Sharif University of Technology School of Mechanical Engineering Center of Excellence in Energy Conversion

Computational Fluid Dynamics

Numerical Methods for Model Equations

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Model Equations

• Here, we will study various methods for solving the followings:

• First order linear wave equation:
$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0$$
 $(a > 0)$
• Transient Diffusion: $\frac{\partial u}{\partial t} - \alpha \frac{\partial^2 u}{\partial x^2} = 0$ $(\alpha > 0)$
• Laplace Equation: $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$
• Burger's Inviscid Equation: $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0$
• Burger's Viscous Equation: $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \mu \frac{\partial^2 u}{\partial x^2}$

Linear Wave Equation

- We will study the following methods:
 - Euler explicit method
 - First order upwind method
 - o Lax method
 - Euler implicit method
 - Leap frog method
 - Lax-Wendroff method (single step and 2-step)
 - Mac-Cormack method
 - 2nd order upwind method (Warming-Beam)
 - Trapezoidal method
 - Runge-Kutta method

Diffusion Equation

- We will study the following methods:
 - Simple explicit method
 - Simple implicit method
 - Crank-Nicholson method
 - o Dufort-Frankel method
 - $\circ \quad heta$ -methods
 - Keller-Box method
 - o ADI method

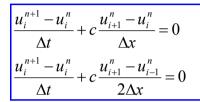
Inviscid Burger Equation

- We will study the following methods:
 - o Lax method
 - Lax-Wendroff method
 - Mac-Cormack method
 - Warming-Kutler-Lomax method
 - Beam-Warming method

Linear Wave Equation

Euler Explicit Method

• The method is (c > 0)



1st order in t and \boldsymbol{x}

1st order in t and 2nd order in x

• It is unconditionally unstable.

First Order Upwind Method

• The method is

$$\frac{\frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} + c \frac{u_{i}^{n} - u_{i-1}^{n}}{\Delta x} = 0 \qquad c > 0$$

$$\frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} + c \frac{u_{i}^{n} - u_{i+1}^{n}}{\Delta x} = 0 \qquad c < 0$$

• Or in general,

$$u_i^{n+1} = u_i^n - \underbrace{\frac{c \,\Delta t}{2\Delta x} \left(u_{i+1}^n - u_{i-1}^n \right)}_{\text{C} \Delta x} + \underbrace{\frac{|c| \Delta t}{2\Delta x} \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n \right)}_{\text{C} \Delta x}$$

• The method is stable provided that

$$0 \le v = \frac{c\,\Delta t}{\Delta x} \le 1$$

• Remember that its modified equation is

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = \frac{c\Delta x}{2} (1 - v) u_{xx} - \frac{c\Delta x^2}{6} (2v^2 - 3v + 1) u_{xxx} + O[\Delta x^3, \Delta x^2 \Delta t, \Delta x \Delta t^2, \Delta t^3]$$

First Order Upwind Method ...

• The amplification factor and phase angle are:

$$G = (1 - \nu - \nu \cos \beta) - i(\nu \sin \beta) = |G| \exp(i\phi)$$
$$\phi = \tan^{-1} \frac{\operatorname{Im}(G)}{\operatorname{Re}(G)} = \tan^{-1} \left(\frac{-\nu \sin \beta}{1 - \nu - \nu \cos \beta} \right)$$

• The exact solution for the problem is $u = \exp[i\kappa_m(x-ct)]$, thus

$$G = \frac{u(t + \Delta t)}{u(t)} = \frac{\exp\{i\kappa_m [x - c(t + \Delta t)]\}}{\exp\{i\kappa_m [x - ct]\}} = \exp(-i\kappa_m c \,\Delta t) \equiv \exp(i\phi_e)$$
$$|G_e| = 1 \qquad \phi_e = -\kappa_m c \,\Delta t = -\beta v$$

- This means that
 - If the initial wave amplitude is A_0 , then after N steps the total dissipation error is given by $(1-|G|^N)A_0$
 - \circ The total dispersion (phase) error is given by $N(\phi_e-\phi)$
 - Note that after one step, the relative shift error is

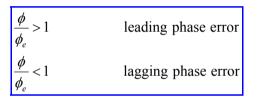
$$\frac{\phi}{\phi_e} = \frac{-1}{\beta v} \tan^{-1} \left(\frac{-v \sin \beta}{1 - v + v \cos \beta} \right)$$

First Order Upwind Method ...

