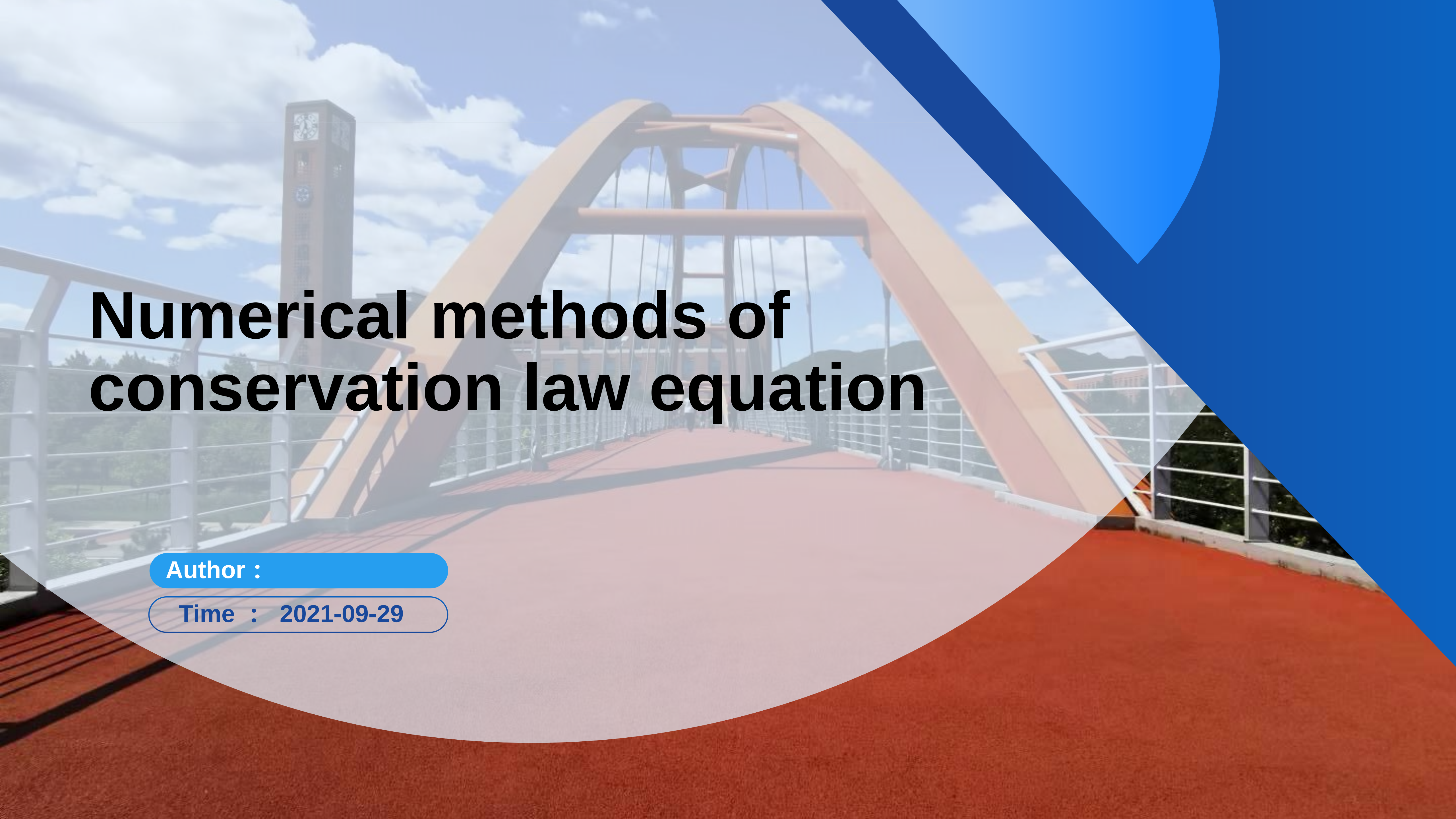


Numerical methods of conservation law equation

Author :

Time : 2021-09-29

以有限差分法求解一维的守恒型方程为例，介绍数值求解偏微分方程(PDE)

的一些基本知识

Outline

I. 线性的一维对流扩散方程

II. 导数的有限差分近似

III. 代数方程组

IV. Fortran codes

One-dimensional model equation

(1) The Advection-Diffusion Equation (最基本的模型方程)

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

非稳态项 → 时间项的离散

对流项 → 对流项的离散

扩散项 → 扩散项的离散

物理方程

FTCS

BTCS

CNCS

有限差分的离散过程：基于泰勒展开，用差商代替微商

代数方程组 → **编程求解**

非稳态对流扩散方程远比Navier-Stokes 方程简单，

但却包含了NS方程中重要的三项

One-dimensional model equation

(1) The Advection-Diffusion Equation (最基本的模型方程)

对于一维的非稳态线性对流扩散方程，一个特解如下：

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

$$f(x,t) = \frac{1}{\sqrt{4t+1}}\exp\left(-\frac{(x-1-Ut)^2}{D(4t+1)}\right)$$

问题描述：

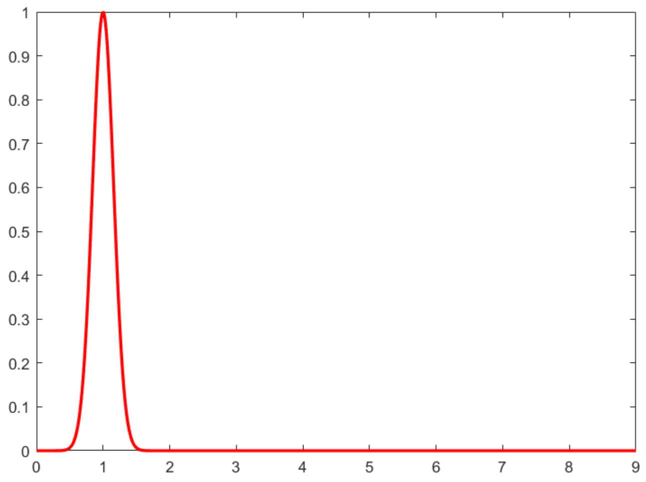
用数值方法求解当$U = 1.0, D = 0.05, x \in [0,9]$时，一维非稳态对流扩散方程的解，并与$t = 2.5$时的解析解进行对比。

初始条件：

$$f(x,0) = \exp\left(-\frac{(x-1)^2}{D}\right), x \in [0,9]$$

边界条件：

$$\begin{cases} f(0,t) = \dfrac{1}{\sqrt{4t+1}}\exp\left(-\dfrac{(1+Ut)^2}{D(4t+1)}\right) \\ f(9,t) = \dfrac{1}{\sqrt{4t+1}}\exp\left(-\dfrac{(8-Ut)^2}{D(4t+1)}\right) \end{cases}$$



