Chapter 5

Numerical Solution to Partial Differential Equation

5.0.1 数值求导

求f'(x)数值格式

微分是一个很敏感的问题,一些小扰动可能会产生很大的误差,在进行数值求导的过程中也需要考虑其稳定性。请用Taylor公式验证上述格式的精度分别为o(h)以及 $o(h^2)$.

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

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

求f''(x)数值格式

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展升:

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

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

5.1 初值问题

n 阶常微分方程

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

可以化成一阶方程组:

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

其分量形式为:

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

定解条件: $\mathbf{y}(t_0) = \mathbf{y}_0$

例5.1.1. F = ma在给定初始位置s(0)和初始速度s'(0)后位移s(t)可解.

例 10.5 稳定边值问题 考虑常微分方程的初值问题

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} \lambda & 0 \\ 0 & -\lambda \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \quad \mathbf{y}(0) = \mathbf{y}_0.$$

其中 $Re\lambda \neq 0$,它的两种模式中的一个按指数增长,所以是不稳定的. 但如果 $Re\lambda < 0$,并且给出在区间[0,6]上的边界条件

$$y_1(0)=1$$
, $y_2(b)=1$,

则即使 6 非常大,边值问题也是稳定的,因为解的增长将受到约束条件的限制.

定理5.1.1 (初值问题解的存在唯一性). 当 $\mathbf{f}: \mathbf{R}^{n+1} \to \mathbf{R}^n$ 是区域D上是Lipschitz连续,即

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

时,对给定区域D内任意初始点,初值问题存在唯一解。

对初值问题来说,问题的数据为初值 y_0 及函数 f. 设 $\hat{y}(t)$ 为初值问题 $\hat{y}' = f(t,\hat{y})$ 的解,带有扰动的初始条件为 $\hat{y}(t_0) = \hat{y}_0$. 可以证明,对任意 $t \ge t_0$.有

$$\|\hat{\mathbf{y}}(t) - \mathbf{y}(t)\| \leqslant e^{L(t-t_0)} \|\hat{\mathbf{y}}_0 - \mathbf{y}_0\|.$$

如果函数 f 也带有扰动,初值问题变为 $\hat{y}' = \hat{f}(t,\hat{y})$,则对任意 $t \ge t_0$,有

$$\parallel \hat{\boldsymbol{y}}(t) - \boldsymbol{y}(t) \parallel \leqslant e^{L(t-t_0)} \parallel \hat{\boldsymbol{y}}_0 - \boldsymbol{y}_0 \parallel + \frac{e^{L(t-t_0)} - 1}{L} \parallel \hat{\boldsymbol{f}} - \boldsymbol{f} \parallel,$$

其中 $\|\hat{f} - f\| = \max_{(t,y) \in D} \|\hat{f}(t,y) - f(t,y)\|$. 上述关于扰动的估计表明初值问题的惟一解是关于问题数据的连续函数,因而问题是适定的.

稳定性

Stiffness ODE的Jacobi矩阵特征值相互差别极大,则称它是刚性的!

5.1.1 数值方法一览

Euler法、Taylor级数法、Runge-Kutta法、线性多步法

例 9.6 解的稳定性 对于例 9.2, 当 n=1 时, 常微分方程为 y'=b,b 为给定常数, 它的解是一族斜率为 6 的平行直线,如图 9.1 所示. 这个常微分方程的解是稳定的,但并 不渐近稳定. 进一步, 当λ为常数时,常微分方程

$$y' = \lambda y$$

的解为

 $y(t) = y_0 e^{\lambda t}$,

其中 $t_0 = 0$ 是初始时间, $y(0) = y_0$ 是初始值. 例 9.5 是 y_0 这个常微分方程在λ=1时的特殊情形,图 9.2 画出了 它的部分解、当λ>0时,由于所有非零解都按指数递 增,如图 9.2 所示,所以任何两个解之间都不相互收 敛,因而每个解都是不稳定的.另一方面,当 λ <0时,所 有非零解都按指数下降,如图 9.3 所示,任何两个解都 点 相互收敛. 因而在这种情形,每个解不仅稳定,而且渐 近稳定. 如果 $\lambda = a + ib$ 是复数,则由 1.3.11 节知

