ივანე ჯავახიშვილის სახელობის
თბილისის სახელმწიფო უნივერსიტეტი

ლექცია 3

FD Methods

Domain of Influence (elliptic, parabolic, hyperbolic)

Conservative formulation

Complications:

- Mixed Derivatives
- Higher Dimensions (2+)
- Source Terms

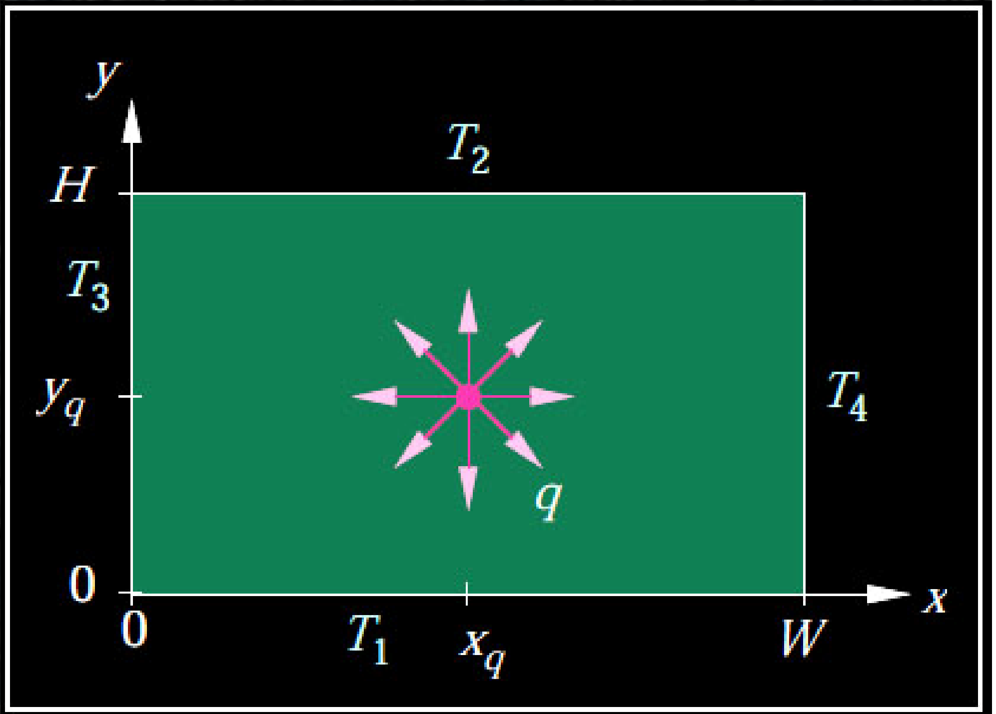
FD: Domain of influence

Elliptic PDE **Laplace equation**

$$\frac{\partial^2}{\partial x^2}\mathrm{U}(x,y)+\frac{\partial^2}{\partial y^2}\mathrm{U}(x,y)=0$$