$f(x, t = 0)$的图像

One-dimensional model equation

(2) The Conservation Equation

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

非守恒形式的对流扩散方程

$$F = Uf - D\frac{\partial f}{\partial x}$$

F 表示对流项和扩散项的通量

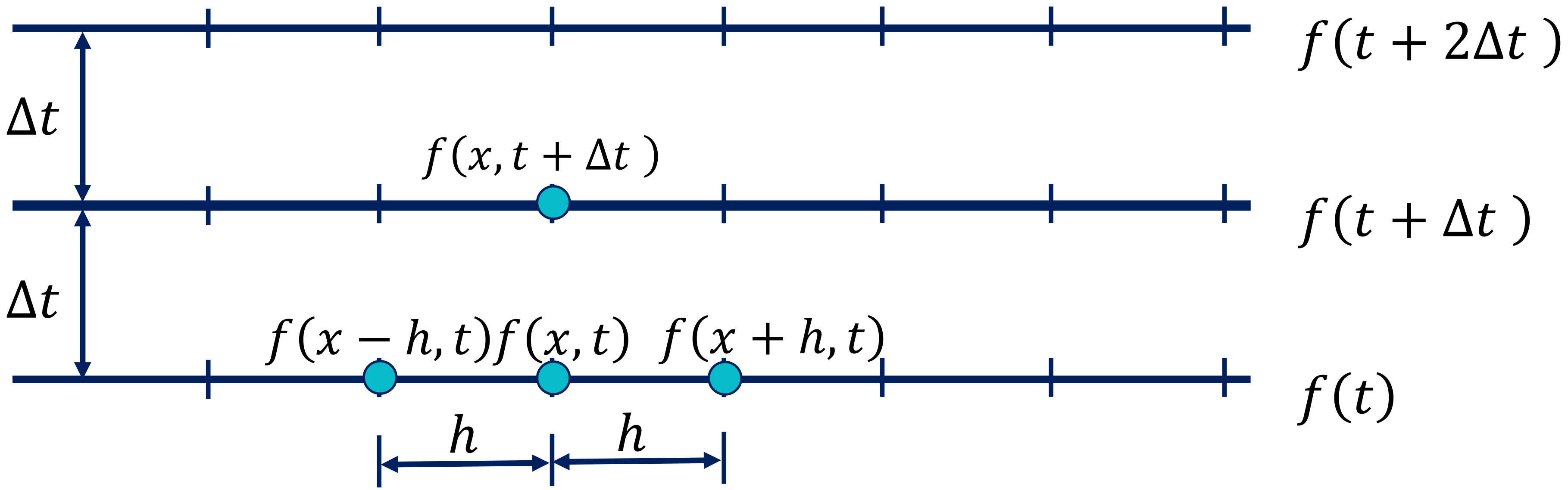
$$\frac{\partial f}{\partial t} + \frac{\partial F}{\partial x} = 0$$

守恒形式的对流扩散方程

One-dimensional model equation

(3) 导数的有限差分近似

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$



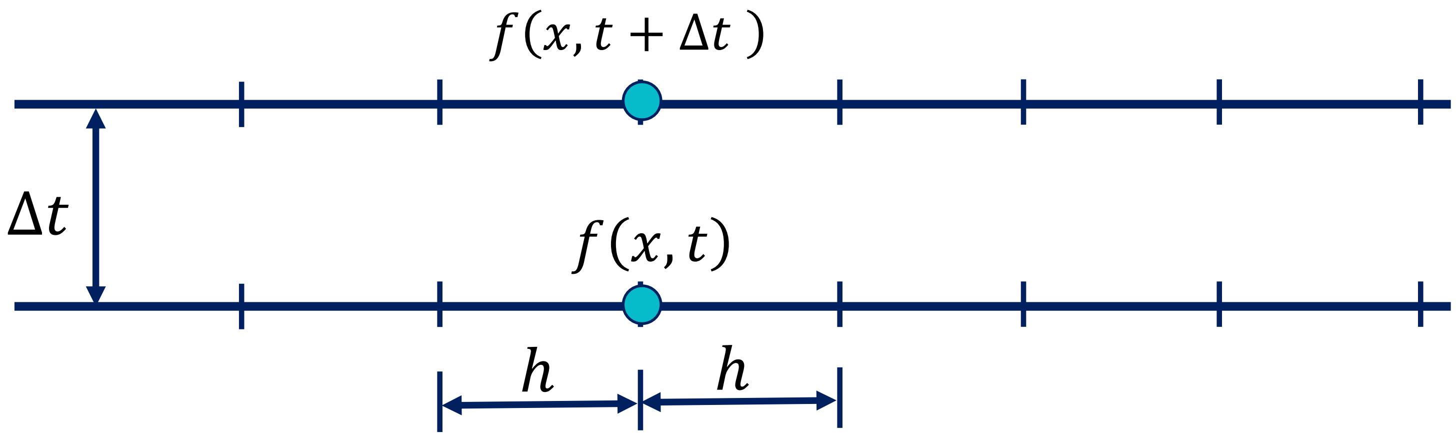
时空离散示意图

One-dimensional model equation

(3.1) 时间项的有限差分近似

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

最简单的时间离散格式：Forward Euler



时空离散示意图

One-dimensional model equation

(3.1) 时间项的有限差分近似

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

最简单的时间离散格式：Forward Euler

泰勒展开：

$$f(t+\Delta t) = f(t) + \frac{\partial f(t)}{\partial t}\Delta t + \frac{\partial^2 f(t)}{\partial t^2}\frac{\Delta t^2}{2} + \cdots$$

$$\frac{\partial f(t)}{\partial t} = \frac{f(t+\Delta t) - f(t)}{\Delta t} - \frac{\partial^2 f(t)}{\partial t^2}\frac{\Delta t}{2} + \cdots$$