• For small wave numbers (small β) we can write

$$\frac{\phi}{\phi_e} \approx 1 - \frac{1}{6} \left(2\nu^2 - 3\nu + 1 \right) \beta^2$$

Note that



• For the upwind method, we get

0 < v < 0.5	leading phase error
0.5 < v	lagging phase error

Lax Method

• The method reads

$$\frac{1}{\Delta t} \left(u_i^{n+1} - \frac{u_{i+1}^n - u_{i-1}^n}{2} \right) + \frac{c}{2\Delta x} \left(u_{i+1}^n - u_{i-1}^n \right) = 0$$

• Where

$$G = \cos \beta - i\nu \sin \beta$$
$$\frac{\phi}{\phi_e} = \frac{\tan^{-1}(-\nu \tan \beta)}{-\nu\beta}$$

Euler Implicit Method

• The method reads

$$\frac{1}{\Delta t} \left(u_i^{n+1} - u_i^n \right) + \frac{c}{2\Delta x} \left(u_{i+1}^{n+1} - u_{i-1}^{n+1} \right) = 0$$

- The method is second order in space and first order in time.
- It is unconditionally stable.
- The modified equation is

$$u_t + c u_x = \left(\frac{c^2 \Delta t}{2}\right) u_{xx} - \left(\frac{c \Delta x^2}{6} + \frac{c^3 \Delta t}{3}\right) u_{xxx} + \dots$$

• The amplification factor and phase error are

$$G = \frac{1 - i\nu\sin\beta}{1 + i\nu^2\sin^2\beta}$$
$$\frac{\phi}{\phi_e} = \frac{\tan^{-1}(-\nu\sin\beta)}{-\nu\beta}$$

Leap-Frog Method

• This 2nd order method is

$$\frac{1}{2\Delta t} \left(u_i^{n+1} - u_i^{n-1} \right) + \frac{c}{2\Delta x} \left(u_{i+1}^n - u_{i-1}^n \right) = 0$$

- It is neutrally stable for $|\nu| \le 1$.
- The modified equation shows a <u>predominantly dispersive</u> behavior.

$$u_t + c u_x = \left(\frac{c \Delta x^2}{6}\right) (v^2 - 1) u_{xxx} - \left(\frac{c \Delta x^4}{120}\right) (9v^4 - 10v^2 + 1) u_{xxxxx} + \dots$$

• The amplification factor and phase error are

$$G = \pm \sqrt{1 - v^2 \sin^2 \beta} - iv \sin \beta$$
$$\frac{\phi}{\phi_e} = \frac{\tan^{-1}(\mp v \sin \beta / \sqrt{1 - v^2 \sin^2 \beta})}{-v\beta}$$

Lax-Wendroff Method

• The method (2nd order in time and space) is derived from the Taylor expansion in time:

$$u_i^{n+1} = u_i^n - \underbrace{\frac{c \,\Delta t}{2\Delta x} \left(u_{i+1}^n - u_{i-1}^n \right)}_{2\Delta x} + \underbrace{\frac{c^2 \,\Delta t^2}{2\Delta x^2} \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n \right)}_{2\Delta x^2}$$

- It is stable for $|v| \leq 1$.
- The modified equation is

$$u_{t} + c u_{x} = \left(\frac{c \Delta x^{2}}{6}\right) (v^{2} - 1) u_{xxx} - \left(\frac{c \Delta x^{3}}{8}\right) v (-v^{2} + 1) u_{xxxx} + \dots$$

• The amplification and phase errors are:

$$G = \left[1 - v^2 \left(1 - \cos \beta\right)\right] - i\left(v \sin \beta\right)$$
$$\frac{\phi}{\phi_e} = \frac{\tan^{-1}\left\{-v \sin \beta / \left[1 - v^2 \left(1 - \cos \beta\right)\right]\right\}}{-v\beta}$$

• Note that the method has a <u>predominantly lagging phase error</u> except for large wave numbers with $\sqrt{0.5} < \nu < 1$

Two-step Lax-Wendroff Method

 For nonlinear equations such as the inviscid flow equations, a 2-step variation of the original Lax-Wendroff method can be used:

$$\frac{1}{\Delta t/2} \left(u_{i+1/2}^{n+1/2} - \frac{u_{i+1}^n + u_i^n}{2} \right) + \frac{c}{\Delta x} \left(u_{i+1}^n - u_i^n \right) = 0 \quad (\text{step 1})$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{c}{\Delta x} \left(u_{i+1/2}^{n+1/2} - u_{i-1/2}^{n+1/2} \right) = 0 \quad (\text{step 2})$$

- The scheme is 2nd order in time and space.
- It is stable for $|v| \le 1$.
- For the linear wave equation, the method becomes exactly like the original Lax-Wendroff equation.

