Numerical Partial Differential Equation

Lecture Notes

By

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Historical Background

- Not pure theoretical analysis, close to experimental branch
- Mathematical theory for numerical solutions of nonlinear P.D.E. is inadequate

1910 L.F. Richardson： (1)Point iterative scheme for Laplace and biharmonic equations
(2)Distinguish the scheme for hyperbolic and elliptic problems

1928 Courant, Friedrichs, Lewy： CFL stability analysis for hyperbolic P.D.E. numerical solution

1918 Liebmann：Relaxation method

1940 Southwell：Residual relaxiation

1950 von Neumann, O'Brien, Hyman, Kaplan：
(1)Stability analysis for time marching problem
(2)Widely used technique in C.F.D. for determining stability

1954 Peter Lax： (1)shock-capturing procedure for shock
(2)applied in conservation-law form of the governing equations
(3)No special requirement is needed

1950 von Neumann, Richtmyer： (1)shock smearing procedure
(2)adding artificial viscosity (explicit)

1950 Frankel： (1)SOR for Laplace equation
(2)significant improvement in convergence rate

1955 Peaceman, Rachford, Douglas：
(1)ADI schemes for parabolic and elliptic equation
(2)ADI is probably the most popular method for incompressible vorticity transport equations

1953 DuFort, Frankel： (1)Leap frog method for parabolic equation
(2)Fully explicit
(3)Arbitarily large time step if no advection Term is appeared

1957 Evans, Harlow at Los Alamos：
(1)Particle In Cell (PIC)
(2)Implicit dissipation to smear out the shock

1962 Gary： (1)technique for fitting the moving shock
(2)avoid smearing in shock-capturing procedure

1966 Moretti, Abbett, Moretti, Bleich：
shock fitting procedure for supersonic flow over various configuration

1960 Lax, Wendroff： (1) 2nd order scheme
(2) A avoid excessive smearing in previous work
(3)Implicit dissipation terms

1969 MacCormack shock smearing

Review Articles

Books

1957 Richtmyer

1967 Richtmyer and Morton------Parabolic, Hyperbolic (Marching Problem)

1960 Forsythe-----------Elliptic problem

1965 Wasow

1969 Ames---------------Nonlinear numerical methods Papers

1981 Hall

1965 Macagno, Harlow, Fromm

1982 Levine

Governing Equations

Conservation Form

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}+\frac{\partial H}{\partial z}=N$$

$$U=\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho w\\ \rho\hat{u}\end{bmatrix}\qquad N=\begin{bmatrix}0\\ \rho B_x\\ \rho B_y\\ \rho B_Z\\ \rho(uB_x+vB_y+wB_z)\end{bmatrix}$$

$$F=\begin{bmatrix}\rho u\\ u\rho u+\sigma_x\\ v\rho u+\tau_{xy}\\ w\rho u+\tau_{xz}\\ \hat{u}\rho u+u\sigma_x+v\tau_{xy}+w\tau_{xz}+\kappa T_x\end{bmatrix}$$

$$G=\begin{bmatrix}\rho v\\ u\rho v+\tau_{yx}\\ v\rho v+\sigma_y\\ w\rho v+\tau_{yz}\\ \hat{u}\rho v+u\tau_{yx}+v\sigma_y+w\tau_{yz}+\kappa T_y\end{bmatrix}$$

$$H=\begin{bmatrix}\rho w\\ u\rho w+\tau_{zx}\\ v\rho w+\tau_{zy}\\ w\rho w+\sigma_z\\ \hat{u}\rho w+u\tau_{zx}+v\tau_{zy}+w\sigma_z+\kappa T_z\end{bmatrix}$$

