[\mathcal{F}(Q_i^n, Q_{i+1}^n) - \mathcal{F}(Q_i^n, Q_{i+1}^n)\big],$$
where $\mathcal{F}(Q_i^n, Q_{i+1}^n) \approx F^n_{i+\frac{1}{2}} = h(Q^-_{i+\frac{1}{2}}, Q^+_{i+\frac{1}{2}})$.

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

(Weighted) Essentially Non-Oscillatory$\big($(W)ENO$\big)$ 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: $u_t + c(x)u_x = 0$

```
% 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
```

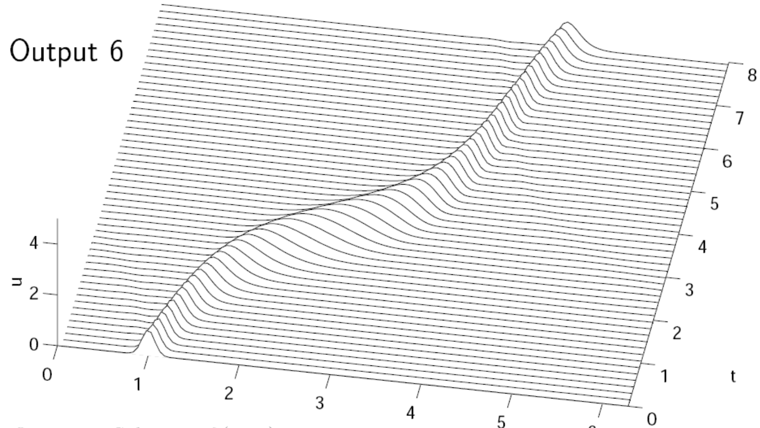
Remark: The examples and figures are from: Trefethen, spectral method in matlab.

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.

Textbook for Computational Electrodynamics



Output 6: Solution of (3.13).

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

- A. Taflove and S. C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method, 3rd ed.

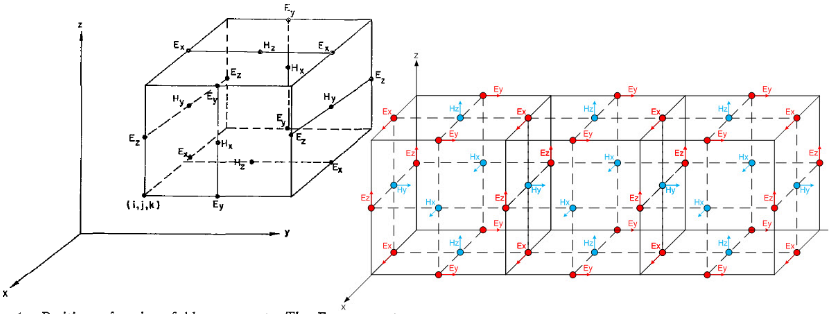
软件包与参考教材

- 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.

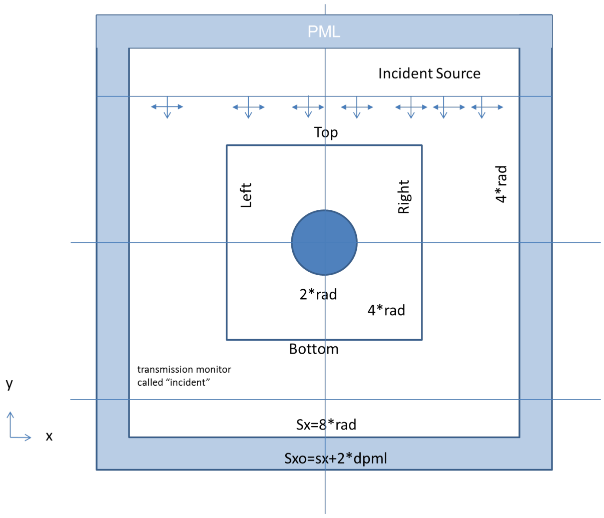
Please do not reproduce this text; all rights are reserved. Copies can be obtained for \$22 or £15 each (including shipping) by contacting me directly. Professors who are using the book in class may contact me to obtain solutions to most of the problems. [This is no longer true – the book is freely available online at `http://web.comlab.ox.ac.uk/oucl/work/nick.trefethen/pdetext.html`.]

Nick Trefethen
July 1996

http://people.maths.ox.ac.uk/trefethen/pdetext.html



ı. 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.



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.

11,644 total Google Scholar (GS) citations for the three editions of *Computational Electrodynamics: The Finite-Difference Time-Domain Method* (Books #2, #4, and #5) as of 7/23/2013.

This ranks 7th on the Google Scholar search conducted in September 2012 by the Institute of Optics of the University of Rochester for the all-time most-cited books in physics.

1. K. R. Umashankar and A. Taflove, *Computational Electromagnetics: Integral Equation Approach.* Norwood, MA: Artech House, 1993.

2. A. Taflove, *Computational Electrodynamics: The Finite-Difference Time-Domain Method.* Norwood, MA: Artech House, 1995. (Download the 1995 book front matter.pdf)

3. A. Taflove, ed., *Advances in Computational Electrodynamics: The Finite-Difference Time-Domain Method.* Norwood, MA: Artech House, 1998. (Download the 1998 book front matter.pdf)

4. A. Taflove and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method, 2nd ed.* Norwood, MA: Artech House, 2000. (Download the 2000 book front matter.pdf)

5. A. Taflove and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method, 3rd ed.* Norwood, MA: Artech House, 2005. (Download the 2005 book front matter.pdf ; visit the Publisher's webpage ; read the book reviews: IEEE EMC review.pdf and IEEE APS review.pdf)

6. A. Taflove, A. Oskooi, and S. G. Johnson, eds., *Advances in FDTD Computational Electrodynamics: Photonics and Nanotechnology*. Norwood, MA: Artech House, 2013. (Download the 2013 book front matter.pdf ; visit the Publisher's webpage)