MacCormack Method

• This method is a predictor-corrector type method (1969):

$$\overline{u}_{i}^{n+1} = u_{i}^{n} - \frac{c \Delta t}{\Delta x} \left(u_{i+1}^{n} - u_{i}^{n} \right)$$
(predictor)
$$u_{i}^{n+1} = \frac{1}{2} \left[u_{i}^{n} + \overline{u}_{i}^{n+1} - \frac{c \Delta t}{\Delta x} \left(\overline{u}_{i}^{n+1} - \overline{u}_{i-1}^{n+1} \right) \right]$$
(corrector)

• For the linear wave equation, this method is equivalent to the original Lax-Wendroff method with the same accuracy and stability limit.

2nd Order Upwind Method

• This is also called Warming and Beam method (1975):

$$\bar{u}_{i}^{n+1} = u_{i}^{n} - \frac{c \,\Delta t}{\Delta x} \left(u_{i}^{n} - u_{i-1}^{n} \right) \qquad \text{(predictor)}$$

$$u_{i}^{n+1} = \frac{1}{2} \left[u_{i}^{n} + \bar{u}_{i}^{n+1} - \frac{c \,\Delta t}{\Delta x} \left(\bar{u}_{i}^{n+1} - \bar{u}_{i-1}^{n+1} \right) - \frac{c \,\Delta t}{\Delta x} \left(u_{i}^{n} - 2u_{i-1}^{n} + u_{j-2}^{n} \right) \right] \qquad \text{(corrector)}$$

• For the linear wave equation, substituting the predictor into the corrector gives:

$$u_i^{n+1} = u_i^n - \nu \left(u_i^n - u_{i-1}^n \right) + \frac{\nu (\nu - 1)}{2} \left(u_i^n - 2u_{i-1}^n + u_{i-2}^n \right)$$

• The modified equation is

$$u_{t} + c u_{x} = \left(\frac{c \Delta x^{2}}{6}\right)(1 - v)(2 - v)u_{xxx} - \left(\frac{\Delta x^{4}}{8\Delta t}\right)v(1 - v)^{2}(2 - v)u_{xxxx} + \dots$$

- The stability condition is $0 \le v \le 2$
- Also

$$G = 1 - 2\nu \left[\nu + 2(1 - \nu)\sin^2\frac{\beta}{2} \right] \sin^2\frac{\beta}{2} - i(\nu\sin\beta) \left[1 + 2(1 - \nu)\sin^2\frac{\beta}{2} \right]$$

2nd Order Upwind Method...

• Note that

$0 < \nu < 1$	a predominantly leading phase error
1 < v < 2	a predominantly lagging phase error

• For $0 < \nu < 1$ the phase errors of the 2nd order upwind method and the Lax-Wendroff scheme are opposite. Fromm's method (1968) uses this fact to produce a method free of dispersive error.

Trapezoidal Differencing Method

 The method is developed by using Taylor series for time and central differences for spatial derivatives: (time-centered & space-centered)

$$u_i^{n+1} = u_i^n - \frac{\nu}{4} \left(u_{i+1}^{n+1} + u_{i+1}^n - u_{i-1}^{n+1} - u_{i-1}^n \right)$$

- The method is second order in space and time.
- It is also unconditionally stable.
- It's modified equation is:

$$u_t + c u_x = -\left(\frac{c^3 \Delta t^2}{12} + \frac{c \Delta x^2}{6}\right) u_{xxx} - \left(\frac{c \Delta x^4}{120} + \frac{c^3 \Delta t^2 \Delta x^2}{24} + \frac{c^4 \Delta t^4}{80}\right) u_{xxxx} + \dots$$

Also

$$G = \left(1 - \frac{i\nu}{2}\sin\beta\right) / \left(1 + \frac{i\nu}{2}\sin\beta\right)$$

Runge-Kutta Methods

• These methods transform the PDE to an ODE as

$$\frac{\partial u}{\partial t} = R(u) \qquad \text{where} \qquad R(u) = -c \frac{\partial u}{\partial x}$$