$$\sigma_x = -P + 2\mu u_x - \frac{2}{3}\mu \nabla \cdot \overline{V}$$

$$\sigma_y = -P + 2\mu v_y - \frac{2}{3}\mu \nabla \cdot \overline{V}$$

$$\sigma_z = -P + 2\mu w_z - \frac{2}{3}\mu \nabla \cdot \overline{V}$$

$$\tau_{xy} = \tau_{yx} = \mu(v_x + u_y)$$

$$\tau_{xz} = \tau_{zx} = \mu(u_z + w_x)$$

$$\tau_{yz} = \tau_{zy} = \mu(w_y + v_z)$$

$$\hat{u} = \hat{u}(P, \rho)$$

$$T = T(P, \rho)$$

$$\mu = \mu(P, \rho)$$

$$\kappa = \kappa(P, \rho)$$

$\overline{B}$ = body force per unit mass

Primitive Varible Form

$$\frac{\partial U}{\partial t} + A\frac{\partial U}{\partial x} + B\frac{\partial U}{\partial y} + C\frac{\partial U}{\partial z} = N$$

$$U = \begin{pmatrix} \rho \\ u \\ v \\ w \\ \hat{u} \end{pmatrix} \qquad N = \frac{1}{\rho}\begin{pmatrix} 0 \\ \rho B_x + \frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \\ \rho B_y + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \\ \rho B_z + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \sigma_z}{\partial z} \\ \nabla\cdot(\kappa T) - P\nabla\cdot\bar{V} + \mu\Phi \end{pmatrix}$$

$$A = \begin{pmatrix} u & \rho & 0 & 0 & 0 \\ 0 & u & 0 & 0 & 0 \\ 0 & 0 & u & 0 & 0 \\ 0 & 0 & 0 & u & 0 \\ 0 & 0 & 0 & 0 & u \end{pmatrix}$$

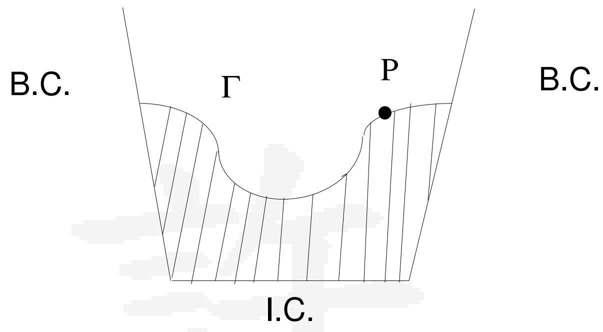
$$B = \begin{pmatrix} v & 0 & \rho & 0 & 0 \\ 0 & v & 0 & 0 & 0 \\ 0 & 0 & v & 0 & 0 \\ 0 & 0 & 0 & v & 0 \\ 0 & 0 & 0 & 0 & v \end{pmatrix}$$

$$C = \begin{pmatrix} w & 0 & 0 & \rho & 0 \\ 0 & w & 0 & 0 & 0 \\ 0 & 0 & w & 0 & 0 \\ 0 & 0 & 0 & w & 0 \\ 0 & 0 & 0 & 0 & w \end{pmatrix}$$

$$\Phi = 2(u_x^2 + v_y^2 + w_z^2) - \frac{2}{3}(\nabla\cdot\bar{V})^2 + (u_y + v_x)^2 + (v_z + w_y)^2 + (u_z + w_x)^2$$

Consider $$a_1u_x+b_1u_y+c_1v_x+d_1v_y=f_1$$
$$a_2u_x+b_2u_y+c_2v_x+d_2v_y=f_2$$

where a1,..........d2,f1,f2 are functions of x,y,u,v
and the domain of interest is



question：Is the behavior of the solution just above P uniquely determined by the information below and on the curve? or are those data sufficient to determine the directional derivatives at P in directions that lie above Γ?

Since $$du=u_xdx+u_ydy$$
$$dv=v_xdx+v_ydy$$

$$\rightarrow \quad \begin{bmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{bmatrix} \begin{bmatrix} u_x \\ u_y \\ v_x \\ v_y \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ du \\ dv \end{bmatrix}$$

a_1,........f_2 are known since u,v are known at P
dx,dy are known since the direction of Γ is known
du,dv are known since u,v are known along Γ

$\rightarrow$ A unique solution for u_x,u_y,v_x,v_y exits
If the determinent is not zero, it implies the directional derivatives have the same value above and below Γ.