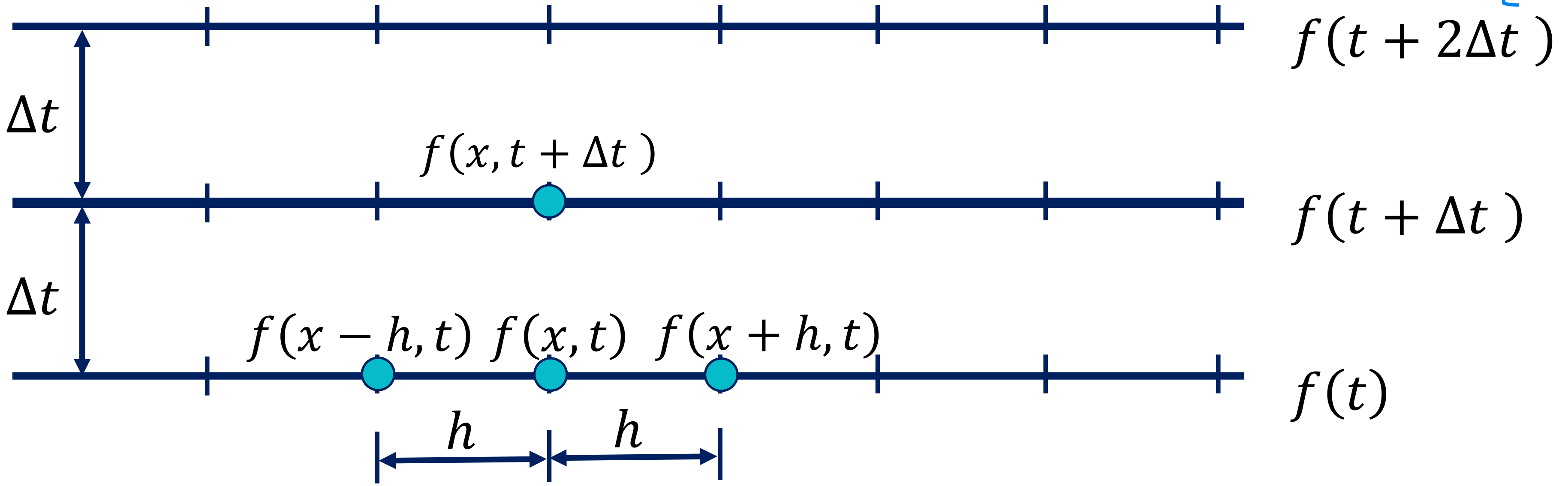
One-dimensional model equation

(3.2) 一阶空间导数项的有限差分近似

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

1. 对流项的物理意义：流体质点的运动导致物理量发生变化
2. 好的离散格式应该能够反映算子(如空间导数)本身的物理意义
3. 风从哪边吹过来，哪边的影响就更显著！

$$\text{对流项}\begin{cases}\text{迎风型格式} & ☑ \\ \text{背风型格式} & ☒\end{cases}$$



时空离散示意图

4. 对流项的离散格式在计算流体力学中具有不可撼动的地位，简单起见，这里采用中心对称格式进行离散

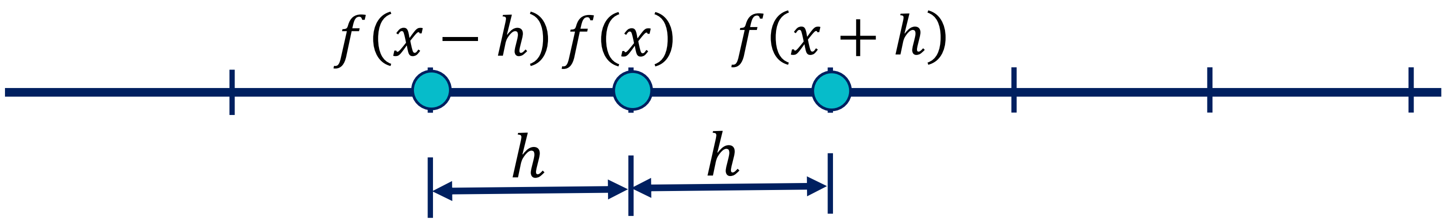
One-dimensional model equation

(3.2) 一阶空间导数项的有限差分近似

$$f(x+h) = f(x) + \frac{\partial f(x)}{\partial x}h + \frac{\partial^2 f(x)}{\partial x^2}\frac{h^2}{2} + \frac{\partial^3 f(x)}{\partial x^3}\frac{h^3}{6} + \frac{\partial^4 f(x)}{\partial x^4}\frac{h^4}{24} + \cdots$$

$$f(x-h) = f(x) - \frac{\partial f(x)}{\partial x}h + \frac{\partial^2 f(x)}{\partial x^2}\frac{h^2}{2} - \frac{\partial^3 f(x)}{\partial x^3}\frac{h^3}{6} + \frac{\partial^4 f(x)}{\partial x^4}\frac{h^4}{24} + \cdots$$

$$f(x+h) - f(x-h) = 2\frac{\partial f(x)}{\partial x}h + 2\frac{\partial^3 f(x)}{\partial x^3}\frac{h^3}{6} + \cdots$$



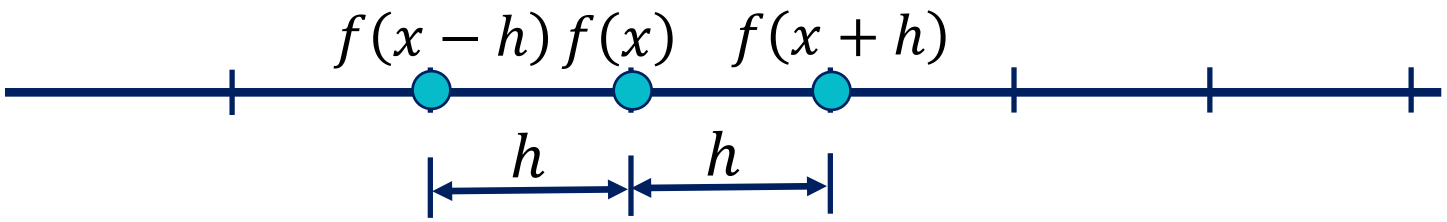
One-dimensional model equation

(3.2) 一阶空间导数项的有限差分近似

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

$$f(x+h) - f(x-h) = 2\frac{\partial f(x)}{\partial x}h + 2\frac{\partial^3 f(x)}{\partial x^3}\frac{h^3}{6} + \cdots$$

$$\frac{\partial f(x)}{\partial x} = \frac{f(x+h) - f(x-h)}{2h} - \frac{\partial^3 f(x)}{\partial x^3}\frac{h^2}{3} + \cdots$$



