含参数的偏微分方程

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含参数的偏微分方程

- 偏微分方程

$$\mathcal{L}(t,x,u)=0 \quad x\in\Omega$$

t：时间
x：空间坐标
Ω：计算区域
$u(t,x)$：状态变量

- 边界条件

$$\mathcal{B}(t,x,u)=0 \quad x\in\partial\Omega$$

- 初值条件

$$u(0,x)=u_0$$

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$$\mathcal{L}(t, x, u, \mu) = 0 \quad x \in \Omega_\mu$$

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- 边界条件

$$\mathcal{B}(t, x, u, \mu) = 0 \quad x \in \partial\Omega_\mu$$

- 初值条件

$$u(0, x) = u_0(\mu)$$

含参数的偏微分方程

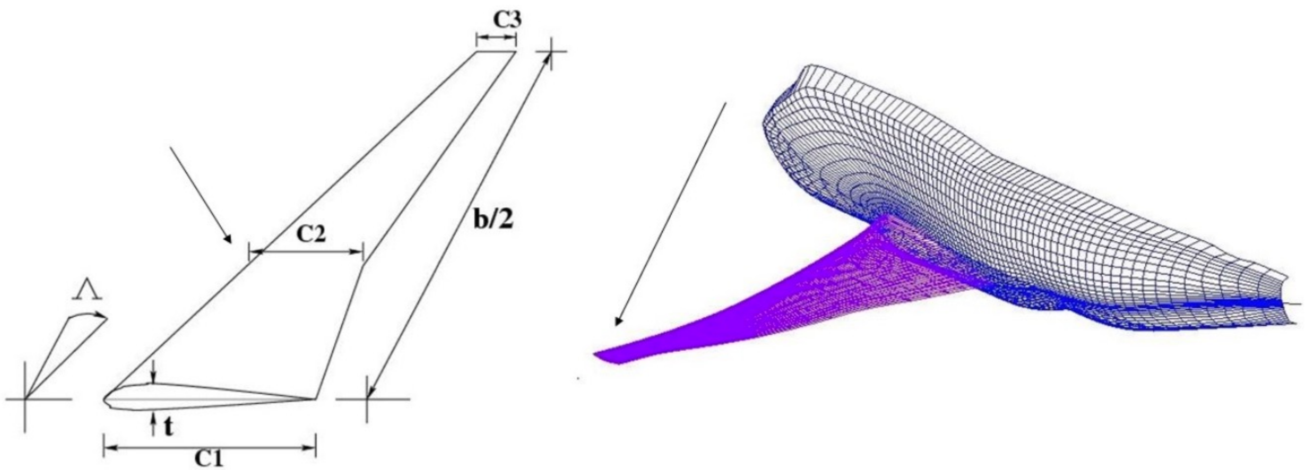
- 参数 μ

边界条件参数： $\mathcal{B}(t,x,u,\mu)=0$

初始条件参数： $u(0,x)=u_0(\mu)$

方程参数边： $\mathcal{L}(t,x,u,\mu)=0$

形状参数： Ω_μ



含参数的偏微分方程

- 参数 μ

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初始条件参数：$u(0, x) = u_0(\mu)$