・If the determinant is equal to zero, discontinuities in the partial derivatives occur when acrossing Γ.

det $\equiv 0 \rightarrow$ characteristic equation

$$(a_1c_2-a_2c_1)(dy)^2-(a_1d_2-a_2d_1+b_1c_2-b_2c_1)dxdy+(b_1d_2-b_2d_1)(dx)^2=0$$

or
$$a(\frac{dy}{dx})^2 - b(\frac{dy}{dx}) + c = 0$$

where $a=a_1c_2-a_2c_1$

$b=a_1d_2-a_2d_1+b_1c_2-b_2c_1$

$c=b_1d_2-b_2d_1$

(i) Two real roots (or two directions)

$\rightarrow$ hyperbolic d.e.

$\frac{dy}{dx} = [-b \pm (b^2-4ac)^{\frac{1}{2}} / 2a]$ is called characterist

Any discontinuity which exists will propagate along lines dy/dx

(ii) Two coincident roots

$\rightarrow$ parabolic d.e.

(iii) Complex roots

$\rightarrow$ elliptic d.e.

There are no directions dy/dx along which the solution can not be expanded.

Example Consider the quasilinear second-order equation

$$au_{xx}+bu_{xy}+cu_{yy}=f$$

where a,b,c,f are functions of x,y,u,u_x,u_y

since $d(u_x)=u_{xx}dx+u_{xy}dy$

$d(u_y)=u_{yx}dx+u_{yy}dy$

$$\rightarrow \begin{bmatrix} a & b & c \\ dx & dy & 0 \\ 0 & dx & dy \end{bmatrix} \begin{bmatrix} u_{xx} \\ u_{xy} \\ u_{yx} \end{bmatrix} = \begin{bmatrix} f \\ d(u_x) \\ d(u_y) \end{bmatrix}$$

The characteristic equation can thus be found

Example   Consider 2D steady flow

$$\begin{cases} uu_x + vu_y + \dfrac{1}{\rho}P_x = 0 & \text{-------(1)} \\ uv_x + vv_y + \dfrac{1}{\rho}P_y = 0 & \text{-------(2)} \\ (\rho u)_x + (\rho v)_y = 0 \\ v_x - u_y = 0 \\ P\rho^{-\gamma} = \text{const} \\ \dfrac{dP}{d\rho} = c^2 \end{cases}$$

operate $\rho u \cdot (1) + \rho v \cdot (2)$

$$\rightarrow \begin{cases} (u^2 - c^2)u_x + (uv)u_y + (uv)v_x + (v^2 - c^2)v_y = 0 \\ v_x - u_y = 0 \end{cases}$$

where $5C^2=6C^2-(u^2+v^2)$

Define

$$u^n = u/c^*,\ v^n = v/c^*,\ c^n = c/c^*$$

$$x^n = x/e,\ \ y^n = y/e$$

dropping " ' " for simplicity

$$\rightarrow \begin{cases} (u^2 - c^2)u_x + (uv)u_y + uv(v_x) + (v^2 - c^2)v_y = 0 \\ -u_y + v_x = 0 \end{cases}$$

where $C^{*2}=1.2-0.2(u^2+v^2)$

$\rightarrow$ Characteristic equation

$$\begin{bmatrix} u^2-c^2 & uv & uv & v^2-c^2 \\ 0 & -1 & 1 & 0 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{bmatrix} \begin{bmatrix} u_x \\ u_y \\ v_x \\ v_y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ du \\ dv \end{bmatrix}$$

$$\rightarrow \frac{dy}{dx} = \frac{uv \pm c\sqrt{u^2 + v^2 - c^2}}{u^2 - c^2}$$

(i) if $u^2+v^2 < c^2$ $\rightarrow$ elliptic

(ii) if $u^2+v^2=c^2$ $\rightarrow$ parabolic

(iii) if $u^2+v^2 > c^2$ $\rightarrow$ hyperbolic

Classification of system of equations

The equation most frequently encountered in C.F.D. will be the following written as first order system.

$$\frac{\partial \underline{u}}{\partial t}+[A]\frac{\partial \underline{u}}{\partial x}+[B]\frac{\partial \underline{v}}{\partial y}+\underline{r}=0$$

where [A],[B] are functions of x,y,t.