One-dimensional model equation

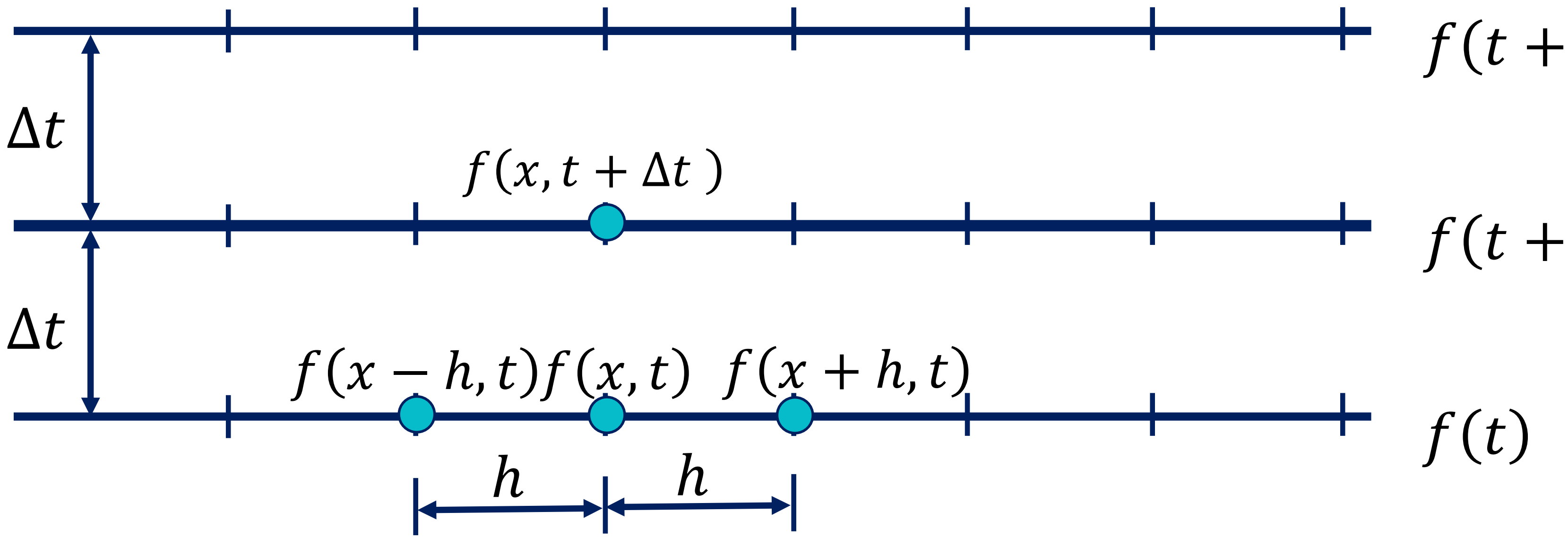
(3.2) 二阶空间导数项的有限差分近似

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

扩散项的物理意义：空间不同位置处的势差导致的物理量的变化，如温度差、浓度差

扩散项的特点：没有方向偏好，向四周均匀传播

中心对称型格式 ☑



时空离散示意图

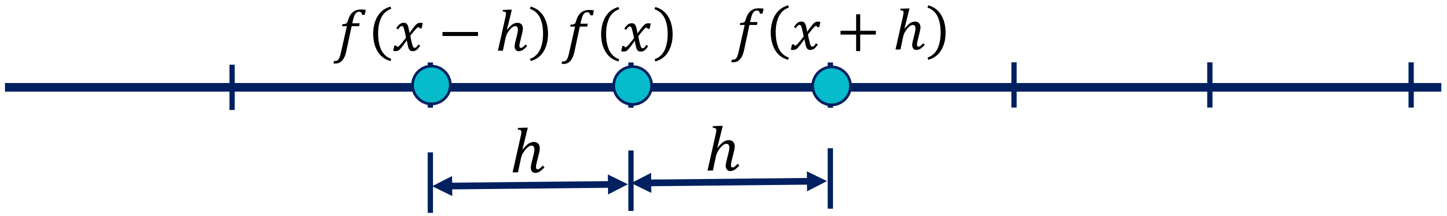
One-dimensional model equation

(3.2) 二阶空间导数项的有限差分近似

$$f(x+h) = f(x) + \frac{\partial f(x)}{\partial x} h + \frac{\partial^2 f(x)}{\partial x^2}\frac{h^2}{2} + \frac{\partial^3 f(x)}{\partial x^3}\frac{h^3}{6} + \frac{\partial^4 f(x)}{\partial x^4}\frac{h^4}{24} + \cdots$$

$$f(x-h) = f(x) - \frac{\partial f(x)}{\partial x} h + \frac{\partial^2 f(x)}{\partial x^2}\frac{h^2}{2} - \frac{\partial^3 f(x)}{\partial x^3}\frac{h^3}{6} + \frac{\partial^4 f(x)}{\partial x^4}\frac{h^4}{24} + \cdots$$

$$f(x+h) + f(x-h) = 2f(x) + 2\frac{\partial^2 f(x)}{\partial x^2}\frac{h^2}{2} + 2\frac{\partial^4 f(x)}{\partial x^4}\frac{h^4}{24} + \cdots$$



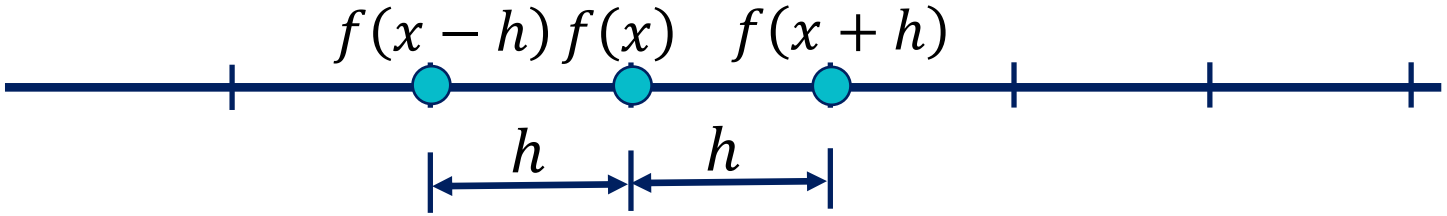
One-dimensional model equation

(3.2) 二阶空间导数项的有限差分近似

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

$$f(x+h) + f(x-h) = 2f(x) + 2\frac{\partial^2 f(x)}{\partial x^2}\frac{h^2}{2} + 2\frac{\partial^4 f(x)}{\partial x^4}\frac{h^4}{24} + \cdots$$

$$\frac{\partial^2 f(x)}{\partial x^2} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{\partial^4 f(x)}{\partial x^4}\frac{h^2}{12} + \cdots$$