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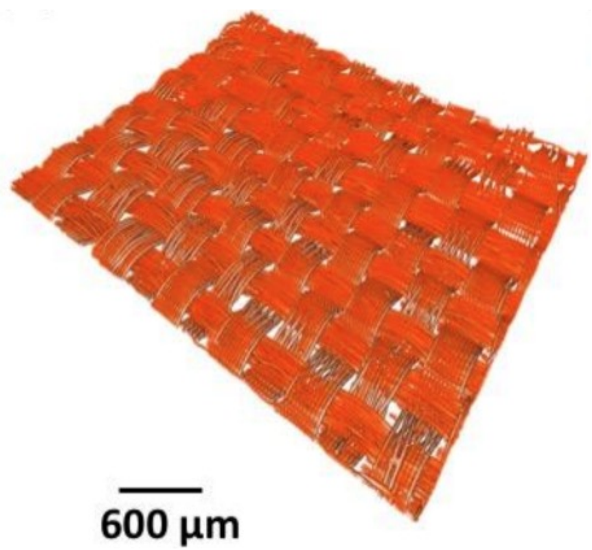
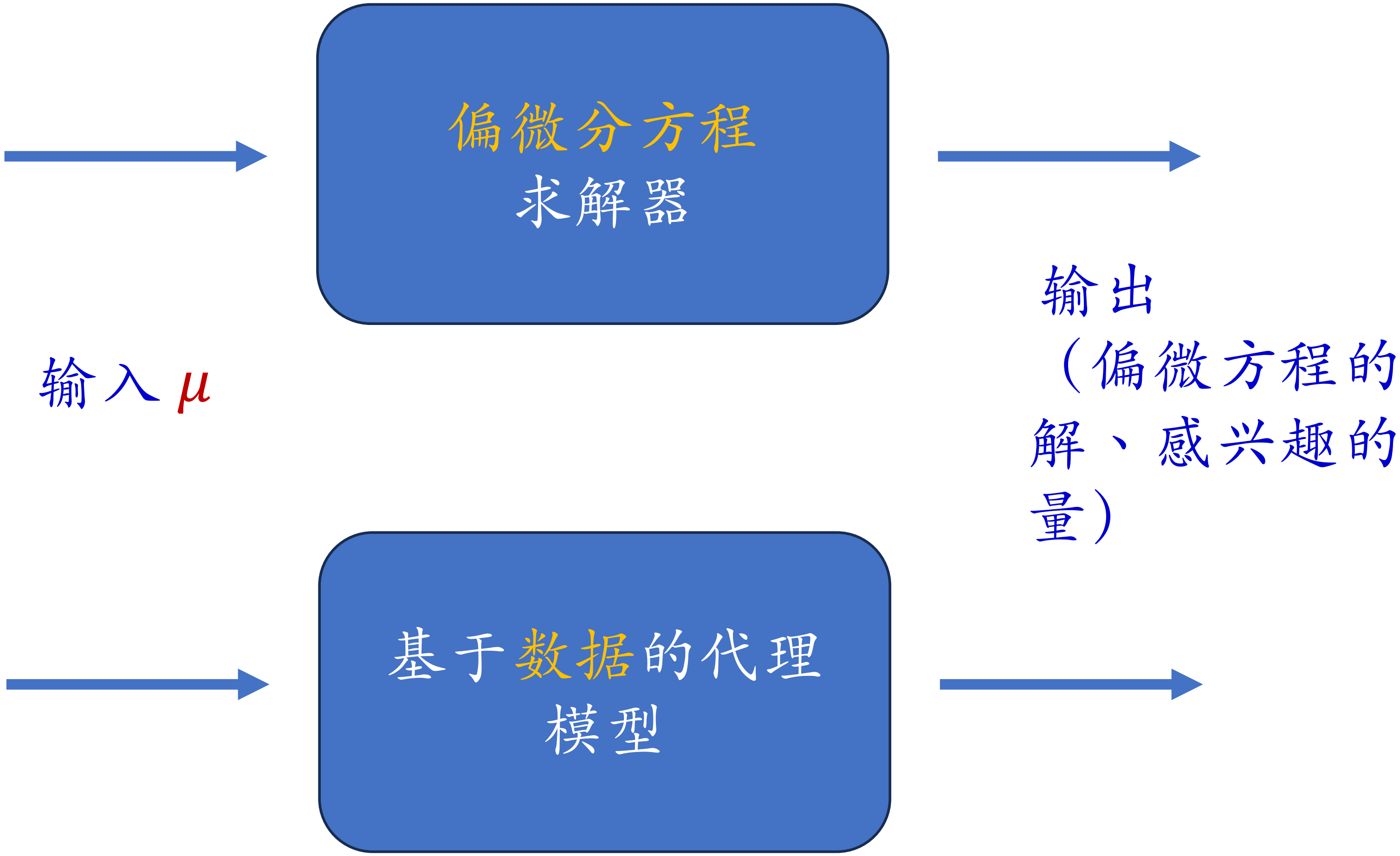
形状参数：Ω_μ

模型误差：$\mathcal{M}_\mu$

$$\sigma = \mathcal{M}_\mu(\epsilon) \qquad \epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$



- 代理模型(Surrogate models)



科学机器学习

- 模型校准、不确定性量化：找到最好的μ（或它的概率分布），输出能和数据更好拟合

- 工程设计优化、控制：找到最好的μ（或它的概率分布），输出能满足一定目标

传统偏微分方程数值方法

➢ 数值方法

- 有限体积方法 (finite volume method)
- 有限元方法 (finite element method)
- 有限差分方法 (finite difference method)
- 谱方法 (spectral method)

  ……

$$\frac{d\boldsymbol{u}}{dt} = f(\boldsymbol{u}, t, x; \mu)$$

$$\boldsymbol{u}(0; \mu) = u_0(\mu)$$

其中 $\boldsymbol{u}(t; \mu) \in R^N$

有限体积方法

- 对流扩散(advection-diffusion)方程

$$\partial_t u + \partial_x(au) = \partial_x(\nu\partial_x u) \qquad x \in (0,1)$$