$$0 < x < W$$

$$0 < y < H$$



FD: Domain of influence

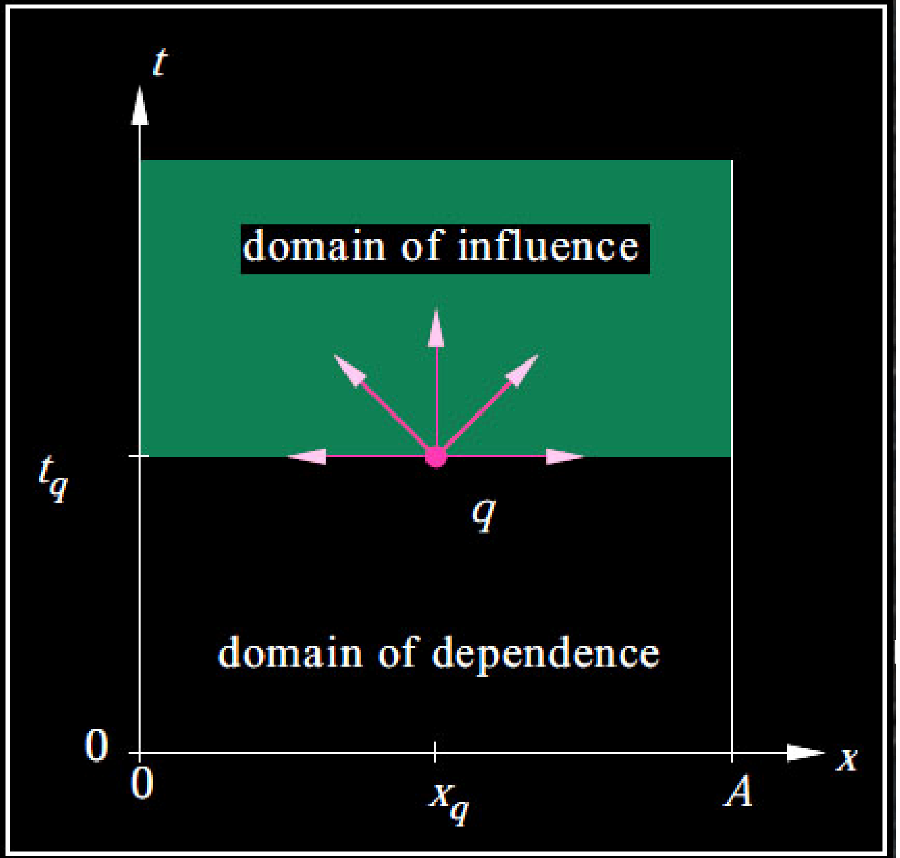
Parabolic PDE **Heat equation**

$$\frac{\partial}{\partial t}\mathrm{U}(t,x) = k\frac{\partial^2}{\partial x^2}\mathrm{U}(t,x)$$

$$U(t,0) = u_0$$

$$U(t,A) = u_A$$

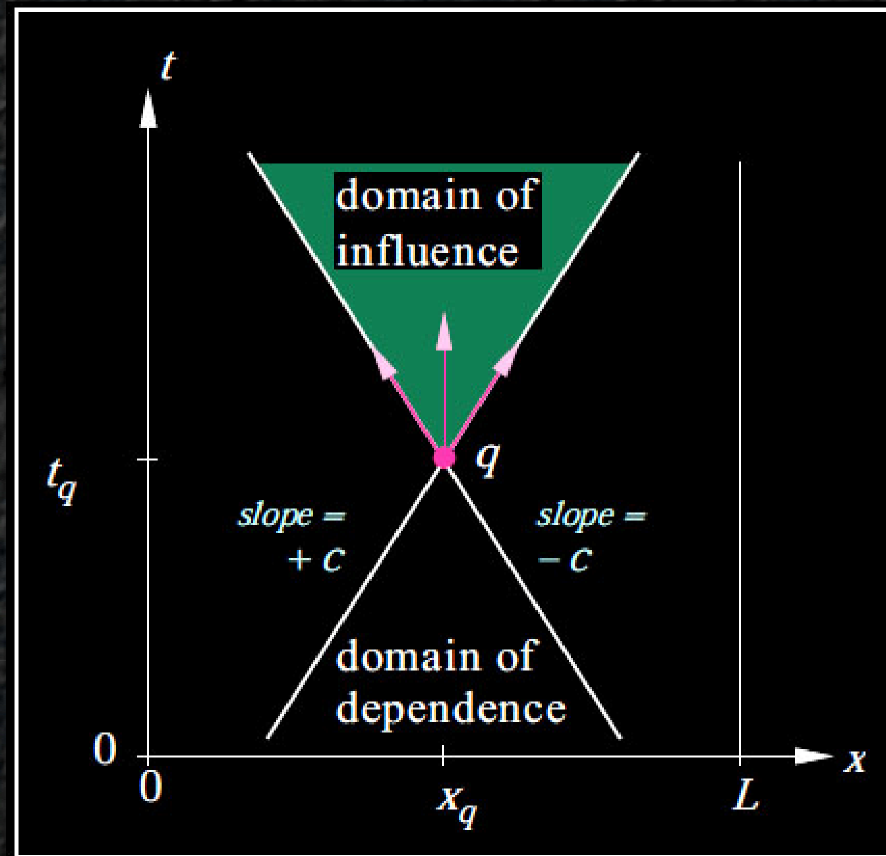
$$U(0,x) = g(x)$$



FD: Domain of influence

Hyperbolic PDE **Wave equation**

$$\frac{\partial^2}{\partial t^2}\mathrm{U}(t,x) = C^2 \frac{\partial^2}{\partial x^2}\mathrm{U}(t,x)$$