One-dimensional model equation

(4) 代数方程组

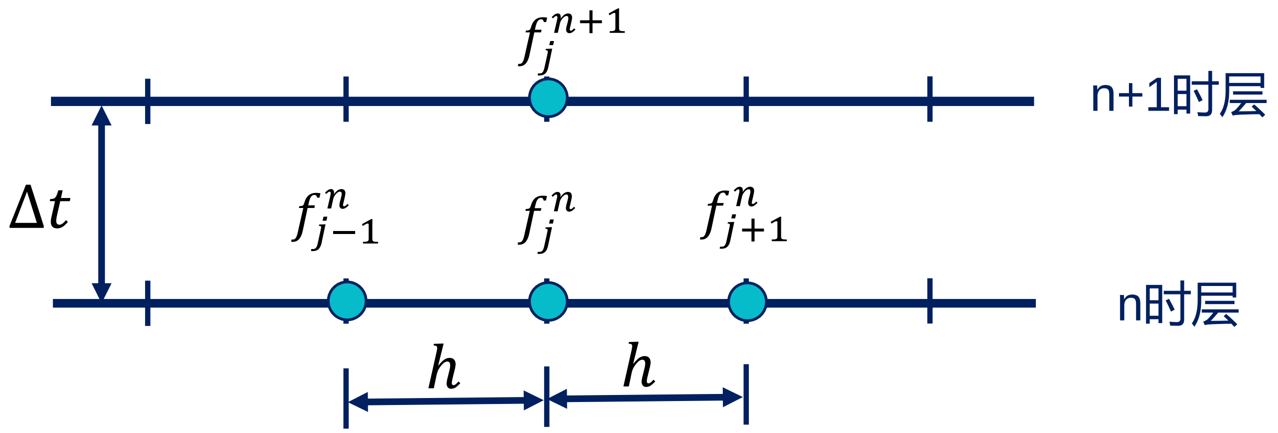
先引入几个基本的记号： $f^n = f(t)$

$$f_j^n = f(x_j, t)$$

$$f_{j-1}^n = f(x_j - h, t)$$

$$f_{j+1}^n = f(x_j + h, t)$$

$$f_j^{n+1} = f(x_j, t + \Delta t)$$



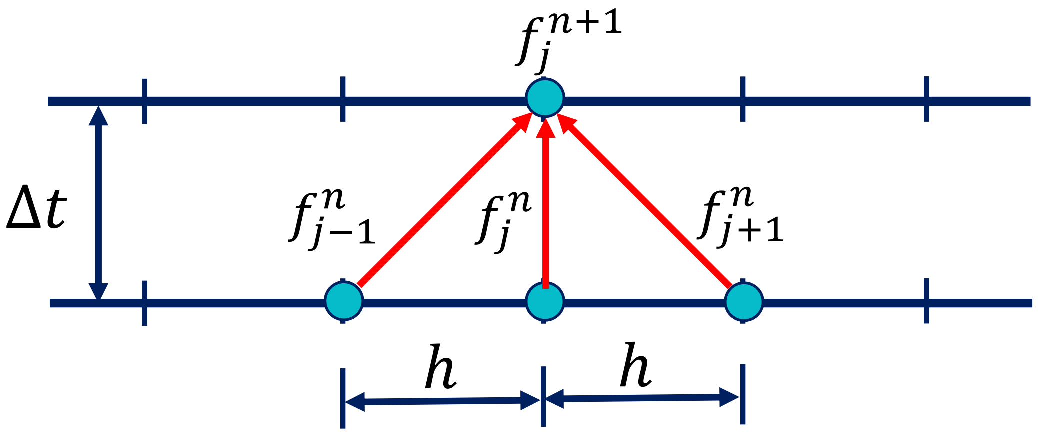
One-dimensional model equation

(4) 代数方程组 (FTCS scheme)

Forward in Time, Centered in Space (FTCS scheme)

用当前时层(n时层)的已知值
将下一个时层(n+1时层)的值**显式**地表示出来

$$\left(\frac{\partial f}{\partial t}\right)_j^n + U\left(\frac{\partial f}{\partial x}\right)_j^n = D\left(\frac{\partial^2 f}{\partial x^2}\right)_j^n$$



$$\left(\frac{\partial f}{\partial t}\right)_j^n = \frac{f_j^{n+1} - f_j^n}{\Delta t} + O(\Delta t)$$

$$\left(\frac{\partial f}{\partial x}\right)_j^n = \frac{f_{j+1}^n - f_{j-1}^n}{2h} + O(h^2)$$

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_j^n = \frac{f_{j+1}^n - 2f_j^n + f_{j-1}^n}{h^2} + O(h^2)$$

$$f_j^n = f(x_j, t)$$

$$f_{j-1}^n = f(x_j - h, t)$$

$$f_{j+1}^n = f(x_j + h, t)$$

$$f_j^{n+1} = f(x_j, t + \Delta t)$$

One-dimensional model equation

(4) 代数方程组 (FTCS scheme)

$$\left(\frac{\partial f}{\partial t}\right)_j^n + U\left(\frac{\partial f}{\partial x}\right)_j^n = D\left(\frac{\partial^2 f}{\partial x^2}\right)_j^n$$

截断误差：
时间上具有一阶精度
空间上具有二阶精度

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U\frac{f_{j+1}^n - f_{j-1}^n}{2h} = D\frac{f_{j+1}^n - 2f_j^n + f_{j-1}^n}{h^2} + O(\Delta t, h^2)$$

$$f_j^{n+1} = f_j^n - \frac{U\Delta t}{2h}\left(f_{j+1}^n - f_{j-1}^n\right) + \frac{D\Delta t}{h^2}\left(f_{j+1}^n - 2f_j^n + f_{j-1}^n\right)$$

One-dimensional model equation

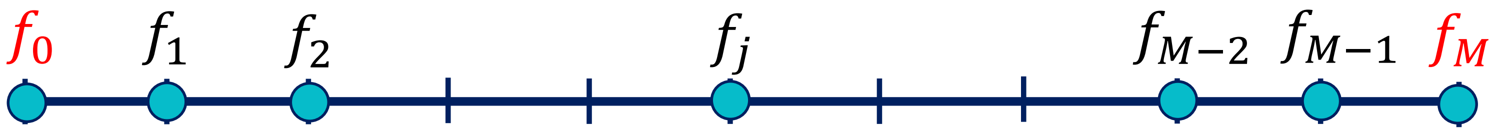
(4) 代数方程组 (FTCS scheme)

$$f_j^{n+1} = (\beta + \lambda) f_{j-1}^n + (1 - 2\beta) f_j^n + (\beta - \lambda) f_{j+1}^n$$

$$\lambda = \frac{U\Delta t}{2h}, \beta = \frac{D\Delta t}{h^2}$$

对应的矩阵: $Ax = B$

$$\begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & 1 & \\ & & & & 1 \end{pmatrix} \begin{pmatrix} f_1^{n+1} \\ f_2^{n+1} \\ \vdots \\ \vdots \\ f_{M-2}^{n+1} \\ f_{M-1}^{n+1} \end{pmatrix} = \begin{pmatrix} (\lambda+\beta) f_0^n + (1\text{-}2\beta) f_1^n + (\beta\text{-}\lambda) f_2^n \\ (\lambda+\beta) f_1^n + (1\text{-}2\beta) f_2^n + (\beta\text{-}\lambda) f_3^n \\ \vdots \\ \vdots \\ (\lambda+\beta) f_{M-3}^n + (1\text{-}2\beta) f_{M-2}^n + (\beta\text{-}\lambda) f_{M-1}^n \\ (\lambda+\beta) f_{M-2}^n + (1\text{-}2\beta) f_{M-1}^n + (\beta\text{-}\lambda) f_M^n \end{pmatrix}$$



其中：f_0^n、f_M^n为边界处的已知值

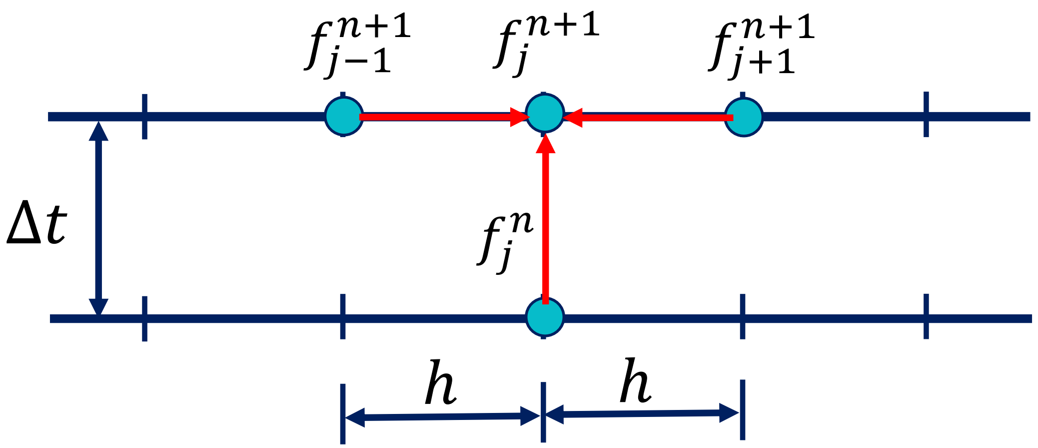
One-dimensional model equation

(4) 代数方程组 (BTCS scheme)