初值条件：$u(0,x) = u_0 \qquad x \in (0,1)$

周期边界：$u(t,0) = u(t,1)$

守恒律：

$$\frac{d}{dt}\int_0^1 u(t,x)dx = \int_0^1 \partial_x(\nu\partial_x u) - \partial_x(ax)dx = 0$$

有限体积方法

➢ 对流扩散(advection-diffusion)方程

$$\partial_t u + \partial_x(au) = \partial_x(\nu\partial_x u) \qquad x \in (0,1)$$

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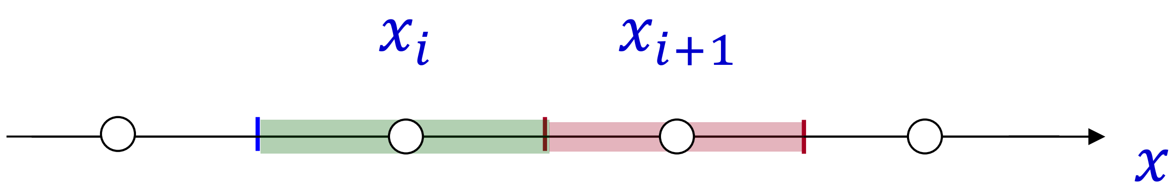
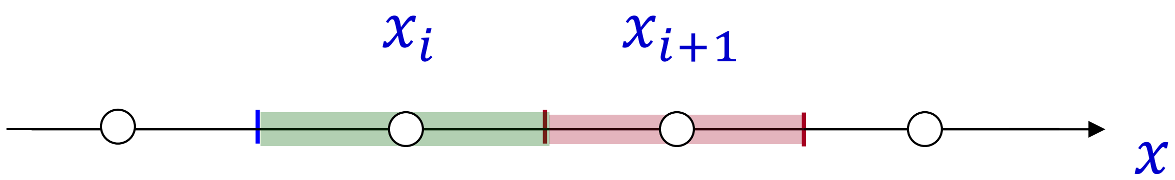


$$u_i(t) = \frac{1}{\Delta x_i}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u(t,x)dx \qquad u_i \approx u(t,x_i)(\text{二阶精度})$$

$$\text{守恒律：} \int_0^1 u(t,x)dx = \sum u_i \Delta x_i$$

有限体积方法



$$\frac{du_i(t)}{dt} = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \partial_t u(t,x)dx$$

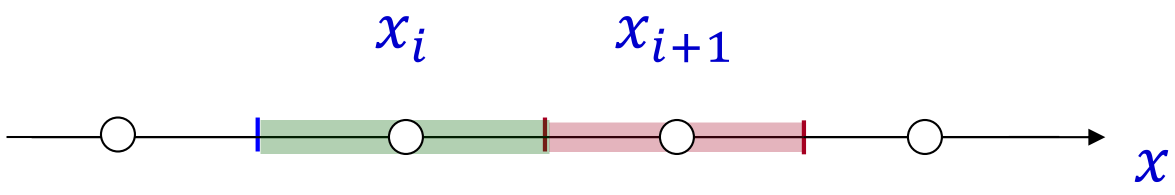
$$= \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \partial_x(\nu\partial_x u) - \partial_x(au)dx$$

$$= \frac{[\nu\,\partial_x u - au](x_{i+1/2}) - [\nu\,\partial_x u - au]\left(x_{i-1/2}\right)}{\Delta x_i}$$

守恒律： $\frac{d}{dt}\int_0^1 u(t,x)dx = \sum \frac{du_i(t)}{dt}\Delta x_i = 0$

有限体积方法

➤ 计算 $[\nu\, \partial_x u - au](x_{i+1/2})$



$$\partial_x u(t, x_{i+1/2}) \approx \frac{u(t, x_{i+1}) - u(t, x_i)}{\Delta x}$$

$$au(t, x_{i+1/2}) \approx \begin{cases} au(t, x_i) & a \geq 0 \\ au(t, x_{i+1}) & a \leq 0 \end{cases} \quad \text{(一阶迎风格式)}$$