(一) hyperbolic

The above system is said to be hyperbolic at points (x,t) and (y,t) if the eigenvalues of [A] and [B] are real and distinct.

ex: Consider a wave equation

$$\begin{cases} v_t = cW_x \\ W_t = cv_t \end{cases}$$

$$\rightarrow \quad \frac{\partial \underline{u}}{\partial t}+[A]\frac{\partial \underline{u}}{\partial x}=0$$

where $\underline{u}=\begin{bmatrix} u \\ v \end{bmatrix}$, $[A]=\begin{bmatrix} 0 & -c \\ c & 0 \end{bmatrix}$

Richtymer and Morton (1967) indicated that a system of equation is said to be hyperbolic if the eigenvalues are all real and [A] can be written as $[A]=[T][X][T]^{-1}$, where [X]is the diagonal matrix of the eigenvalues of [A]

The eigenvalues of the investigated wave equation is

$\det\left|[A]-\lambda[I]\right|=0$

$\rightarrow \quad \lambda_1 = c, \quad \lambda_2 = -c$

Homework：find the corresponding [T]

=> Eignenvalues $dx/dt = \pm c$ of [A] represent the characteristic differential equations of the wave equation

(二) Elliptic

The above system of equation is said to be elliptic at a point (x,t) if the eigenvalues of [A] are all complex.

ex：consider Cauchy-Rieman equation

$$\begin{cases} u_x = v_y \\ u_y = -v_x \end{cases}$$

$$\rightarrow \quad \frac{\partial \underline{w}}{\partial x} + [A]\frac{\partial \underline{w}}{\partial y} = 0$$

where $\underline{w} = \begin{bmatrix} u \\ v \end{bmatrix}, \quad [A] = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$

The eigenvalue of [A] is λ_1=i,λ_2=-i

- classification of second-order P.D.E. is very complex
- mixed system of equations has roots of characteristics(i) real (ii)complex
- The above set of equations may exhibit the hyperbolic behavior in (x,t) space and elliptic in (y,t) space, depending on the eigenvalue structure of A, B, matrices

Consistency

A finite difference representation of a P.D.E. has consistency property if

$$\lim_{\text{mesh}\to 0}(PDE - FDE) = 0$$

Stability

A stable numerical scheme is one for which errors resulting from any source (round-off, truncation) are not permitted to grow in the sequence of numerical procedures from one marching step to another (For hyperbolic or parabolic marching problems)

For equilibrim problems,
(1)Truncation convergence for iterative process
(2)The error inherent in the direct method won't grow as mesh size is refined

Convergence

$$\lim_{\text{mesh}\to 0}\underbrace{(\text{solution of F.D.E.}) = \text{true P.D.E. solution}}_{\text{with the same B.C. and I.C.}}$$

- Generally, a consistent and stable scheme is convergent

Round-off error

Any computed solution may be affected by rounding to a finite number of digits in the arithmetic operations

Discretization error

Error in the solution of PDE is caused by replacing the continuous problem by a discrete one

In general, second-order accurate methods can provide enough accuracy for most of the practical problems

Conservative Property

Conservative property of a scheme means a good approxiamtion to P.D.E., not only in small, local neighborhood involving a few grid points but also in an arbitrarily large regions

・A difference formulation based on nondivergence form may lead to numerical difficulties in situations where the coefficients may be discontinous in flows containing shock waves

Finite Difference form of P.D.E.

(a)Taylor series expansion

(b)Polynominal fitting

(c)Integral method

(d)Control volume approach

In many cases (simple, linear equations), the resulting difference equations can be identical

Differencing scheme and its error

First-derivative approximation with △x=h=const

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{h} + O(h)$$ Forward difference

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{h} + O(h)$$ Backward difference

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2h} + O(h^2)$$ Central difference

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{-3u_{i,j} + 4u_{i+1,j} - u_{i+2,j}}{2h} + O(h^2)$$

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{3u_{i,j} - 4u_{i-1,j} + u_{i-2,j}}{2h} + O(h^2)$$