• A 2nd order Runge-Kutta method becomes:

$$u^{(1)} = u^{n} + \Delta t R^{n} \qquad (\text{step 1})$$

$$u^{n+1} = u^{n} + \frac{\Delta t}{2} (R^{n} + R^{(1)}) \qquad (\text{step 2})$$
where
$$R^{(1)} = -c \left(\frac{\partial u}{\partial x}\right)^{(1)} = -c \left[\left(\frac{\partial u}{\partial x}\right)^{n} + \Delta t \left(\frac{\partial R}{\partial x}\right)^{n}\right] = -c \left(\frac{\partial u}{\partial x}\right)^{n} + c^{2} \Delta t \left(\frac{\partial^{2} u}{\partial x^{2}}\right)^{n}$$

• Or simply we have

$$u^{n+1} = u^n + \frac{\Delta t}{2} \left(-2c u_x^n + c^2 \Delta t u_{xx}^n \right)$$

• Using 2nd-order central differences, we obtain the 2nd order Lax-Wendroff scheme.

Runge-Kutta Methods...

• One of the most popular Runge-Kutta method is its 4-step version (2nd order in time and 4th order in space when 2nd order spatial differences are used):

$u^{(1)} = u^n + \frac{\Delta t}{2} R^n$	(step 1)
$u^{(2)} = u^n + \frac{\Delta t}{2} R^{(1)}$	(step 2)
$u^{(3)} = u^n + \Delta t R^{(2)}$	(step 3)
$u^{n+1} = u^n + \frac{\Delta t}{6} (R^n + 2R^{(1)} + 2R^{(2)} + R^{(3)})$	(step 4)

Diffusion Equation

Diffusion Equation

• In 1D, we have

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

• This is a <u>parabolic</u> equation whose exact solution for an initial condition u(x,0) = f(x) and boundary conditions u(0,t) = u(1,t) = 0 is given by

> $u(x,t) = \sum_{n=1}^{\infty} A_n \exp(-\alpha k_n^2 t) \sin(k_n x)$ where $(k_n = n\pi)$ $A_n = 2 \int_0^1 f(x) \sin(k_n x) dx$

• The exact amplification is

$$G_e = \frac{u(t + \Delta t)}{u(t)} = \exp(-\alpha k_m^2 \Delta t) = \exp(-r\beta^2)$$

Simple Explicit Method

• Using first order in time and second order in space, we get

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

• The scheme is stable for

$$0 \le r = \frac{\alpha \,\Delta t}{\Delta x^2} \le 1/2$$

• The amplification factor is

$$G = 1 + 2r(\cos\beta - 1)$$

• The modified equation becomes:

$$u_t - \alpha u_{xx} = \left(\frac{-\alpha^2 \Delta t}{2} + \frac{\alpha \Delta x^2}{12}\right) u_{xxxx} + \left(\frac{\alpha^3 \Delta t^2}{3} - \frac{\alpha^2 \Delta t \Delta x^2}{12} + \frac{\alpha \Delta x^4}{360}\right) u_{xxxxxx} + \dots$$

Simple Implicit Method

• This method is first order in time and second order in space:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2}$$

- It is unconditionally stable.
- The modified equation is

$$u_t - \alpha u_{xx} = \left(\frac{\alpha^2 \Delta t}{2} + \frac{\alpha \Delta x^2}{12}\right) u_{xxxx} + \left(\frac{\alpha^3 \Delta t^2}{3} + \frac{\alpha^2 \Delta t \Delta x^2}{12} + \frac{\alpha \Delta x^4}{360}\right) u_{xxxxxx} + \dots$$

• The amplification factor is

$$G = \frac{1}{1 + 2r(1 - \cos\beta)}$$

Crank-Nicolson Method

• The method (1947) reads

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{\alpha}{2\Delta x^2} \left[\left(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1} \right) + \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n \right) \right]$$

• Its modified equation is

$$u_t - \alpha u_{xx} = \left(\frac{\alpha \Delta x^2}{12}\right) u_{xxxx} + \left(\frac{\alpha^3 \Delta t^2}{12} + \frac{\alpha \Delta x^4}{360}\right) u_{xxxxxx} + \dots$$