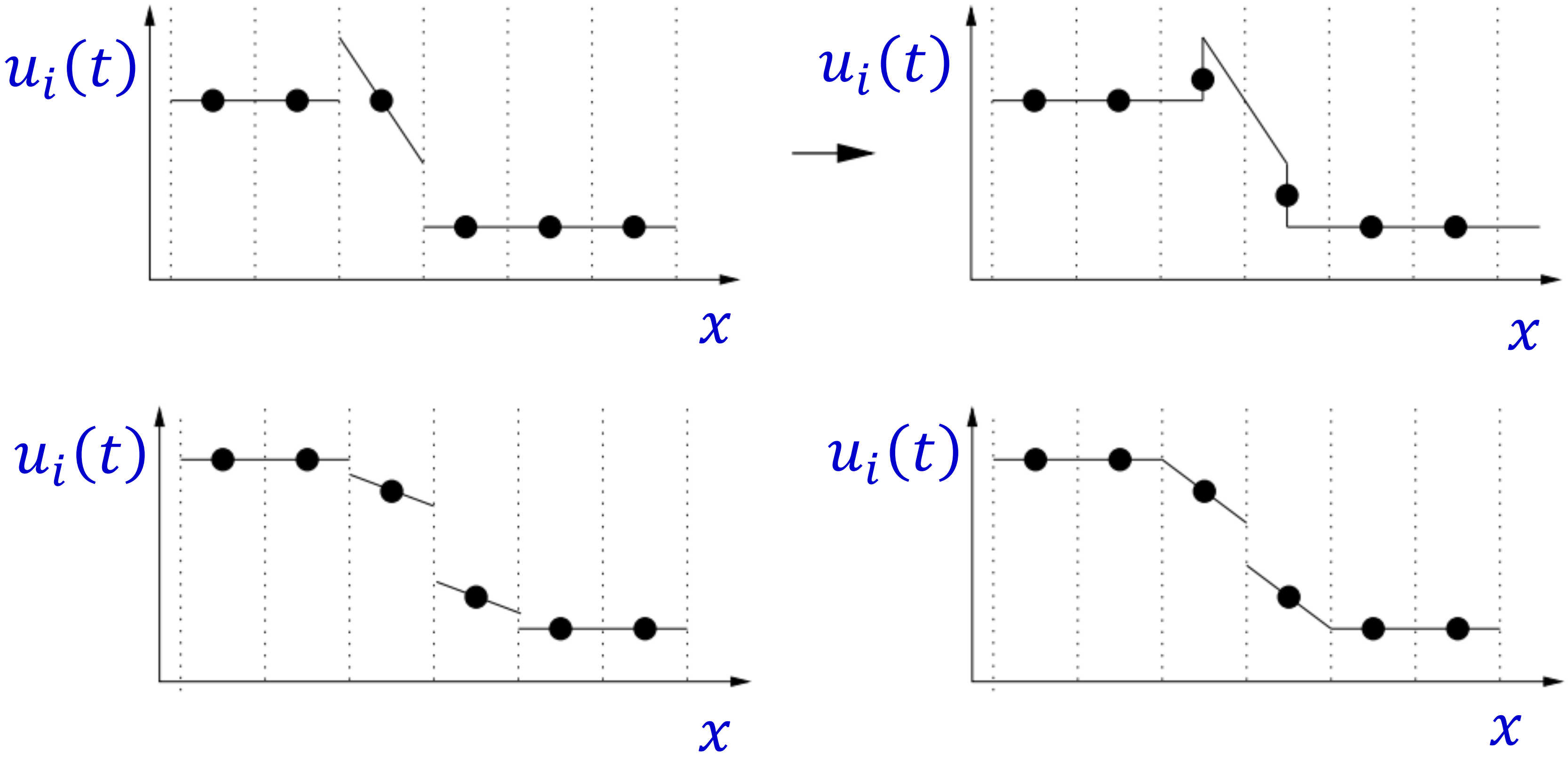
a ：流场速度

有限体积方法

➢ 限制器(limiter)

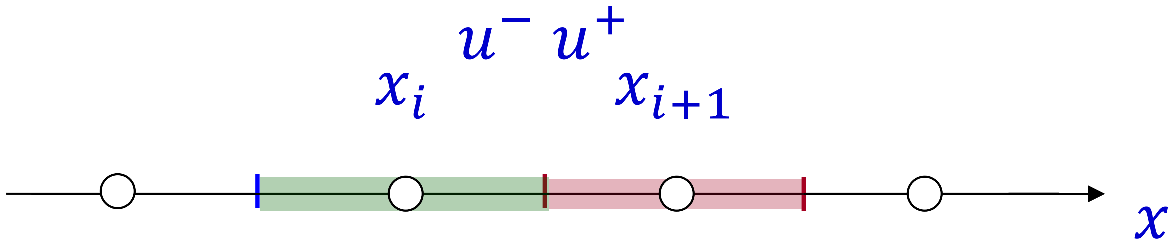
$$u_i(t) = \frac{1}{\Delta x_i}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u(t,x)dx$$

$$u_i(t), u_{i+1}(t), u_{i+2}(t) \rightarrow u(t,x) \qquad x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$$