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{1}{2h}\left(\frac{\overline{\delta_x} u_{i,j}}{1 + \frac{\delta_x^2}{6}}\right) + O(h^4)$$

where

$$\overline{\delta_x} u_{i,j} = u_{i+1,j} - u_{i-1,j}$$

$$\overline{\delta_x} u_{i,j} = u_{i+1/2,j} - u_{i-1/2,j}$$

Three-point second-derivative approximation for constant △x=const=h

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} = \frac{u_{i,j} - 2u_{i+1,j} + u_{i+2,j}}{h^2} + O(h)$$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} = \frac{u_{i,j} - 2u_{i-1,j} + u_{i-2,j}}{h^2} + O(h)$$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + O(h^2)$$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} = \frac{\delta_x^2 u_{i,j}}{h^2 (1 + \delta_x^2 / 12)} + O(h^4)$$

If the upstream differencing method is employed to the 1-D convection equation

$$u_t + cu_x = 0 \qquad ; c>0$$

then we can obtain the differencing equation

$$u_t + cu_x = \frac{c\Delta x}{2}(1-\nu)u_{xx} - \frac{c(\Delta x)^2}{6}(2\nu^2 - 3\nu + 1)u_{xxx} + O((\Delta x)^3, (\Delta x)^2\Delta t, \Delta x(\Delta t)^2, (\Delta t)^3)$$

(i) Implicit artifical viscosity $\left(\frac{c\Delta x}{2}(1-\nu)u_{xx}\right)\nu$

The numerical errors of even order derivatives (e.g. second order derivative) generated inherently in the differencing procedure

(ii) Explict artificial viscosity
The even order derivatives which are purposely added to a differencing scheme

(iii) Artifical viscosity tends to reduce all gradients in the solution whether it is physically correct or numerically induced

Dissipation error： (Amplitude error) direct result of the even derivatives terms in the truncation error which is related to the amplitude error

Dispersion error： The direct result of the odd derivatives terms in the (phase error) truncation error which is related to the relative phase error (phase relations between various waves are distorted)

Diffusion—The combined effect of dissipation and dispersion

Shift condition—The finite difference algorithm, exhibiting the behavior of btaining the same result by employing the method of characteristic, is said to obtain the shift condition.

ex： 1D convection equation solved by the upstream difference method with Courant number=1.

Stability

・Strong stability：overall error due to round-off doesn't grow

・Weak stability：A single general round-off error doesn't grow

Let N：numerical solution of discretization

D：exact solution of discretization equation

A：exact solution of P.D.E.

Von Neumann (Fourier) analysis of a single equation

(1) Considering $u_t=\alpha u_{xx}$

explicit approximation (j,n)

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}=\frac{\alpha}{(\Delta x)^2}\left(u_{j+1}^n-2u_j^n+u_{j-1}^n\right) \qquad \text{(FTCS scheme)}$$

or $$u_j^{n+1}=u_j^n+\frac{\alpha\Delta t}{(\Delta x)^2}\left(u_{j+1}^n-2u_j^n+u_{j-1}^n\right)\text{------------------(3-101)}$$

substitute N=D+ε into (3-101) and D satisfing (3-101)

$$\rightarrow \frac{\varepsilon_j^{n+1}-\varepsilon_j^n}{\Delta t}=\alpha/_{\Delta x^2}\left(\varepsilon_{j+1}^n-2\varepsilon_j^n+\varepsilon_{j-1}^n\right)\text{-----------------------(3-103)}$$

i.e.,the error satisfies the original difference form or the numerical error and the exact numerical solution both posses the same growth property in time

Assuming a distribution of error at any time in a mesh

$$\varepsilon(x,t)=\sum_m^{\infty} b_m(t)e^{ik_m x}$$

where the wave number is difined as $k_m=\frac{m\pi}{L}$ m=0,1,2,........,M

M：number of inervals △x

L：M△x ; 2L-The period of fundamental frequency m=1

frequency $f_m \equiv \frac{k_m}{2\pi}=\frac{m}{2L}$

Since the difference equation (3-103) is linear, superposition may be used. We examine the behavior of a single term for simplicity(weak stability)

$$\varepsilon_m(x,t) = b_m(t)e^{ik_m x}$$

suppose $b_m(t)=e^{at}$

Then, $\varepsilon_m(x,t) = e^{at}e^{ik_m x}$ ---------------------------------(3-105)