• The amplification factor is

$$G = \frac{1 - r(1 - \cos \beta)}{1 + r(1 - \cos \beta)}$$

Dufort-Frankel Method

• This method is given by ($r = \alpha \Delta t / \Delta x^2$)

$$u_i^{n+1}(1+2r) = u_i^{n-1} + 2r(u_{i+1}^n - u_i^{n-1} + u_{i-1}^n)$$

- Remember that the method is not consistent with the diffusion equation if $\Delta t / \Delta x \rightarrow cte$.
- The modified equation becomes

$$u_t - \alpha u_{xx} = \left(\frac{\alpha \Delta x^2}{12} - \frac{\alpha^3 \Delta t^2}{\Delta x^2}\right) u_{xxxx} + \left(\frac{\alpha \Delta x^4}{360} - \frac{\alpha^3 \Delta t^2}{3} + \frac{2\alpha^5 \Delta t^4}{\Delta x^4}\right) u_{xxxxxx} + \dots$$

Also, the amplification factor is

$$G = \frac{2r\cos\beta \pm \sqrt{1 - 4r^2\sin^2\beta}}{1 + 2r}$$

• The method is unconditionally stable (for $r \ge 0$) and can be easily extended to 2D and 3D cases.

θ - Methods

• By combining the formulation of the simple explicit, simple implicit and Crank-Nicolson methods, we obtain

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{\alpha}{\Delta x^2} \Big[\theta \, \delta_x^2 \, u_i^{n+1} + (1 - \theta) \, \delta_x^2 \, u_i^n \Big] \qquad 0 \le \theta \le 1$$

where
$$\delta_x^2 \, u_i^n = u_i^{n+1} - 2u_i^n + u_{i-1}^n$$

• The method is 2nd order in time and space except for special cases:

$$\begin{aligned} Crank - Nicolson \ (\theta = 1/2) & T.E. = O[\Delta t^2, \Delta x^2] \\ (\theta = \frac{1}{2} - \frac{\Delta x^2}{12 \alpha \Delta t}) & T.E. = O[\Delta t^2, \Delta x^4] \\ (\theta = \frac{1}{2} - \frac{\Delta x^2}{12 \alpha \Delta t}), \ \frac{\Delta x^2}{\alpha \Delta t} = \sqrt{20} & T.E. = O[\Delta t^2, \Delta x^6] \end{aligned}$$

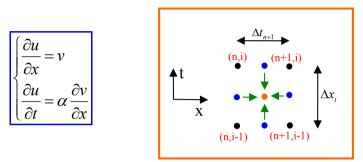
Its modified equation is

$$u_{t} - \alpha u_{xx} = \left[\left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t + \frac{\alpha \Delta x^{2}}{12} \right] u_{xxxx} + \left[\left(\theta^{2} - \theta + \frac{1}{3}\right) \alpha^{3} \Delta t^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{\alpha \Delta x^{4}}{360} \right] u_{xxxxx} + \dots + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{2}\right) \alpha^{2} \Delta t \Delta x^{2} + \frac{1}{6} \left(\theta - \frac{1}{6}\right) \alpha^{2} \Delta t \Delta$$

- The method is unconditionally stable if $1/2 \le \theta \le 1$.
- When $0 \le \theta \le 1/2$ the method is stable if $0 \le r \le (2-4\theta)^{-1}$

Keller-Box Method

• In this method, we split the equation into the followings:



• Then, the method becomes

$$\frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x_i} = \frac{v_i^{n+1} + v_{i-1}^{n+1}}{2}$$
$$\frac{u_i^{n+1} + u_{i-1}^{n+1}}{\Delta t_{n+1}} = \frac{\alpha}{\Delta x_i} \left(v_i^{n+1} - v_{i-1}^{n+1} \right) + \frac{u_i^n + u_{i-1}^n}{\Delta t_{n+1}} + \frac{\alpha}{\Delta x_i} \left(v_i^n - v_{i-1}^n \right)$$

• This method is 2nd order in time and space.

ADI Method

• The Alternating Direction Implicit method consists of two steps:

$$\frac{u_{i,j}^{n+1/2} - u_{i,j}^{n}}{\Delta t/2} = \alpha \left(\overline{\delta}_{x}^{2} u_{i,j}^{n+1/2} + \overline{\delta}_{y}^{2} u_{i,j}^{n} \right) \qquad (\text{step 1})$$

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n+1/2}}{\Delta t/2} = \alpha \left(\overline{\delta}_{x}^{2} u_{i,j}^{n+1/2} + \overline{\delta}_{y}^{2} u_{i,j}^{n+1} \right) \qquad (\text{step 2})$$
where
$$\overline{\delta}_{x}^{2} = \delta_{x}^{2}/\Delta x^{2} \qquad \overline{\delta}_{y}^{2} = \delta_{y}^{2}/\Delta y^{2}$$