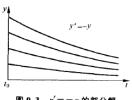


图 9.3 y'=-y 的部分解

$$e^{\lambda t} = e^{(\alpha + ib)t} = e^{\alpha t} e^{ibt} = e^{\alpha t} (\cos(bt) + i\sin(bt))$$

这样,解是按指数增加还是减少将由 ReA 的符号确定. 特别地,若 ReA>0,则解是不稳定 的;若 Rea<0,则解是渐近稳定的;如果 Rea=0,则解是振荡的,但由于相互之间保持一 定距离,所以虽然稳定,但不渐近稳定。

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

1. 欧拉(Euler)法

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%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5.1.2 (Euler). Considering the following initial problem:

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

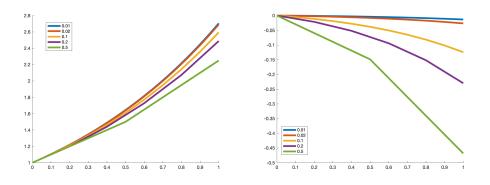


Figure 5.1: (Left) The Euler solution, (Right) Errors

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:

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

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):

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

2. Taylor级数法

例5.1.3 (Taylor series). Considering the following nonlinear ODE:

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

The Taylor series of above equation is:

$$y = y_0 + hy_0' + \frac{h^2}{2}y_0'' + \dots,$$

where $y_0' = 0, y_0'' = -2, y'' = 2y^2(4x^2y - 1)$

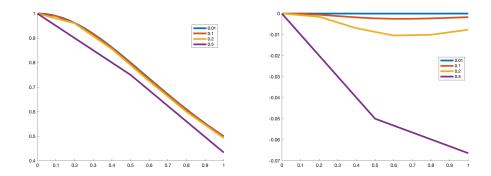


Figure 5.2: (Left) The Taylor series solution, (Right) Errors

3. Runge-Kutta方法- 显式

 $ia_{i,j}, c_i(i-2,3,\ldots,s;j< i)$ 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:

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

其中,

$$k_1 = f(x_m, y_m),$$

$$k_2 = f(x_m + c_2h, y_m + ha_{2,1}k_1),$$

$$k_3 = f(x_m + c_3h, y_m + h(a_{3,1}k_1 + a_{3,2}k_2)),$$

$$\dots$$

$$k_s = f(x_m + c_sh, y_m + h(a_{s,1}k_1 + \dots + a_{s,s-1}k_s - 1))$$

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。

例5.1.4 (explicit Runge-Kutta method(example 9.12)). Using Heun method to solve the following ODE:

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

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

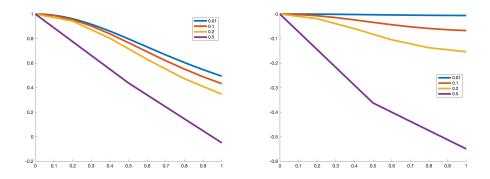


Figure 5.3: (Left) The Runge-Kutta solution with Heun formula, (Right) Errors

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

$$y_{k+1} = y_k + \frac{h_k}{6} (k_1 + 2k_2 + 2k_3 + k_4), \tag{5.1}$$

with the definition of momentum

$$k_1 = f(t_k, y_k),$$

$$k_2 = f(t_k + \frac{1}{2}h_k, y_k + \frac{1}{2}h_k k_1),$$

$$k_3 = f(t_k + \frac{1}{2}h_k, y_k + \frac{1}{2}h_k k_2),$$

$$k_4 = f(t_k + h_k, y_k + h_k k_3),$$

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:

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

3. Runge-Kutta方法- 隐式

如果 k_i 的计算中用到了所有的k值,即:

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

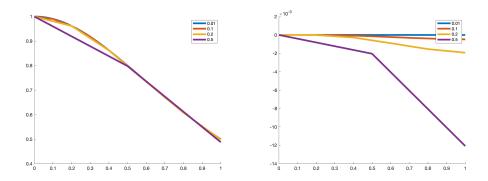


Figure 5.4: (Left) The Runge-Kutta solution with Hammer formula, (Right) Errors

其中k;满足:

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

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。

单步法。以上的方法都属于单步法,即形如:

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

其中○被称为单步法的增量函数。单步法的截断误差可表示为

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

稳定性与收敛性

定义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。

定义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。

定义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

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

4.线性多步法

对于y' = f(x, y), $i \exists y_m = y(x_m), f_m = f(x_m, y_m), 则:$

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

其中 $k \in \mathbb{N}^+$, $\{\alpha_i\}$ 是给定实数, h是步长。则截断误差为:

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

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:

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

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.

5.2 抛物型

一维(空间)模型 热传导过程的数学建模

$$u_t = \nu u_{xx}, \quad x \in (0,1), \quad t > 0$$
 (5.2)

$$u(x,0) = f(x), x \in [0,1]$$
 (5.3)

$$u(0,t) = a(t), \qquad t \ge 0 \tag{5.4}$$

$$u(1,t) = b(t), t \ge 0 (5.5)$$

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

$$\frac{\partial u}{\partial t}(x_{j}, t_{n}) \approx \frac{u(x_{j}, t_{n+1}) - u(x_{j}, t_{n})}{\tau} \Gamma := \frac{U_{j}^{n+1} - U_{j}^{n}}{\tau}$$

$$\frac{\partial^{2} u}{\partial x^{2}}(x_{j}, t_{n}) \approx \frac{u(x_{j+1}, t_{n}) - 2u(x_{j}, t_{n}) + u(x_{j-1}, t_{n})}{(h)^{2}}$$

$$:= \frac{U_{j+1}^{n} - 2U_{j}^{n} + U_{j-1}^{n}}{(h)^{2}}$$

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 $t_2=0$. 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 y_2 处的值,得到相应的导数值 $y_2'=-0.5971$. 在相应的隐式方法中(在这里为梯形公式) 将这些预估值代人,得到解的校正值

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

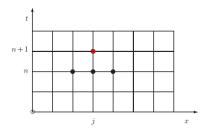
用这个新的 y_2 再计算 f 的值,得到改进值 $y_2' = -0.6528$,以便在下一步计算时使用. 到这里,完成了 PECE 程序的一步. 如果需要的话,还可以反复校正,直到收敛. 这个问题的精确解为 $y(t) = 1/(1+t^2)$,因而在积分点上的真值为 y(0.25) = 0.9412, y(0.5) = 0.8.

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

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

和隐式四阶 Adams-Moulton 校正格式

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



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

$$U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n), \tag{5.6}$$

It is preferred as an **explicit Scheme**.