有限体积方法

- 限制器(limiter)



$$u^-(x_{i+1/2}) \approx u_i + \frac{\Delta x_i}{2} s_i\ ,\ \ s_i = \mathrm{minmod}\{\frac{2(u_{i+1}-u_i)}{\Delta x_{i+1}+\Delta x_i}, \frac{2(u_i-u_{i-1})}{\Delta x_i+\Delta x_{i-1}}\}$$

$$\mathrm{minmod}\{a,b\} = \begin{cases} a & 当 ab>0，且 |a| \le |b| \\ b & 当 ab>0，且 |b| \le |a| \\ 0 & 其它 \end{cases}$$

$$u^+(x_{i+1/2}) \approx u_{i+1} - \frac{\Delta x_{i+1}}{2} s_{i+1}$$

$$au(t,x_{i+1/2}) \approx \begin{cases} au^-(t,x_{i+1/2}) & a \ge 0 \\ au^+(t,x_{i+1/2}) & a \le 0 \end{cases}$$

有限体积方法

- 时间离散

$$\boldsymbol{u} = [u_1(t); u_2(t); u_3(t) \cdots; u_n(t)]$$

$$\frac{d\boldsymbol{u}}{dt} = f(\boldsymbol{u}, t, x) \qquad \boldsymbol{u}(0) = [u_0(x_1); u_0(x_1); \cdots; u_n(x_1)]$$

向前Euler方法

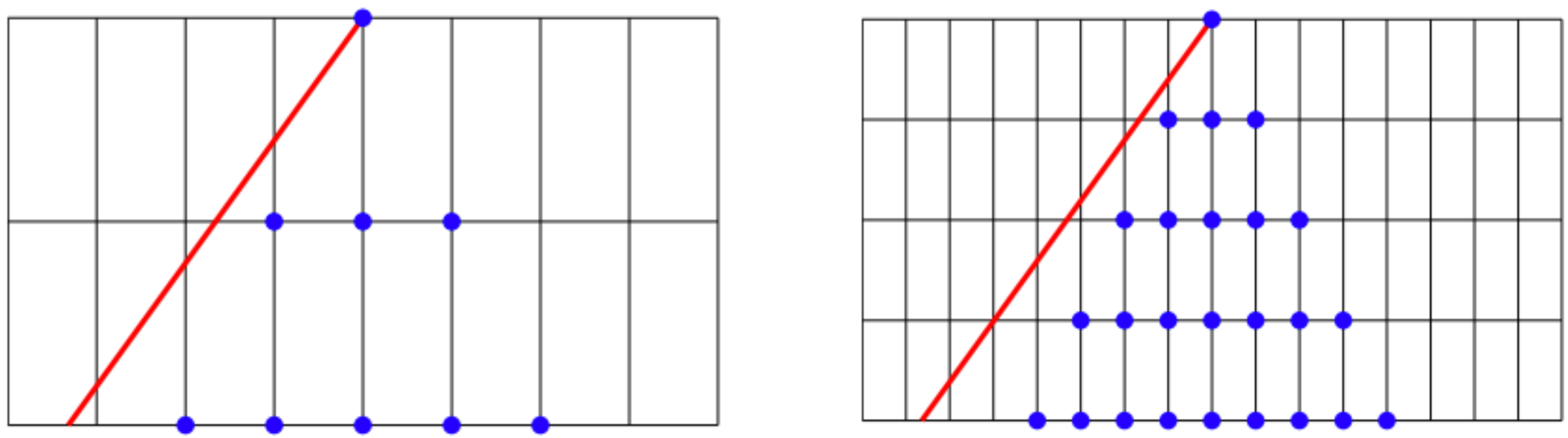
$$\boldsymbol{u}(t+\Delta t) = \boldsymbol{u}(t) + \Delta t f(\boldsymbol{u}(t), t, x)$$

Runge-Kutta方法

$$\boldsymbol{u}\left(t + \frac{\Delta t}{2}\right) = u(t) + \frac{\Delta t}{2} f(\boldsymbol{u}(t), t, x)$$

$$\boldsymbol{u}(t+\Delta t) = u(t) + \Delta t f\left(\boldsymbol{u}(\frac{\Delta t}{2}), t, x\right)$$