- In the first step a tri-diagonal system is solved for each *j* row and during the 2nd step a tri-diagonal system is solved for each *i* row of grid points.
- The method is 2^{nd} order in t, x, y. And

$$G = \frac{\left[1 - r_x(1 - \cos\beta_x)\right]\left[1 - r_y(1 - \cos\beta_y)\right]}{\left[1 + r_x(1 - \cos\beta_x)\right]\left[1 + r_y(1 - \cos\beta_y)\right]}$$

where
$$r_x = \frac{\alpha \,\Delta t}{\Delta x^2}, \quad r_y = \frac{\alpha \,\Delta t}{\Delta y^2}, \quad \beta_x = \kappa_m \Delta x, \quad \beta_y = \kappa_m \Delta y$$

• The method is unconditionally stable.

ADI Method ...

• For a 3D problem, Douglas and Gunn suggest the following formulation:

$\left(1 - \frac{r_x}{2}\delta_x^2\right)\Delta u^* = \left(r_x\delta_x^2 + r_y\delta_y^2 + r_z\delta_z^2\right)u^n$	(step 1)
$\left(1 - \frac{r_y}{2}\delta_y^2\right)\Delta u^{**} = \Delta u^*$	(step 2)
$\left(1 - \frac{r_z}{2}\delta_z^2\right)\Delta u = \Delta u^{**}$	(step 3)
where	
$\Delta u_{i,j} = u_{i,j}^{n+1} - u_{i,j}^n$	

Inviscid Burger Equation

General

• The inviscid Burger equation

$$\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0 \quad with \quad F = u^2 / 2$$

- Is analog to the Euler equations for the flow of an inviscid fluid. It also represents a nonlinear wave equation, where each point on the wave front can propagate with a different speed. As a result this equation can show the coalescence of characteristics and therefore accept the formation of discontinuous solutions, similar to shock waves in fluid dynamics.
- The characteristic of the Burger's equation is

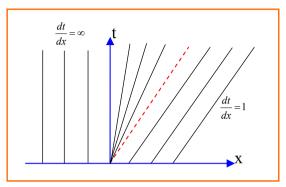
$$\frac{dt}{dx} = \frac{1}{u}$$

The solution to the Burger's equation under a specific initial condition is

$$\begin{cases} u(x,0) = 0 & x < 0 \\ u(x,0) = 1 & 0 \le x \end{cases} \longrightarrow \begin{cases} u = 0 & x \le 0 \\ u = x/t & 0 < x < t \\ u = 1 & t \le x \end{cases}$$

General...

• The solution can be shown as below



If the initial condition was

$$\begin{cases} u(x,0) = u_1 & x \le a \\ u(x,0) = u_2 < u_1 & x > a \end{cases}$$

• Then, a shock wave like discontinuity will be traveling in the domain at the average value of the $(u_1 + u_2)/2$ function across the wave front.

Lax Method

• This is a first order method:

$$u_i^{n+1} = \left(\frac{u_{i+1}^n + u_{i-1}^n}{2}\right) - \frac{\Delta t}{2\Delta x} \left(F_{i+1}^n - F_{i-1}^n\right) = 0$$

• Its amplification factor is

$$G = \cos\beta - i\frac{\Delta t}{\Delta x}\frac{dF}{du}\sin\beta$$

• The stability limit is

$$\left|\frac{\Delta t}{\Delta x}u_{\max}\right| \le 1$$

• When using a finite volume method, a first order method in t is

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} \left(F_{i+1/2}^n - F_{i-1/2}^n \right)$$

Using the Lax method, we get

$$F_{i+1/2} = \frac{1}{2} \left[F_i^n + F_{i+1}^n - \frac{\Delta x}{\Delta t} (u_{i+1} - u_i) \right]$$

• This flux function is consistent in the sense that

$$F(u_i, u_{i+1}) = F(u_i)$$
 when $u_i = u_{i+1}$

Lax-Wendroff Method

- This method is developed using the Taylor series and is 2nd order accurate in space and time.
- The method reads: $(\partial F / \partial u)_{i+1/2} \equiv A_{i+1/2} = A((u_i + u_{i+1}) / 2)$

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2\Delta x} \left(F_{i+1}^n - F_i^n \right) + \frac{1}{2} \left(\frac{\Delta t}{\Delta x} \right)^2 \left[A_{i+1/2}^n \left(F_{i+1}^n - F_i^n \right) - A_{i-1/2}^n \left(F_i^n - F_{i-1}^n \right) \right]$$

We also have

$$G = 1 - 2\left(A\frac{\Delta t}{\Delta x}\right)^2 (1 - \cos\beta) - 2iA\frac{\Delta t}{\Delta x}\sin\beta$$

• The stability requirement is

$$\left|\frac{\Delta t}{\Delta x}u_{\max}\right| \le 1$$

• As the Courant number $u\Delta t / \Delta x$ is reduced from 1.0, the quality of the solution is degraded and more oscillations are produced.