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 \begin{array}{|c|c|c|c|c|}\hline \mathbf{1} & \text{Given } \nu, f, [a,b] \text{ and } N, T, \tau; \\ \mathbf{2} & h = (b-a)/N \text{ and set } x_j = j*h, \forall j = 0, 1, \cdots, N; \\ \mathbf{3} & \mathbf{u} = \operatorname{zeros}(N+1, T+1) ; \\ \mathbf{4} & \text{for } n = 1, 2, \cdots, T \text{ do} \\ \mathbf{5} & u(0,n) = a(n\tau); u(N,n) = b(n\tau); \\ \mathbf{6} & \text{for } j = 1, 2, \cdots, N-1 \text{ do} \\ \mathbf{7} & U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n); \\ \mathbf{8} & \text{end} \\ \mathbf{9} & \text{end} \\ \end{array}
```

- 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):

$$T(x,t) = \frac{u(x,t+\tau) - u(x,t)}{\tau} - \nu \frac{(u(x+h,t) - 2u(x,t) + u(x-h,t))}{h^2}$$

$$= (u_t(x,t) + \frac{\tau}{2}u_{tt}(x,t) + \ldots) - \nu (u_{xx} + \frac{h^2}{12}u_{xxxx} + \ldots)$$

$$\approx \frac{\tau}{2}u_{tt}(x,t) - \frac{\nu h^2}{12}u_{xxxx}$$

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

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

- 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 $E^n \leq \frac{1}{2}\tau \left(M_{tt} + \frac{1}{6\mu}M_{xxxx}\right)$ 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 $\mu := \frac{\tau}{h^2} \leq \frac{1}{2}$.

Fourier(误差)分析方法 Using Fourier mode

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

as the solution of the finite difference scheme (5.6) it yields

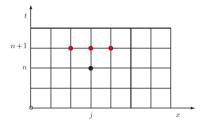
$$\lambda := \lambda(k) = 1 + \mu(e^{ikh} - 2 + e^{-ikh})$$
$$= 1 - 2\mu(1 - \cos(kh))$$
$$= 1 - 4\mu \sin^2 \frac{1}{2}kh$$

- 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 $\mu = \frac{\tau}{h^2} \leq \frac{1}{2}$ 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

$$U_j^{n+1} = U_j^{n+1} + \mu(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1})$$
 (5.7)



The implicit scheme yields

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

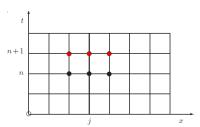
 U_0^{n+1} and U_N^{n+1} are known with the boundary condition.

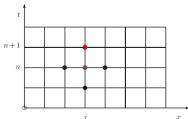
- Thomas algorithm is most efficient for tri-diagonal system
- $\bullet\,$ using Fourier mode $U^n_j=(\lambda)^n e^{ik(jh)}$ yields

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

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)

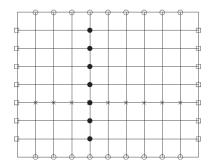
空间变量多元情形 Let Ω be a rectangular domain $(0,X) \times (0,Y)$ Find a function u(x,y,t) defined on Ω

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

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 $\triangle y$

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



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.

At last, split into two steps as

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

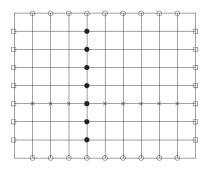
$$(1 - \frac{1}{2}\mu_y \delta_y^2) U^{n + 1} = (1 + \frac{1}{2}\mu_x \delta_x^2) U^{n + \frac{1}{2}}$$

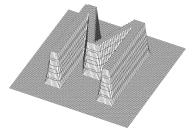
延伸: 算子分裂法 一个算例

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

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 非规则区域的边界处理
- 1. Set up equation at P with non-uniform finite difference scheme
- 2. Firstly $\mathbf{Extrapolating}($ 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

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($a \le x \le b$)?

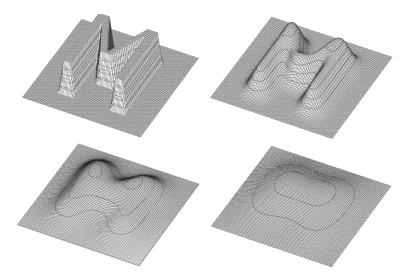
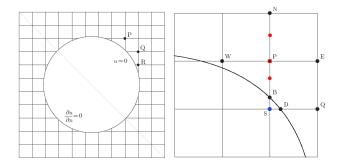


Figure 5.5: Numerical solution at t=0 (Upper Left), t=0.001 (Upper right), t=0.004 (Lower Left) and t=0.01 (Lower Right)



2. Riemann Problem/Solver

The hyperbolic equation with initial data

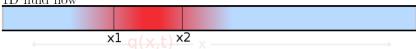
$$q_0(x) = \begin{cases} q_l & x < 0 \\ q_r & x > 0 \end{cases}$$

is known as the Riemann problem.

For the linear constant-coefficient system, the solution is

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

1D fluid flow



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

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

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

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

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

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 $C_i := [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}])$:

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

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:

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

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)

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.

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