Backward in Time, Centered in Space (BTCS scheme)

用当前时层(n时层)的已知值
将下一个时层(n+1时层)的值**隐式**地表示出来

$$\left(\frac{\partial f}{\partial t}\right)_j^{n} + U\left(\frac{\partial f}{\partial x}\right)_j^{n+1} = D\left(\frac{\partial^2 f}{\partial x^2}\right)_j^{n+1}$$



$$\left(\frac{\partial f}{\partial t}\right)_j^{n} = \frac{f_j^{n+1} - f_j^n}{\Delta t} + O(\Delta t)$$

$$\left(\frac{\partial f}{\partial x}\right)_j^{n+1} = \frac{f_{j+1}^{n+1} - f_{j-1}^{n+1}}{2h} + O(h^2)$$

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_j^{n+1} = \frac{f_{j+1}^{n+1} - 2f_j^{n+1} + f_{j-1}^{n+1}}{h^2} + O(h^2)$$

$$f_j^n = f(x_j, t)$$

$$f_j^{n+1} = f(x_j, t + \Delta t)$$

$$f_{j+1}^{n+1} = f(x_j + h, t + \Delta t)$$

$$f_{j-1}^{n+1} = f(x_j - h, t + \Delta t)$$

One-dimensional model equation

(4) 代数方程组 (BTCS scheme)

$$\left(\frac{\partial f}{\partial t}\right)_j^n + U\left(\frac{\partial f}{\partial x}\right)_j^{n+1} = D\left(\frac{\partial^2 f}{\partial x^2}\right)_j^{n+1}$$

截断误差：
时间上具有一阶精度
空间上具有二阶精度

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U\frac{f_{j+1}^{n+1} - f_{j-1}^{n+1}}{2h} = D\frac{f_{j+1}^{n+1} - 2f_j^{n+1} + f_{j-1}^{n+1}}{h^2} + O(\Delta t, h^2)$$

$$\left(\frac{U\Delta t}{2h} - \frac{D\Delta t}{h^2}\right)f_{j+1}^{n+1} + \left(1 + \frac{2D\Delta t}{h^2}\right)f_j^{n+1} - \left(\frac{U\Delta t}{2h} + \frac{D\Delta t}{h^2}\right)f_{j-1}^{n+1} = f_j^n$$

One-dimensional model equation

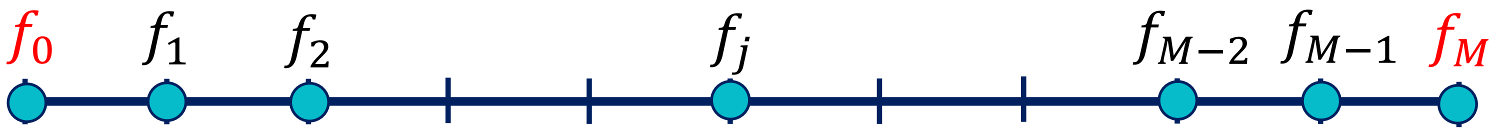
(4) 代数方程组 (BTCS scheme)

$$(\lambda-\beta)f_{j+1}^{n+1}+(1+2\beta)f_j^{n+1}-(\lambda+\beta)f_{j-1}^{n+1}=f_j^n$$

$$\lambda=\frac{U\Delta t}{2h},\beta=\frac{D\Delta t}{h^2}$$

对应的矩阵: $Ax=B$

$$\begin{pmatrix} 1+2\beta & \lambda\text{-}\beta & 0 & \cdots & 0 & 0 \\ -\lambda\text{-}\beta & 1+2\beta & \lambda\text{-}\beta & 0 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & 0 & -\lambda\text{-}\beta & 1+2\beta & \lambda\text{-}\beta \\ 0 & 0 & \cdots & 0 & -\lambda\text{-}\beta & 1+2\beta \end{pmatrix}\begin{pmatrix} f_1^{n+1} \\ f_2^{n+1} \\ \vdots \\ \vdots \\ f_{M-2}^{n+1} \\ f_{M-1}^{n+1} \end{pmatrix}=\begin{pmatrix} f_1^n+(\lambda+\beta)f_0^{n+1} \\ f_2^n \\ \vdots \\ \vdots \\ f_{M-2}^n \\ f_{M-1}^n+(\beta-\lambda)f_M^{n+1} \end{pmatrix}$$



其中： f_0^n、f_M^n**为边界处的已知值**

One-dimensional model equation

(4) 代数方程组 (CNCS scheme)

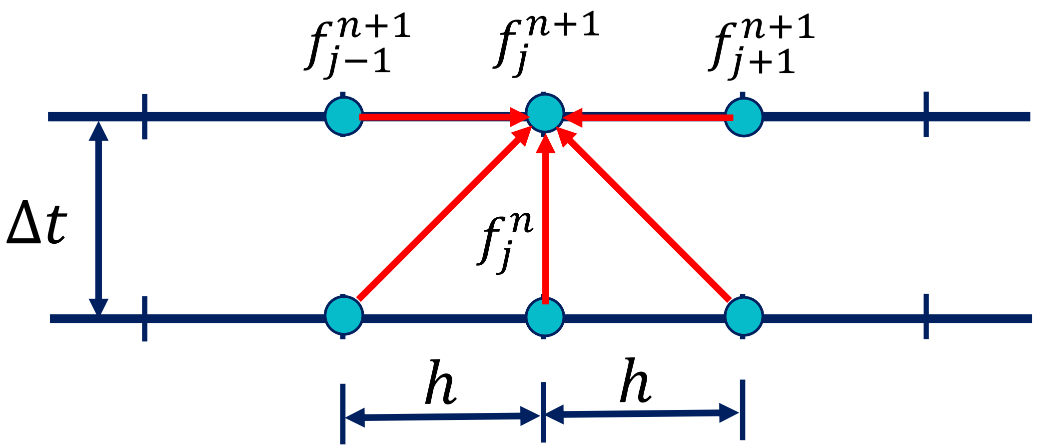
CNCS = FTCS + BTCS

FTCS $f_j^{n+1} = (\beta+\lambda)f_{j-1}^n + (1-2\beta)f_j^n + (\beta-\lambda)f_{j+1}^n$

$$\lambda = \frac{U\Delta t}{2h}, \beta = \frac{D\Delta t}{h^2}$$

BTCS $-(\lambda+\beta)f_{j-1}^{n+1} + (1+2\beta)f_j^{n+1} + (\lambda-\beta)f_{j+1}^{n+1} = f_j^n$