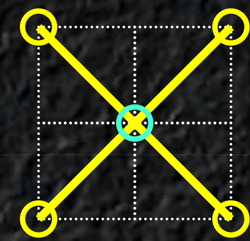


$$U(t,0) = u_0$$

$$U(0,x) = f(x)$$

$$\frac{\partial}{\partial t}U(0,x) = g(x)$$

Mixed Derivatives



Central Derivative Stencil:

$$\text{2D:}\quad \frac{\partial^2 u}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right) = \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)$$

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j} = \frac{\left(\frac{\partial u}{\partial y}\right)_{i+1,j} - \left(\frac{\partial u}{\partial y}\right)_{i-1,j}}{2\Delta x} + \mathcal{O}(\Delta x)^2$$

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1}}{2\Delta y} + \mathcal{O}(\Delta y)^2$$

$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2\Delta y} + \mathcal{O}(\Delta y)^2$$

$$\frac{\partial^2}{\partial x \partial y} \mathrm{U}(x,y) \Rightarrow \frac{\mathrm{U}(i+1,j+1) + \mathrm{U}(i-1,j-1)}{4\Delta x \Delta y} - \frac{\mathrm{U}(i+1,j-1) + \mathrm{U}(i-1,j+1)}{4\Delta x \Delta y}$$

PDE Formulation

Burgers Equation: $$\frac{\partial}{\partial t}\mathrm{U}(t,x)+\mathrm{U}(t,x)\frac{\partial}{\partial x}\mathrm{U}(t,x)=0$$

Straightforward discretization (upwind):