- 对流项Courant, Friedrichs, and Lewy (CFL) 条件

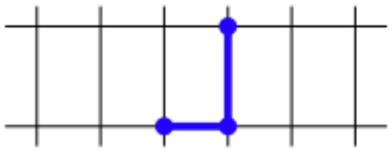


分析对流项：
红色直线：当 $\nu = 0$，我们有$u(t,x) = u_0(x - at)$
蓝色点：向前Euler方法的模版(Stencil)

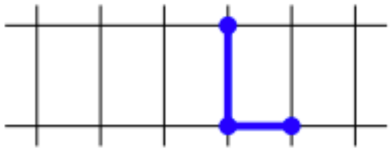
$$\left|\frac{a\Delta t}{\Delta x}\right| \leq 1$$

有限体积方法

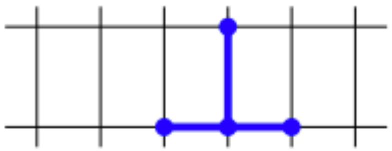
- 对流项Courant, Friedrichs, and Lewy (CFL) 条件



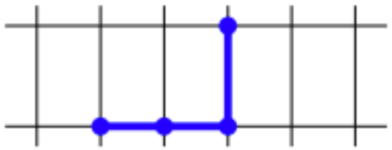
$$0 \leq \frac{a\Delta t}{\Delta x} \leq 1$$



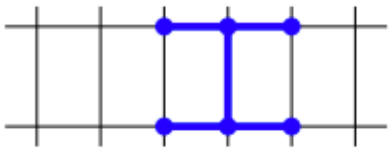
$$-1 \leq \frac{a\Delta t}{\Delta x} \leq 0$$



$$-1 \leq \frac{a\Delta t}{\Delta x} \leq 1$$



$$0 \leq \frac{a\Delta t}{\Delta x} \leq 2$$



$$-\infty \leq \frac{a\Delta t}{\Delta x} \leq +\infty$$

有限体积方法

- 扩散项Courant, Friedrichs, and Lewy (CFL) 条件

向前Euler方法：

$$\boldsymbol{u}(t+\Delta t)=\left(I+\frac{\nu\Delta t}{\Delta x^2}A\right)\boldsymbol{u}(t)$$

$$A=\begin{bmatrix}-2 & 1 & & \\ 1 & -2 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2\end{bmatrix}$$

von Neumann 稳定性分析：

$$|\boldsymbol{u}(t+\Delta t)|_\infty \le \left|I+\frac{\nu\Delta t}{\Delta x^2}A\right|_\infty |\boldsymbol{u}(t)|_\infty$$

$$\frac{2\nu\Delta t}{\Delta x^2}\le 1$$

有限体积方法

➢ Burgers 方程

$$\partial_t u + \partial_x\left(\frac{u^2}{2}\right) = \partial_x(\nu\partial_x u) \qquad x \in (0,1)$$
$$u(0,x) = u_0(x) \qquad x \in (0,1)$$
$$u(t,0) = u(t,1)$$

守恒律：

$$\frac{d}{dt}\int_0^1 u(t,x)dx = \int_0^1 \partial_x(\nu\partial_x u) - \partial_x\left(\frac{u^2}{2}\right)dx = 0$$

有限体积方法

- Burgers 方程

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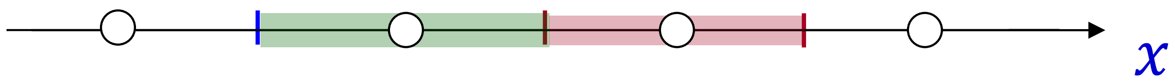


$$u_i(t) = \frac{1}{\Delta x_i}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u(t,x)dx \qquad u_i \approx u(t,x_i)(\text{二阶精度})$$

守恒律：$\int_0^1 u(t,x)dx = \sum u_i \Delta x_i$

有限体积方法

➢ Burgers 方程

$$\frac{du_i(t)}{dt} = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \partial_t u(t,x)dx$$

$$= \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \nu\, \partial_{xx} u - \partial_x\left(\frac{u^2}{2}\right) dx$$

$$= \frac{\left[\nu\, \partial_x u - \frac{u^2}{2}\right](x_{i+1/2}) - \left[\nu\, \partial_x u - \frac{u^2}{2}\right](x_{i-1/2})}{\Delta x}$$