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

FVM的收敛性(Convergence)

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

The method be *consistent*, which promises the local truncation error goes to 0 as $\triangle t \rightarrow 0$. 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 $\Delta t \to 0$ 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 $\Delta t, \Delta x \to 0$

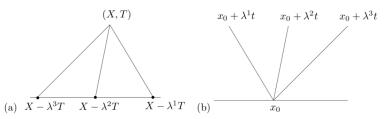
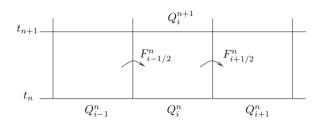


Fig. 3.2. For a typical hyperbolic system of three equations with $\lambda^1 < 0 < \lambda^2 < \lambda^3$, (a) shows the domain of dependence of the point (X, T), and (b) shows the range of influence of the point x_0 .

(R. Leveque, 2002)



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

$$\frac{\triangle x}{\triangle t} \ge \max_{p} |\lambda^{p}|, \qquad p = 1, \dots, m.$$

This condition is necessary but not sufficient!

通量(Flux)函数

To do the calculation,

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

the key step is to compute the numerical flux term

- ¡2-¿ unstable: $\mathcal{F}(Q_{i-1}^n, Q_{i+1}^n) = \frac{1}{2} [f(Q_{i-1}^n) + f(Q_i^n)]$
- ¡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

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

$$\tag{5.8}$$

Roe 的方案 Recall the numerical method for Conservation Law

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

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

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

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

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

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

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

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

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

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

or

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

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

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

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

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

Example

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

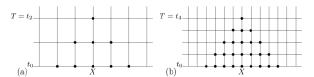


Fig. 4.3. (a) Numerical domain of dependence of a grid point when using a three-point explicit finite difference method, with mesh spacing Δx^a . (b) On a finer grid with mesh spacing $\Delta x^b = \frac{1}{2}\Delta x^a$.

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:

$$\tilde{q}^n(x,t_n) = Q_i^n$$
, 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

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

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

(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

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

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: $u_t + c(x)u_x = 0$

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

4.Maxwell's Equation The governing equations for Electrodynamics are Understanding FDTD:

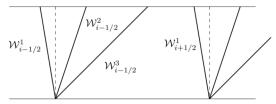
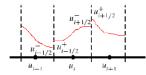


Fig. 4.7. An illustration of the process of Algorithm 4.1 for the case of a linear system of three equations. The Riemann problem is solved at each cell interface, and the wave structure is used to determine the exact solution time Δt later. The wave $W_{i-1/2}^2$, for example, has moved a distance $\lambda^2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



Use ENO/WENO to compute
$$u_{i+1/2}^{\pm}$$
 $u_{i+1/2}^{-} = p_i(x_{i+1/2}) = v_i(u_{i-r},...,u_{i+s})$ $u_{i+1/2}^{+} = p_{i+1}(x_{i+1/2}) = v_{i+1}(u_{i-r},...,u_{i+s})$ technische universiteit eindhoven

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 $\mathbf{E} := (\mathbf{E}_{\mathbf{x}}, \mathbf{E}_{\mathbf{y}}, \mathbf{E}_{\mathbf{z}})$ 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
- 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

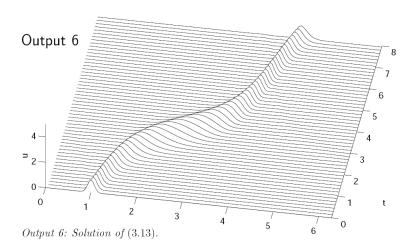
$$e\frac{\partial u}{\partial t} = \nabla \cdot (b\nabla u - \mathbf{a}u) + cu + d,$$

with proper parameter, boundary and initial conditions

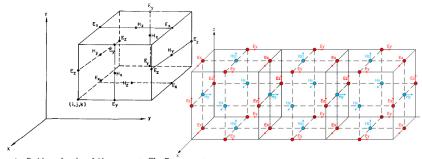
2. Further numerically study of the quenching phenomenon (quenching1d.pdf)

```
% 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 = e|xp(-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;
   data(i+1,:) = v; tdata = [tdata; t];
 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
```

- 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.



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



; 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.