Substitute (3-105) into (3-103)

$\rightarrow \quad e^{a\Delta t} = 1 + 2\gamma(\cos\beta - 1)$

where $\gamma = \alpha\Delta t \big/ (\Delta x)^2$

$\beta = k_m \Delta x$

Employing $\quad \cos\beta = \dfrac{e^{i\beta} + e^{-i\beta}}{2}$

and $\quad \sin^2\dfrac{\beta}{2} = \dfrac{1-\cos\beta}{2}$

$\rightarrow e^{a\Delta t} = 1 - 4\gamma\sin^2\dfrac{\beta}{2}$

Since $\quad \varepsilon_j^{n+1} = e^{a(n+1)\Delta t}e^{ik_m x_j} = e^{a\Delta t}\varepsilon_j^n = (\textit{Amplification}\ \text{Factor})\ \varepsilon_j^n$,

then Amplification factor is

$G = e^{a\Delta t} = 1 - 4\gamma\sin^2\dfrac{\beta}{2}$

Stable requirement means

- The influence of boundary conditions is not included in this analysis. (matrix method accounts for the influence of B.C.)
- In general, the Fourier stability analysis assumes that the periodic

B.C.s are imposed.

(2) Von Neumann analysis of the hyperbolic equation

$u_t + cu_x = 0 \qquad\qquad (3\text{-}108)$

The solution of (3-108) is

u(x-ct)=constant

with the characteristics given by a solution of

x_t=constant

i.e.,the initial data prescribed at t=0 is propagated along the characteristics

Lax scheme for (3-108) is

$$u_j^{n+1} = \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right) - \frac{c\Delta t}{\Delta x}\left(\frac{u_{j+1}^n - u_{j-1}^n}{2}\right)$$

Let $\quad u_j^n = e^{at}e^{ik_m x}$

then $\qquad G = \cos\beta - i\nu\sin\beta$

where $\nu = \text{Courant number} = \dfrac{c\Delta t}{\Delta x}$

stability requirement

$|G| \le 1 \rightarrow |\nu| \le 1$ This is the Courant-Friedrichs-Lewy(CFL) condition

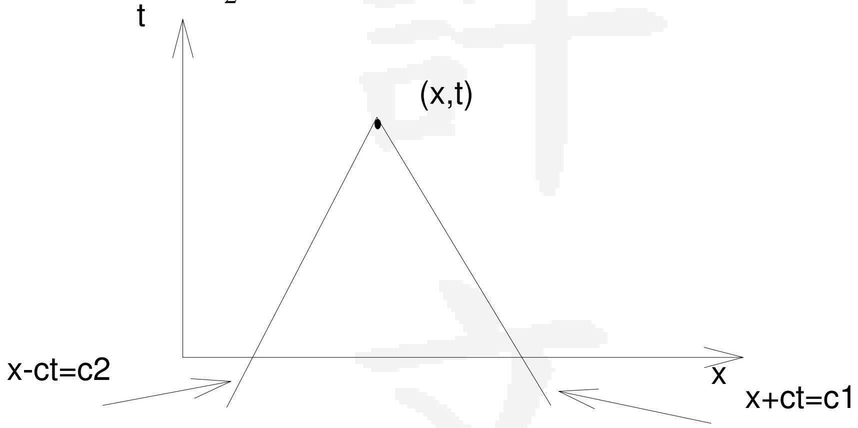
(3) Second-order hyperbolic wave equation

$u_{tt} - c^2 u_{xx} = 0$

The solution at a point (x,t) depends on data contained between the characteristics

x+ct=const C_1

x-ct=const C_2



Stability analysis

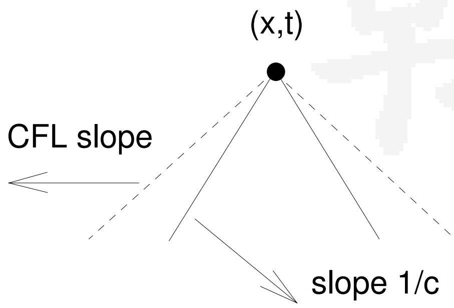
$\rightarrow$CFL condition

$\left| c \, \Delta t / \Delta x \right| \le 1$

i.e. CFL condition requires that the analytic domain of influence lies within the numerical domain of inflluence.