有限体积方法

➢ Burgers 方程

$$\partial_t u + \partial_x\left(\frac{u^2}{2}\right) = \nu\ \partial_{xx} u \qquad x \in (0,1)$$

$$\frac{du_i(t)}{dt} = \frac{\left[\nu\ \partial_x u - \frac{u^2}{2}\right](x_{i+1/2}) - \left[\nu\ \partial_x u - \frac{u^2}{2}\right](x_{i-1/2})}{\Delta x}$$

$$\partial_x u(t, x_{i+1/2}) \approx \frac{u(t, x_{i+1}) - u(t, x_i)}{\Delta x}$$

$$\frac{u(t, x_{i+1/2})^2}{2} \approx \begin{cases} \dfrac{u(t, x_i)^2}{2} & \dfrac{u(t, x_i) + u(t, x_{i+1})}{2} \geq 0 \\ \dfrac{u(t, x_{i+1})^2}{2} & \dfrac{u(t, x_i) + u(t, x_{i+1})}{2} \leq 0 \end{cases}$$

(一阶迎风格式)

传统偏微分方程数值方法

- 数值方法

  - 有限体积方法 (finite volume method)
  - 有限元方法 (finite element method)
  - 有限差分方法 (finite difference method)
  - 谱方法 (spectral method)

  ……

$$\frac{d\boldsymbol{u}}{dt} = f(\boldsymbol{u}, t, x; \mu)$$

$$\boldsymbol{u}(0; \mu) = u_0(\mu)$$

其中 $\boldsymbol{u}(t; \mu) \in R^N$

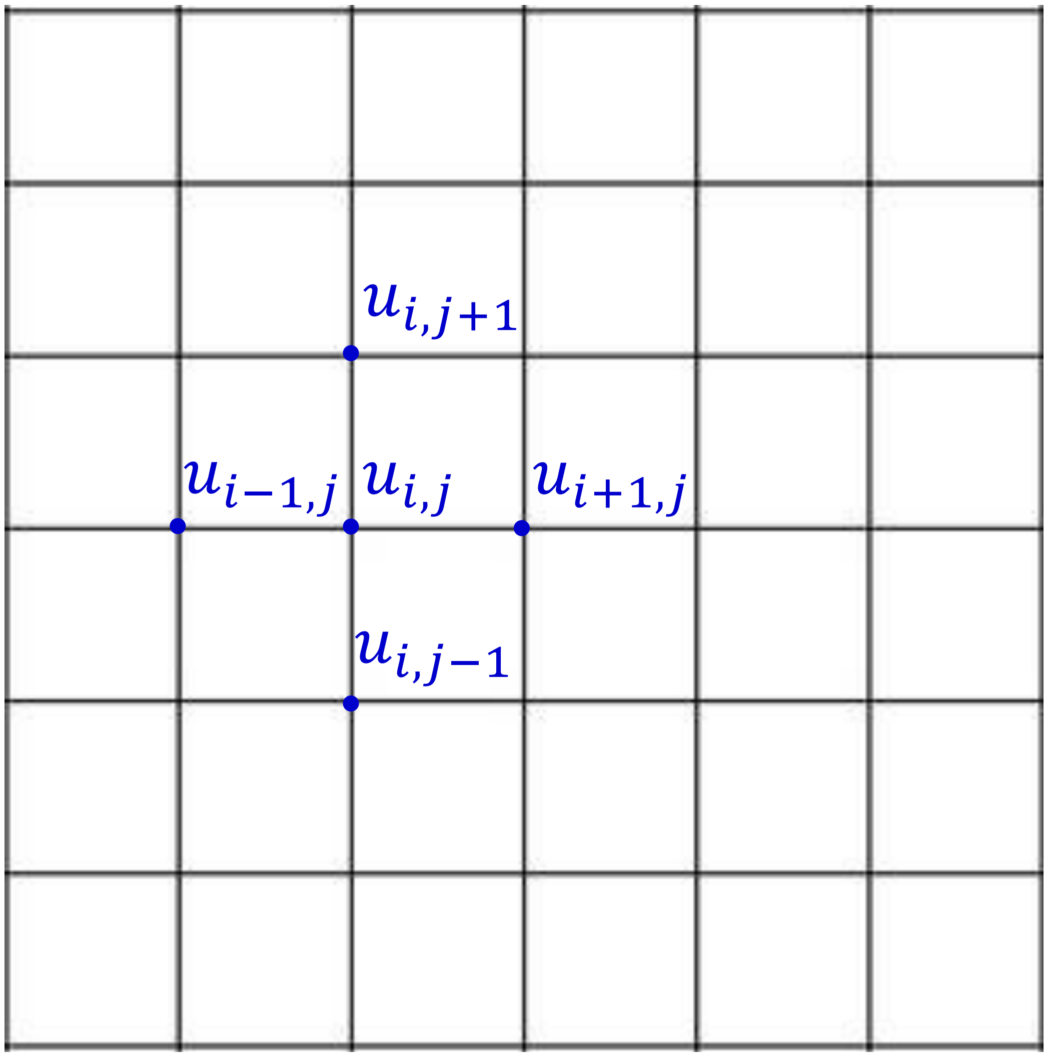
有限差分方法

- Darcy 方程

$$\partial_x(a\partial_x u) + \partial_y\left(a\partial_y u\right) = f(x,y) \qquad (x,y) \in [0,1]^2$$
$$u(x,y) = 0 \qquad (x,y) \in \partial[0,1]^2$$