Lax-Wendroff Method...

• Using the finite volume formulation, we get

$$F_{i+1/2} = \frac{1}{2} \left(F_i + F_{i+1} \right) - \frac{\Delta t}{2\Delta x} \lambda_{i+1/2}^2 \left(u_{i+1} - u_i \right)$$

- Here $\lambda_{i+1/2}$ is the eigenvalue of the Jacobian $A_{i+1/2}$ which is $u_{i+1/2}$ for the Burger's equation.
- We also notice that

$$F_{i+1/2} = \underbrace{\frac{1}{2} \left(F_i + F_{i+1} - \frac{\Delta x}{\Delta t} \left(u_{i+1} - u_i \right) \right)}_{\text{Lax method (first order)}} + \underbrace{\frac{\Delta x}{\Delta t} \left[1 - \left(\frac{\Delta t}{\Delta x} \right)^2 \lambda_{i+1/2}^2 \right] \left(\frac{u_{i+1} - u_i}{2} \right)}_{\text{Constrainty}}$$

• Since Lax method produces no oscillations, we can use a function ϕ to control the amount of the 2nd part to be added to the Lax method to minimize the oscillations.

MacCormack Method

• This method is a predictor-corrector version of the Lax-Wendroff scheme thus easier to implement.

$$\overline{u}_{i}^{n+1} = u_{i}^{n} - \frac{\Delta t}{\Delta x} \left(F_{i+1}^{n} - F_{i}^{n} \right)$$
(predictor)
$$u_{i}^{n+1} = \frac{1}{2} u_{i}^{n} + \overline{u}_{i}^{n+1} - \frac{\Delta t}{\Delta x} \left(\overline{F}_{i}^{n+1} - \overline{F}_{i-1}^{n+1} \right)$$
(corrector)

• The amplification factor and the stability limit are the same as those for the Lax-Wendroff method.

Warming-Kutler-Lomax Method

• This is a 3rd order scheme and uses the MacCormack method for the first two levels. The method (1973) reads

$$u_{i}^{(1)} = u_{i}^{n} - \frac{2\Delta t}{3\Delta x} \left(F_{i+1}^{n} - F_{i}^{n} \right)$$

$$u_{i}^{(2)} = \frac{1}{2} \left[u_{i}^{n} + u_{i}^{(1)} - \frac{2\Delta t}{3\Delta x} \left(F_{i}^{n} - F_{i-1}^{(1)} \right) \right]$$

$$u_{i}^{n+1} = u_{i}^{n} - \frac{\Delta t}{24\Delta x} \left(-2F_{i+2}^{n} + 7F_{i+1}^{n} - 7F_{i-1}^{n} + 2F_{i-2}^{n} \right)$$

$$- \frac{3\Delta t}{8\Delta x} \left(F_{i+1}^{(2)} - F_{i-1}^{(2)} \right) - \frac{\omega}{24} \left(u_{i+2}^{n} - 4u_{i+1}^{n} + 6u_{i}^{n} - 4u_{i-1}^{n} + u_{i-2}^{n} \right)$$

• The stability limit for Burger's equation is given by

$$|v| = \left|\frac{\Delta t}{\Delta x}u_{\max}\right| \le 1$$
 and $4v^2 - v^4 \le \omega \le 3$

Beam and Warming Method

- This is a 2nd order implicit method.
- First use the trapezoidal method,

$$u_i^{n+1} = u_i^n + \frac{\Delta t}{2} \left[(u_t)^n + (u_t)^{n+1} \right] + O[\Delta t^3]$$

Then, substitute the model equation into it

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2} \left[\left(\frac{\partial F}{\partial x} \right)^n + \left(\frac{\partial F}{\partial x} \right)^{n+1} \right]$$