CNCS $-(\lambda+\beta)f_{j-1}^{n+1} + 2(1+\beta)f_j^{n+1} + (\lambda-\beta)f_{j+1}^{n+1} = (\beta+\lambda)f_{j-1}^n + 2(1-\beta)f_j^n + (\beta-\lambda)f_{j+1}^n$



截断误差：
时间和空间上都具有二阶精度

One-dimensional model equation

(4) 代数方程组 (CNCS scheme)

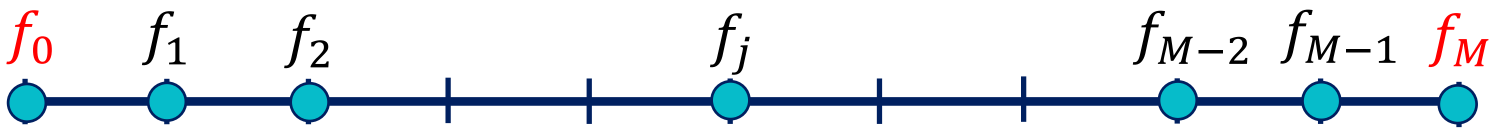
$$\lambda = \frac{U\Delta t}{2h}, \beta = \frac{D\Delta t}{h^2}$$

$$-(\lambda+\beta)f_{j-1}^{n+1} + 2(1+\beta)f_j^{n+1} + (\lambda-\beta)f_{j+1}^{n+1} = (\beta+\lambda)f_{j-1}^{n} + 2(1-\beta)f_j^{n} + (\beta-\lambda)f_{j+1}^{n}$$

对应的矩阵: $Ax = B$

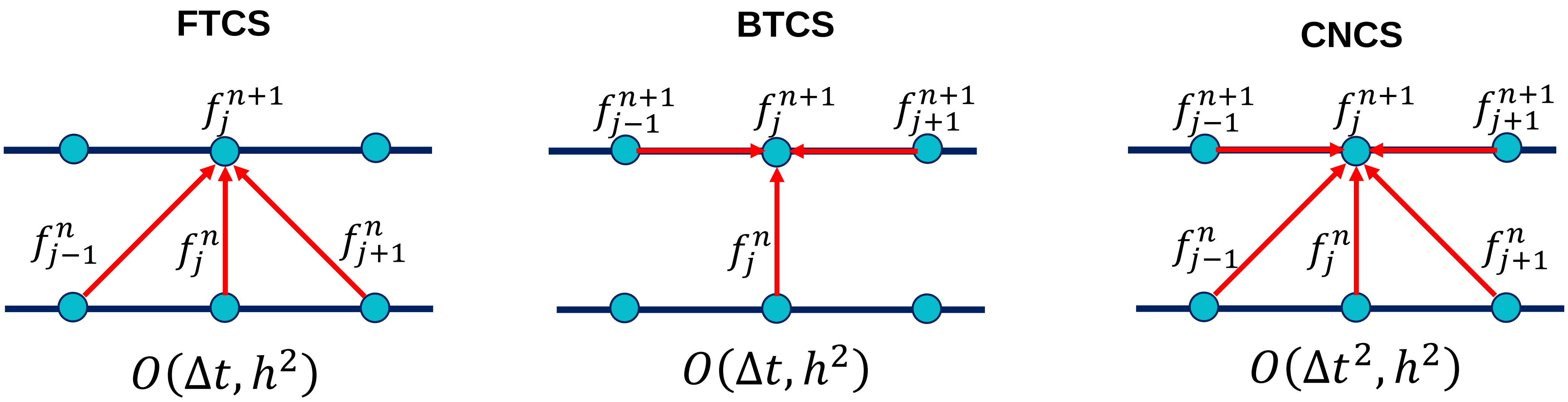
$$\begin{pmatrix} 2+2\beta & \lambda\text{-}\beta & 0 & \cdots & 0 & 0 \\ \text{-}\lambda\text{-}\beta & 2+2\beta & \lambda\text{-}\beta & 0 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & 0 & \text{-}\lambda\text{-}\beta & 2+2\beta & \lambda\text{-}\beta \\ 0 & 0 & \cdots & 0 & \text{-}\lambda\text{-}\beta & 2+2\beta \end{pmatrix} \begin{pmatrix} f_1^{n+1} \\ f_2^{n+1} \\ \vdots \\ \vdots \\ f_{M-2}^{n+1} \\ f_{M-1}^{n+1} \end{pmatrix} = \begin{pmatrix} 2(\lambda+\beta) f_0^{n+1} + 2(1\text{-}\beta) f_1^n + (\beta-\lambda) f_2^n \\ (\lambda+\beta) f_1^n + 2(1\text{-}\beta) f_2^n + (\beta-\lambda) f_3^n \\ \vdots \\ \vdots \\ (\lambda+\beta) f_{M\text{-}3}^n + 2(1\text{-}\beta) f_{M\text{-}2}^n + (\beta-\lambda) f_{M-1}^n \\ (\lambda+\beta) f_{M\text{-}2}^n + 2(1\text{-}\beta) f_{M-1}^n + 2(\beta-\lambda) f_M^{n+1} \end{pmatrix}$$