当a是常数时， $a(\partial_{xx}u + \partial_{yy}u) = f(x,y)$

- Darcy 方程



- Darcy 方程

$$\begin{aligned}
\partial_x(a\partial_x u)(x_i, y_j) \\
&= (a\partial_x u)(x_{i+1/2}, y_j) - (a\partial_x u)(x_{i-1/2}, y_j) \\
&= \frac{a(x_{i+1}, y_j) + a(x_i, y_j)}{2}\,\frac{u(x_{i+1}, y_j) - u(x_i, y_j)}{\Delta x} \\
&- \frac{a(x_i, y_j) + a(x_{i-1}, y_j)}{2}\,\frac{u(x_i, y_j) - u(x_{i-1}, y_j)}{\Delta x}
\end{aligned}$$

$$A\boldsymbol{u} = \boldsymbol{f}$$

有限元分方法

- Darcy 方程

$$\partial_x(a\partial_x u) + \partial_y(a\partial_y u) = f(x,y) \qquad (x,y) \in [0,1]^2$$
$$u(x,y) = 0 \qquad (x,y) \in \partial[0,1]^2$$

弱解：

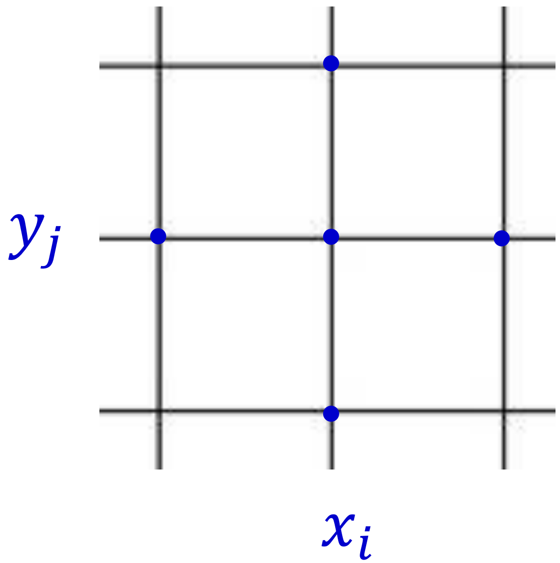
$$-\int a\left(\partial_x u \partial_x \phi + \partial_y u \partial_y \phi\right) d\Omega = \int f(x,y)\phi d\Omega \quad \forall \phi \in V$$
$$u(x,y) = 0 \qquad (x,y) \in \partial\Omega$$

有限元(基函数) $\phi_i(x,y)$：

$$u(x,y) = \sum u_i \phi_i(x,y)$$

有限差分方法

- Darcy 方程



有限元(基函数) $\phi_{i,j}$：

$\phi_{i,j}(x_i, y_j) = 1$

$\phi_{i,j}(x, y)$的支持在包含(x_i, y_j)的4个单元里，且限制在每个单元内是双线性函数

$$\phi_{i,j}\Big|_e = axy + bx + cy + d$$

有限元分方法

- Darcy 方程

求 $u(x,y) = \sum u_{i,j}\, \phi_{i,j}(x,y)$

$$-\int a\left(\partial_x u \partial_x \phi_{i,j} + \partial_y u \partial_y \phi_{i,j}\right) d\Omega = \int f(x,y)\phi_{i,j} d\Omega$$

$$u_{1,j} = u_{N,j} = u_{i,1} = u_{i,N} = 0$$

$$A\boldsymbol{u} = \boldsymbol{f}$$

传统偏微分方程数值方法

- 优势
  - 离散格式满足守恒律
  - 对精度、误差有较好的理解
  - 知道如何选取Δt、Δx
  - 显示格式复杂度有较好理解$O(\frac{1}{\Delta t \Delta x^d})$

  ……

- 劣势
  - 需要知道完整的方程
  - 对于有挑战的问题Δx一般很小
  - 对于有挑战的问题Δt一般很小，需要时间大量迭代
  - 对于有挑战的问题，求解线性(非线性)方程组较为耗时

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