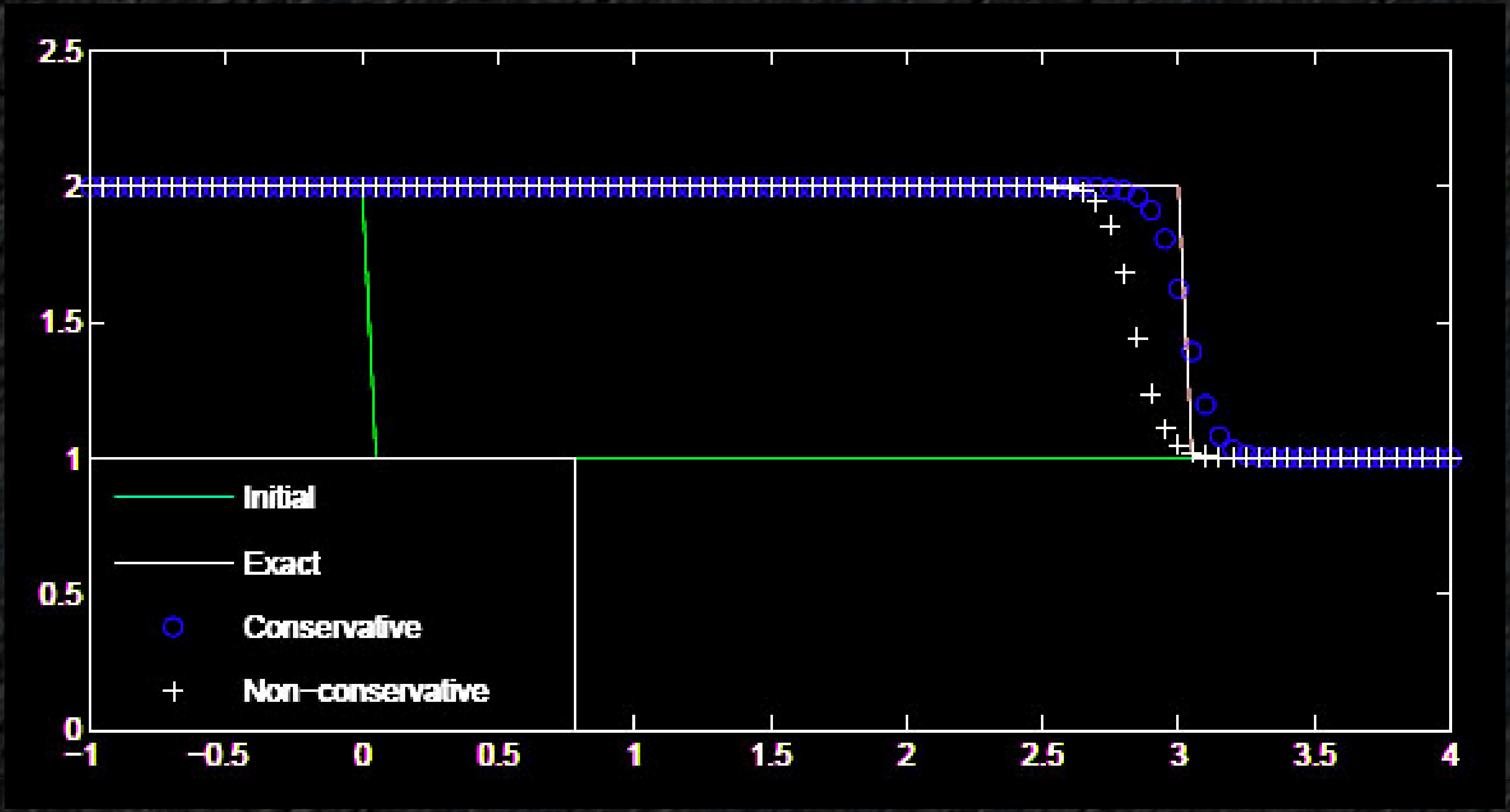
$$\mathrm{U}(i+1,j)=\mathrm{U}(i,j)-\frac{\Delta t}{\Delta x}\mathrm{U}(i,j)\left[\mathrm{U}(i,j+1)-\mathrm{U}(i,j)\right]$$

Conservative Form: $$\frac{\partial}{\partial t}\mathrm{U}(t,x)+\frac{1}{2}\frac{\partial}{\partial x}\left(\mathrm{U}(t,x)\right)^2=0$$

Standard discretization (upwind):

$$\mathrm{U}(i+1,j)=\mathrm{U}(i,j)-\frac{\Delta t}{2\Delta x}\left[\left(\mathrm{U}(i,j+1)\right)^2-\left(\mathrm{U}(i,j)\right)^2\right]$$

Burgers Equation



Lax-Wendroff Theorem

For hyperbolic systems of conservation laws, schemes written in conservation form guarantee that if the scheme converges numerically, then it converges to the analytic solution of the original system of equations.

Lax equivalence:

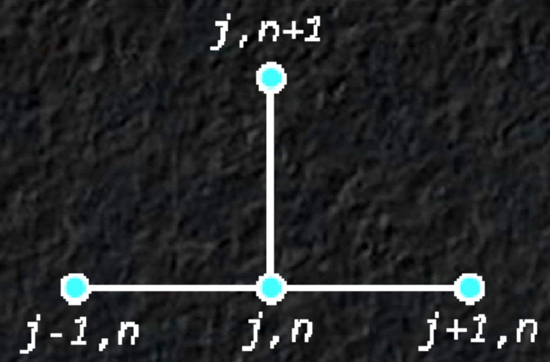
Stable solutions converge to analytic solutions

Implicit and Explicit Methods

Explicit FD method:

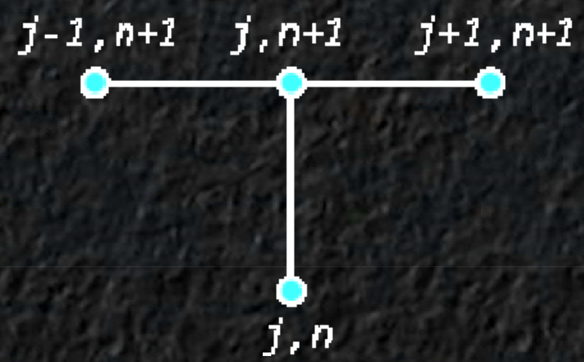
U(n+1) is defined by U(n)

knowing the values at time n, one can obtain the corresponding values at time n+1

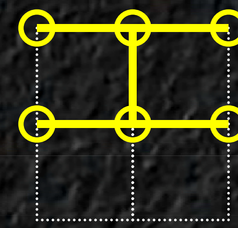


Implicit FD method:

U(n+1) is defined by solution of system of equations at every time step



Implicit Methods



Crank-Nicolson for parabolic equations:

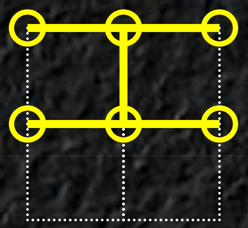
e.g. **Heat Equation**

$$\frac{\partial}{\partial t}\mathrm{U}(t,x) = F\left(U, \frac{\partial U}{\partial x}, \frac{\partial^2 U}{\partial x^2} t, x, \right)$$

1. (i+1) backward derivative

2. (i) forward derivative

Implicit Methods



$$\frac{\partial}{\partial t}\mathrm{U}(t,x) = F\left(U, \frac{\partial U}{\partial x}, \frac{\partial^2 U}{\partial x^2} t, x, \right)$$

1. Forward derivative: $$\frac{U(i+1,j)-U(i,j)}{\Delta t} = F(i,j)$$
2. Backward derivative: $$\frac{U(i+1,j)-U(i,j)}{\Delta t} = F(i+1,j)$$

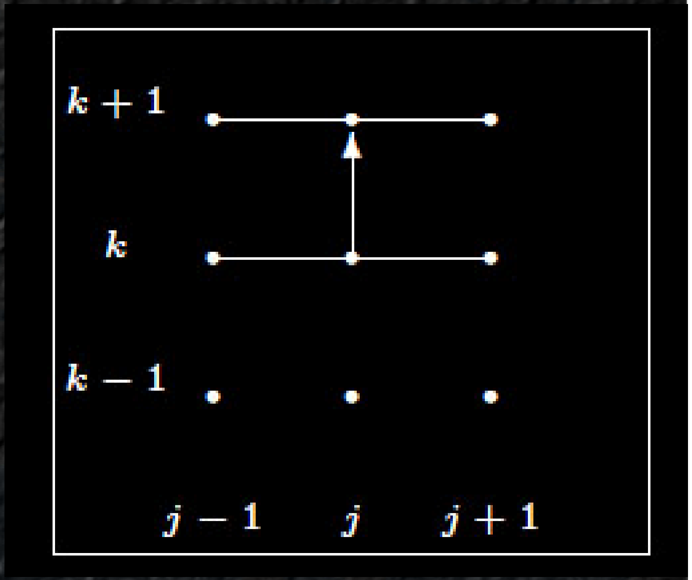
Crank-Nicolson

$$\frac{U(i+1,j)-U(i,j)}{\Delta t} = \frac{1}{2}\left[F(i,j)+F(i+1,j)\right]$$

Implicit and Explicit Methods

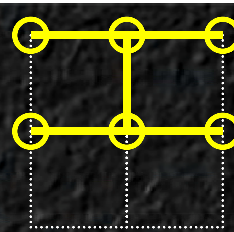
+ Unconditionally Stable
+ Second Order Accurate in Time