其中：f_0^n、f_M^n**为边界处的已知值**



One-dimensional model equation

(4) 代数方程组



时空离散示意图

One-dimensional model equation

(5) TDMA求解流程

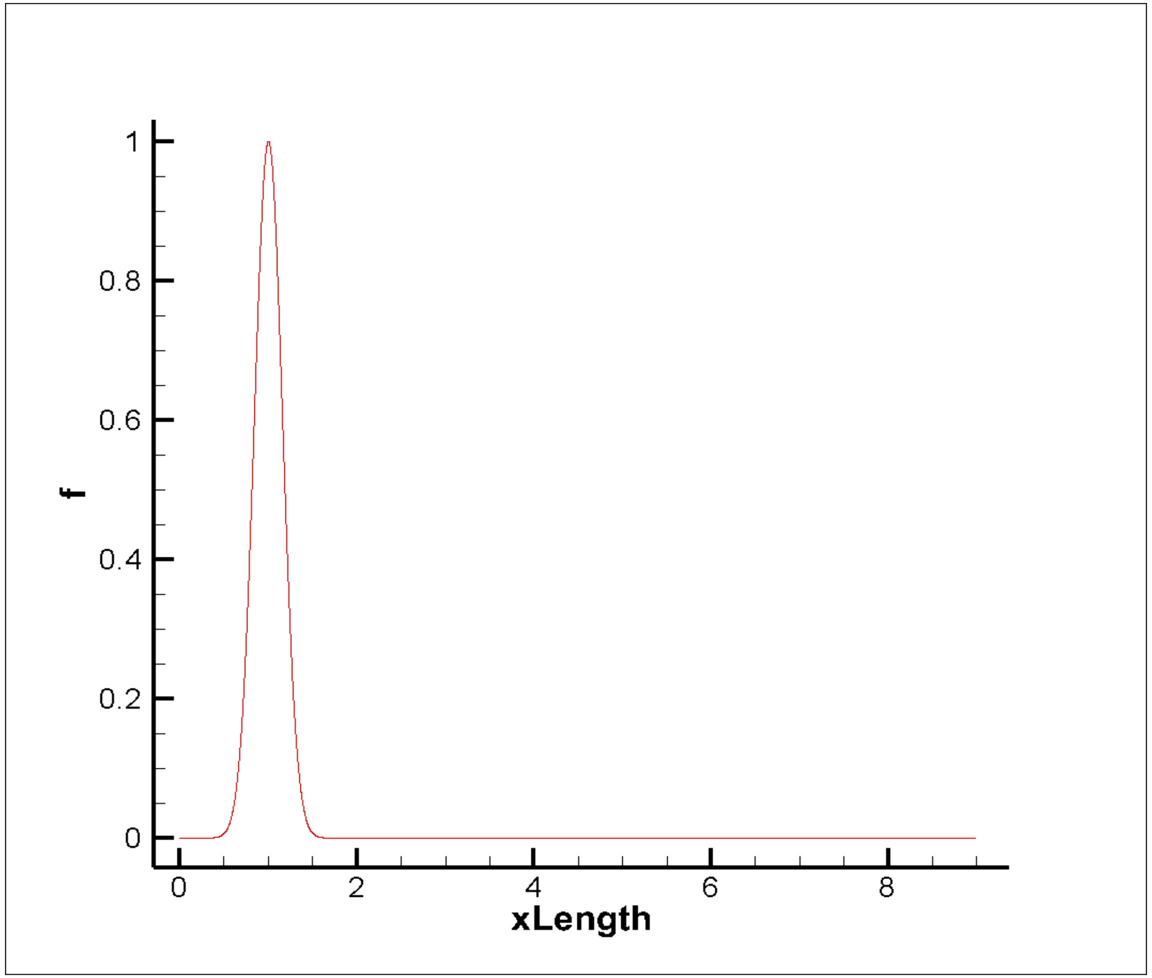
Ref: Tridiagonal Matrix Algorithm

One-dimensional model equation

(6) Computational result with Fortran code

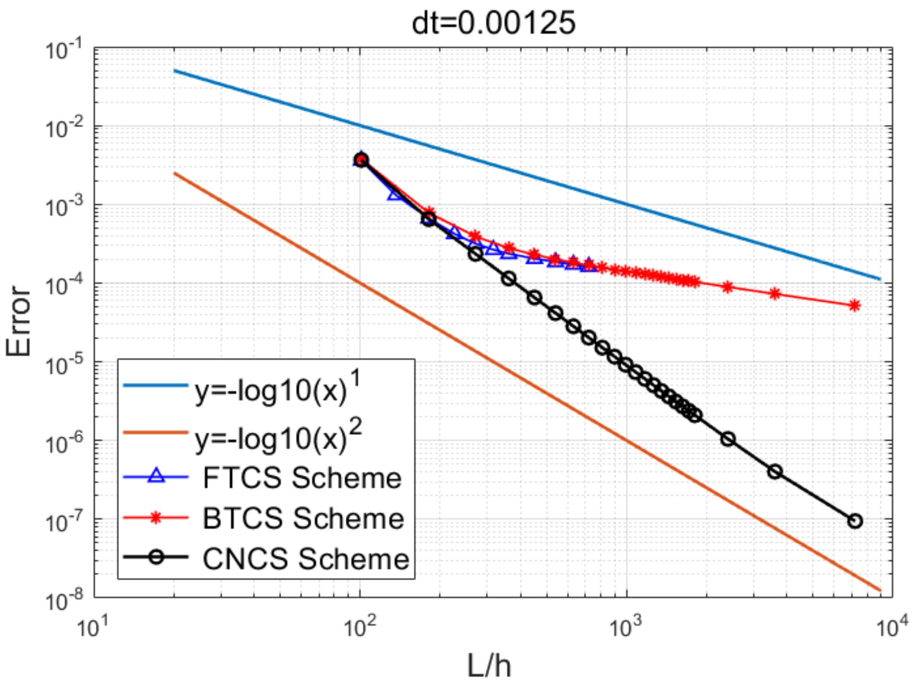
1. 固定时间步长，CFL数随网格数按比例变化

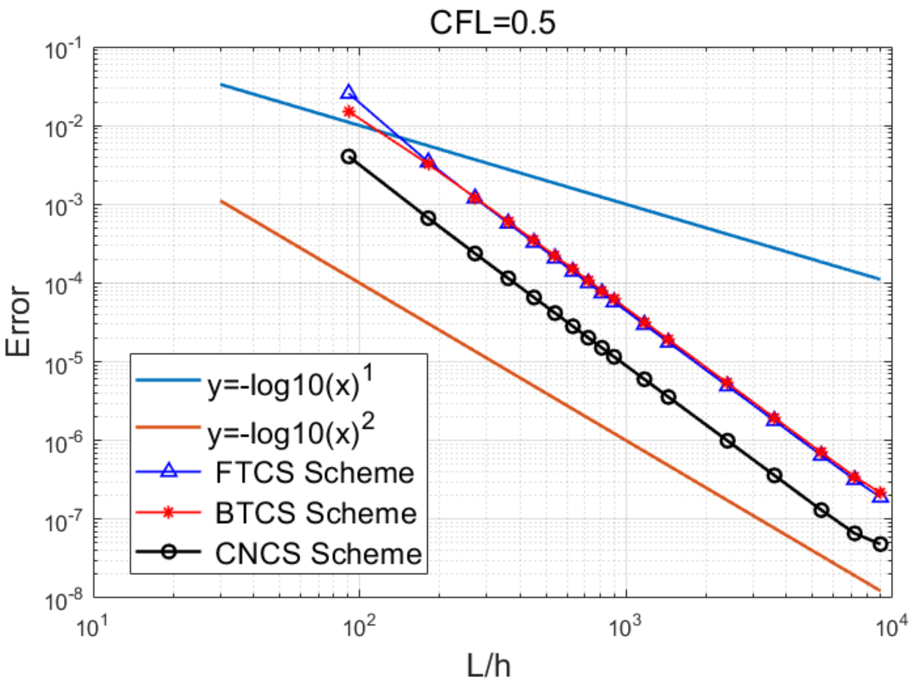
2. 固定CFL数，时间步长随网格数按比例变化



One-dimensional model equation

(7) 误差分析





固定时间步长，CFL数会改变

FTCS, BTCS：误差收敛于一阶精度

CNCS:误差收敛于二阶精度

固定CFL数，时间步长会改变

误差均收敛于二阶精度