• Beam and Warming (1976) suggested that

$$F^{n+1} \approx F^n + \left(\frac{\partial F}{\partial u}\right)^n \left(u^{n+1} - u^n\right) = F^n + A^n \left(u^{n+1} - u^n\right)$$

• Thus, the method becomes

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2} \left[2 \left(\frac{\partial F}{\partial x} \right)^n + \frac{\partial}{\partial x} \left[A(u_i^{n+1} - u_i^n) \right] \right]$$

• Substitute x-derivatives with 2nd order central differences, we get

$$-\left(\frac{\Delta t A_{i-1}^{n}}{4\Delta x}\right)u_{i-1}^{n+1} + u_{i}^{n+1} + \left(\frac{\Delta t A_{i+1}^{n}}{4\Delta x}\right)u_{i+1}^{n+1} = -\left(\frac{\Delta t}{\Delta x}\right)\frac{F_{i+1}^{n} - F_{i-1}^{n}}{2} - \left(\frac{\Delta t A_{i-1}^{n}}{4\Delta x}\right)u_{i-1}^{n} + u_{i}^{n} + \left(\frac{\Delta t A_{i+1}^{n}}{4\Delta x}\right)u_{i+1}^{n} = -\left(\frac{\Delta t}{\Delta x}\right)\frac{F_{i+1}^{n} - F_{i-1}^{n}}{2} - \left(\frac{\Delta t A_{i-1}^{n}}{4\Delta x}\right)u_{i-1}^{n} + u_{i}^{n} + \left(\frac{\Delta t A_{i+1}^{n}}{4\Delta x}\right)u_{i+1}^{n} = -\left(\frac{\Delta t}{\Delta x}\right)\frac{F_{i+1}^{n} - F_{i-1}^{n}}{2} - \left(\frac{\Delta t A_{i-1}^{n}}{4\Delta x}\right)u_{i-1}^{n} + u_{i}^{n} + \left(\frac{\Delta t A_{i+1}^{n}}{4\Delta x}\right)u_{i+1}^{n} = -\left(\frac{\Delta t A_{i-1}^{n}}{4\Delta x}\right)u_{i-1}^{n} + u_{i}^{n} + \left(\frac{\Delta t A_{i+1}^{n}}{4\Delta x}\right)u_{i+1}^{n} = -\left(\frac{\Delta t A_{i-1}^{n}}{4\Delta x}\right)u_{i-1}^{n} + u_{i}^{n} + \left(\frac{\Delta t A_{i+1}^{n}}{4\Delta x}\right)u_{i+1}^{n} = -\left(\frac{\Delta t A_{i-1}^{n}}{4\Delta x}\right)u_{i-1}^{n} + u_{i}^{n} + \left(\frac{\Delta t A_{i+1}^{n}}{4\Delta x}\right)u_{i+1}^{n} = -\left(\frac{\Delta t A_{i-1}^{n}}{4\Delta x}\right)u_{i+1}^{n} + \left(\frac{\Delta t A_{i+1}^{n}}{4\Delta x}\right)u_{i+1}^{n} = -\left(\frac{\Delta t A_{i-1}^{n}}{4\Delta x}\right)u_{i+1}^{n} + \left(\frac{\Delta t A_{i+1}^{n}}{4\Delta x}\right)u_{i+1$$

Beam and Warming Method...

- This leads to a tri-diagonal system and can be solved using the Thomas algorithm.
- This method is <u>stable</u> but produces oscillations.
- To reduce oscillations, an artificial smoothing can be added to the scheme $0 < \omega \le 1$:

$$\frac{-\omega}{8}\left(u_{i+2}^n - 4u_{i+1}^n + 6u_i^n - 4u_{i-1}^n + u_{i-2}^n\right)$$

- An efficient form of the above method can be obtained using $\Delta u_i = u_i^{n+1} u_i^n$
- The trapezoidal formula with the following linearization

$$F_i^{n+1} = F_i^n + A_i^n \Delta u_i$$

• The final form of the scheme becomes

$$-\left(\frac{\Delta t A_{i-1}^n}{4\Delta x}\right) \Delta u_{i-1} + \Delta u_i + \left(\frac{\Delta t A_{i+1}^n}{4\Delta x}\right) \Delta u_{i+1} = -\left(\frac{\Delta t}{\Delta x}\right) \frac{F_{i+1}^n - F_{i-1}^n}{2}$$

• Which is simpler for computation. The method still needs a smoothing to produce an oscillation free solution.