- Complete system should be solved at each time step



Crank-Nicolson method:
stable for larger time steps

Crank-Nicolson



1D Diffusion equation $$\frac{\partial}{\partial t}\mathrm{U}(t,x) = a\frac{\partial^2 U}{\partial x^2}$$

$$\frac{U(i+1,j)-U(i,j)}{\Delta t} = \frac{a}{2}\left[\frac{\partial^2 U}{\partial x^2}(i+1,j) + \frac{\partial^2 U}{\partial x^2}(i,j)\right]$$

$$\frac{U(i+1,j)-U(i,j)}{\Delta t} = \frac{a}{2(\Delta x)^2}\left[\left(U(i+1,j+1)-2U(i+1,j)+U(i+1,j-1)\right)+\left(U(i,j+1)-2U(i,j)+U(i,j-1)\right)\right]$$

$$r \equiv \frac{a\Delta t}{2(\Delta x)^2}$$

$$-rU(i+1,j+1)+(1+2r)U(i+1,j)-rU(i+1,j-1) =$$
$$rU(i,j+1)+(1-2r)U(i,j)+rU(i,j-1)$$

Triagonal Matrix

$$-rU(i+1,j+1)+(1+2r)U(i+1,j)-rU(i+1,j-1)=d(i,j)$$

$$a_j y_{j-1} + b_j y_j + c_j y_{j+1} = d_j$$

$$\begin{bmatrix} b_1 & c_1 & & \\ a_2 & b_2 & c_2 & \\ & . & . & . \\ & & a_n & b_n \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ . \\ y_n \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ . \\ d_n \end{bmatrix}$$

$$a_1 = 0$$

$$c_n = 0$$

1. Computing inverse matrix: $\boldsymbol{y} = \mathbf{T}^{-1} \boldsymbol{d}$
2. Gaussian elimination

Gaussian Elimination

$$a_j y_{j-1} + b_j y_j + c_j y_{j+1} = d_j \qquad a_1 = 0 \quad c_n = 0$$

$$c'_i = \begin{cases} \dfrac{c_i}{b_i} & ; \quad i = 1 \\[2ex] \dfrac{c_i}{b_i - a_i c'_{i-1}} & ; \quad i = 2, 3, \dots, n-1 \end{cases}$$

$$d'_i = \begin{cases} \dfrac{d_i}{b_i} & ; \quad i = 1 \\[2ex] \dfrac{d_i - a_i d'_{i-1}}{b_i - a_i c'_{i-1}} & ; \quad i = 2, 3, \dots, n. \end{cases}$$

$$y_j + c^*_j y_{j+1} = d^*_j \qquad j = 1, \dots, n-1$$

$$y_n = d^*_n \qquad j = n$$

$$y_j = d^*_j - c^*_j y_{j+1} \qquad j = 1, \dots, n-1$$

$$y_n = d^*_n \qquad j = n$$

To do

Derive implicit Crank-Nicolson algorithm and solve equations:

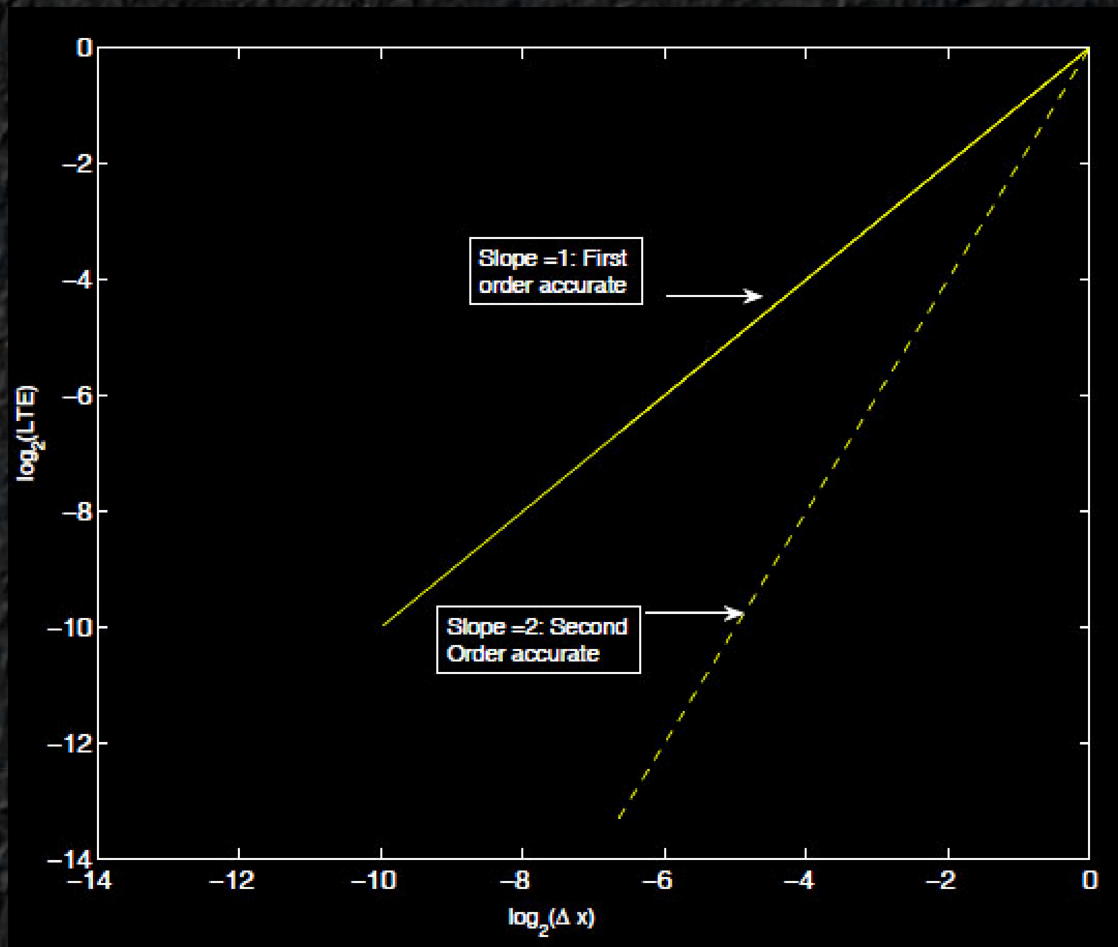
1. $$\frac{\partial}{\partial t}\mathrm{U}(x,t) = a(x)\frac{\partial^2 U(x,t)}{\partial x^2} + f\frac{\partial U(x,t)}{\partial x}$$

2. $$\frac{\partial}{\partial t}\mathrm{U}(x,t) = a(x,t)\frac{\partial^2 U(x,t)}{\partial x^2} + cU(x,t)$$

3. $$\frac{\partial}{\partial t}\mathrm{U}(x,y,t) = a(x,y)\left(\frac{\partial^2 U(x,y,t)}{\partial x^2} + \frac{\partial^2 U(x,y,t)}{\partial y^2}\right)$$

First vs Second Order Accuracy

Local truncation error vs. grid resolution in x



Source Terms

Nonlinear Equation with source term S(U)

$$\frac{\partial}{\partial t}\mathrm{U}(t,x)+\frac{\partial}{\partial x}F(\mathrm{U})=S(\mathrm{U})$$

e.g. HD in curvilinear coordinates

1. Unsplit method
2. Fractional step (splitting method)

Source Terms: unsplit method

One sided forward method:

$$U(i+1,j) = U(i,j) - \frac{\Delta t}{\Delta x}\left[F(U(i,j+1)) - F(U(i,j))\right] + \Delta t S(U(i,j))$$

- Lax-Friedrichs (linear + nonlinear)
- Leapfrog (linear)
- Lax-Wendroff (linear+nonlinear)
- Beam-Warming (linear)

Source Terms: splitting method

Split inhomogeneous equation into two steps:

transport + sources

1) Solve PDE (transport) $$\frac{\partial}{\partial t}\mathrm{U}(t,x)+\frac{\partial}{\partial x}F(\mathrm{U})=0$$

$$\mathrm{U}(i,j)\rightarrow\overline{\mathrm{U}}(i,j)$$

2) Solve ODE (source) $$\frac{\partial}{\partial t}\overline{\mathrm{U}}(t,x)=S(\overline{\mathrm{U}})$$

$$\mathrm{U}(i,j)\rightarrow\overline{\mathrm{U}}(i,j)\rightarrow\mathrm{U}(i+1,j)$$