Since the chearacteristic slope is $dt/dx = \pm 1/c$

such that



the numerical domain may include the analytic zone

Positivity-

Accurate resolution of steep gradients is important in most of the problems

Consider $$\rho_t + v\rho_x = 0 \qquad (1)$$

where v is a constant

If the above equation is discretized in the following form：

$$\rho_i^{n+1} = \rho_i^n - \frac{v\Delta t}{\Delta x}\left(\rho_i^n - \rho_{i-1}^n\right) \quad \leftarrow \text{1st order montone scheme}$$

consider $\left\{\rho_i^n\right\}$ are positive at t=n△t

and $\left| {v\Delta t}/{\Delta x} \right| \le 1$

$\rightarrow \left\{\rho_i^{n+1}\right\}$ at t=(n+1)△t are also positive

Now consider a higher-order scheme for (1)：

$$\rho_i^{n+1} = a_i\rho_{i-1}^n + b_i\rho_i^n + c\rho_{i+1}^n$$

or

$$\rho_i^{n+1} = \rho_i^n - \frac{1}{2}\left[\varepsilon_{i+\frac{1}{2}}\left(\rho_{i+1}^n + \rho_i^n\right) - \varepsilon_{i-\frac{1}{2}}\left(\rho_i^n + \rho_{i-1}^n\right)\right] + \left[\nu_{i+\frac{1}{2}}\left(\rho_{i+1}^n - \rho_i^n\right) - \nu_{i-\frac{1}{2}}\left(\rho_i^n - \rho_{i-1}^n\right)\right]$$

$$\equiv \rho_i^n + \nu_{i+\frac{1}{2}}\left(\rho_{i+1}^n - \rho_i^n\right) - \nu_{i-\frac{1}{2}}\left(\rho_i^n - \rho_{i-1}^n\right) + convection$$

where $$\varepsilon_{i+\frac{1}{2}} = v_{i+\frac{1}{2}}\, {\Delta t}/{\Delta x}$$

$\left\{\nu_{i+\frac{1}{2}}\right\}$ appears as a consequence of numerical diffusion.

$$\rightarrow \quad \begin{aligned} a_i &= \nu_{i-\frac{1}{2}} + \frac{1}{2}\varepsilon_{i-\frac{1}{2}} \\ b_i &= 1 - \frac{1}{2}\varepsilon_{i+\frac{1}{2}} + \frac{1}{2}\varepsilon_{i-\frac{1}{2}} - \nu_{i+\frac{1}{2}} - \nu_{i-\frac{1}{2}} \\ c_i &= \nu_{i+\frac{1}{2}} - \frac{1}{2}\varepsilon_{i+\frac{1}{2}} \end{aligned}$$

＊if $\left\{\nu_{i+\frac{1}{2}}\right\}$ are positive and large enough

$\rightarrow \left\{\rho_i^{n+1}\right\}$ are positive

＊The positive conditions for all i are

$$\left|\varepsilon_{i+\frac{1}{2}}\right| \le 1$$

$$\frac{1}{2}\left|\varepsilon_{i+\frac{1}{2}}\right| \le \nu_{i+\frac{1}{2}} \le \frac{1}{2}$$

=>first-order numerical diffusion rapidly smears a sharp discontinity since

$$\rho_i^{n+1} = \rho_i^n + \nu_{i+1/2}\left(\rho_{i+1}^n - \rho_i^n\right) - \nu_{i-1/2}\left(\rho_i^n - \rho_{i-1}^n\right)$$

and higher-order solution(than one) reduces the numerical diffusion but sacrifices the assureed positivity

The price of guranteed positivity is a severe, unphysical spreading of the discontinuity which should be located at x=vt

=> the requirements of positivity and accuraty seem to be mutually exclusive→nonlinear monotone methods were invented to circumvent this dilemma