Multidimensional Problems

Nonlinear multidimensional PDE:

$$\frac{\partial}{\partial t}\mathrm{U}(t,x)+\frac{\partial}{\partial x}F(\mathrm{U})+\frac{\partial}{\partial y}G(\mathrm{U})+\frac{\partial}{\partial z}H(\mathrm{U})=S(\mathrm{U})$$

Dimensional splitting

x-sweep

y-sweep

z-sweep

source term: splitting method

Dimension Splitting

x-sweep (PDE): $\frac{\partial}{\partial t}\mathrm{U}(t,x)+\frac{\partial}{\partial x}F(\mathrm{U})=0$ $\mathrm{U}(i,j)\rightarrow \mathrm{U}^{*}(i,j)$

y-sweep (PDE): $\frac{\partial}{\partial t}\mathrm{U}^{*}(t,x)+\frac{\partial}{\partial y}G(\mathrm{U}^{*})=0$ $\mathrm{U}^{*}(i,j)\rightarrow \mathrm{U}^{**}(i,j)$

z-sweep (PDE): $\frac{\partial}{\partial t}\mathrm{U}^{**}(t,x)+\frac{\partial}{\partial z}H(\mathrm{U}^{**})=0$ $\mathrm{U}^{**}(i,j)\rightarrow \mathrm{U}^{***}(i,j)$

source (ODE): $\frac{\partial}{\partial t}\mathrm{U}^{***}(t,x)=S(\mathrm{U}^{***})$ $\mathrm{U}^{***}(i,j)\rightarrow \mathrm{U}(i+1,j)$

Dimension Splitting

Upwind method (forward difference)

$$
\begin{aligned}
\mathrm{U}(i+1,j) = \mathrm{U}(i,j) - \frac{\Delta t}{\Delta x}\big[F(\mathrm{U}(i,j+1)) - F(\mathrm{U}(i,j))\big] - \\
- \frac{\Delta t}{\Delta y}\big[G(\mathrm{U}(i,j+1)) - G(\mathrm{U}(i,j))\big] - \\
- \frac{\Delta t}{\Delta z}\big[H(\mathrm{U}(i,j+1)) - H(\mathrm{U}(i,j))\big] + \\
+ \Delta t S(\mathrm{U}(i,j))
\end{aligned}
$$

Dimension Splitting

+ Speed
+ Numerical Stability

- Accuracy

Method of Lines

Conservation Equation: $$\frac{\partial}{\partial t}\mathrm{U}(t,x)+\frac{\partial}{\partial x}F(\mathrm{U})=0$$

Only spatial discretization: $$\frac{d}{dt}\mathrm{U}(j)=f(j)$$

$$f(j)=\frac{1}{\Delta x}\left[F(\mathrm{U}(j+1))-F(\mathrm{U}(j))\right]$$

Solution of the ODE (i=1..N)

- Analytic?
- Runge-Kutta

Method of Lines

Multidimensional problem:

$$\frac{\partial}{\partial t}\mathrm{U}(t,x)+\frac{\partial}{\partial x}F(\mathrm{U})+\frac{\partial}{\partial y}G(\mathrm{U})=S(\mathrm{U})$$

Lines:

$$\frac{d}{dt}\mathrm{U}(j,k)=f(j,k)+g(j,k)+S(\mathrm{U}(j,k))$$

Spatial discretazion:

$$f(j,k)=\frac{1}{\Delta x}\left[F(\mathrm{U}(j+1,k))-F(\mathrm{U}(j,k))\right]$$

$$g(j,k)=\frac{1}{\Delta y}\left[G(\mathrm{U}(j,k+1))-G(\mathrm{U}(j,k))\right]$$

Method of Lines

Analytic solution in time: Numerical error only due to spatial discretization;

+ For some problems analytic solutions exist;
+ Nonlinear equations solved using stable scheme (some nonlinear problems can not be solved using implicit method)

- Computationally extensive on high resolution grids;

Linear schemes

"It is not possible for a linear scheme to be both higher that first order accurate and free of spurious oscillations."

Godunov 1959

First order: numerical diffusion;

Second order: spurious oscillations;

end

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