空气动力学方程组间断有限元方法

1　方程简介

考虑三维 Euler 方程组, 将其写成双曲守恒律形式：

$$\begin{cases} \boldsymbol{u_t} + \nabla \cdot \boldsymbol{f}(\boldsymbol{u}) = 0 \\ \boldsymbol{u}(x,y,z,0) = \boldsymbol{u_0}(x,y,z) \end{cases} \qquad (x,y,z,t) \in \Omega \times (0,T) \tag{1}$$

其中，$\boldsymbol{u}$ 为守恒量，$\boldsymbol{f}(u) = (f_1(u), f_2(u), f_3(u))$ 为通量，

$$\boldsymbol{u} = \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} \rho \\ \rho v_1 \\ \rho v_2 \\ \rho v_3 \\ E \end{bmatrix} \quad f_1(\boldsymbol{u}) = \begin{bmatrix} \rho v_1 \\ \rho v_1^2 + p \\ \rho v_2 v_1 \\ \rho v_3 v_1 \\ (E+p) v_1 \end{bmatrix}, \quad f_2(\boldsymbol{u}) = \begin{bmatrix} \rho v_2 \\ \rho v_1 v_2 \\ \rho v_2^2 + p \\ \rho v_3 v_2 \\ (E+p) v_2 \end{bmatrix}, \quad f_3(\boldsymbol{u}) = \begin{bmatrix} \rho v_3 \\ \rho v_1 v_3 \\ \rho v_2 v_3 \\ \rho v_3^2 + p \\ (E+p) v_3 \end{bmatrix} \tag{2}$$

其中，ρ 表示密度，$\boldsymbol{v} = (v_1, v_2, v_3)$ 为速度，E 为能量，压力

$$p = (\gamma - 1)\left(E - \frac{1}{2}\rho ||\boldsymbol{v}||^2\right) = (\gamma - 1)\left(u_4 - \frac{1}{2u_0}\left(u_1^2 + u_2^2 + u_3^3\right)\right) \tag{3}$$

绝热指数 γ 在计算中一般取为常数 1.4。

下面给出二维 Euler 方程的一个有光滑解的例子，常用来测试算法的精度。在该例子中，计算区域 $\Omega = [0,2]^3$，给定初始条件：

$$\begin{cases} \rho(x,y,z,0) = 1 + 0.2\sin(\pi(x+y+z)) \\ v_1(x,y,z,0) = 0.4, \quad v_2(x,y,z,0) = 0.3 \\ v_3(x,y,z,0) = 0.3, \quad p(x,y,z,0) = 1 \end{cases} \tag{4}$$

取周期边界条件，则密度函数有精确解：

$$\rho(x,y,z,t) = 1 + 0.2\sin(\pi(x+y+z-t))$$

该算例一般可以计算到 $T = 2$。

2　基函数与外法向量

设 $\mathcal{T}_h = \{K\}$ 为区域 Ω 的一个四面体剖分，在 $\mathcal{T}_h$ 中的任意一个四面体 K 上，设 $\{(x_i, y_i, z_i)\}_{i=0}^{3}$ 为四面体的四个顶点的坐标，如图1所示。

设四面体单元 K 的体积为 V，P 为四面体内一点，四面体 $PA_1A_2A_3$，$PA_0A_2A_3$，$PA_0A_1A_3$ 的体积分别为 V_0，V_1，V_2，则有

$$\begin{aligned}
6V &= \begin{vmatrix} 1 & x_0 & y_0 & z_0 \\ 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \end{vmatrix}, \quad 6V_0 = \begin{vmatrix} 1 & x & y & z \\ 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \end{vmatrix}, \\
6V_1 &= \begin{vmatrix} 1 & x_0 & y_0 & z_0 \\ 1 & x & y & z \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \end{vmatrix}, \quad 6V_2 = \begin{vmatrix} 1 & x_0 & y_0 & z_0 \\ 1 & x_1 & y_1 & z_1 \\ 1 & x & y & z \\ 1 & x_3 & y_3 & z_3 \end{vmatrix}.
\end{aligned} \tag{5}$$

令：$\eta_0 = V_0/V$，$\eta_1 = V_1/V$，$\eta_2 = V_2/V$，其中

$$\begin{aligned}
\nabla\eta_0 &= \frac{1}{6V}\left(-\begin{vmatrix} 1 & y_1 & z_1 \\ 1 & y_2 & z_2 \\ 1 & y_3 & z_3 \end{vmatrix}, \begin{vmatrix} 1 & x_1 & z_1 \\ 1 & x_2 & z_2 \\ 1 & x_3 & z_3 \end{vmatrix}, -\begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} \right) \\
\nabla\eta_1 &= \frac{1}{6V}\left(\begin{vmatrix} 1 & y_0 & z_0 \\ 1 & y_2 & z_2 \\ 1 & y_3 & z_3 \end{vmatrix}, -\begin{vmatrix} 1 & x_0 & z_0 \\ 1 & x_2 & z_2 \\ 1 & x_3 & z_3 \end{vmatrix}, \begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} \right) \\
\nabla\eta_2 &= \frac{1}{6V}\left(-\begin{vmatrix} 1 & y_0 & z_0 \\ 1 & y_1 & z_1 \\ 1 & y_3 & z_3 \end{vmatrix}, \begin{vmatrix} 1 & x_0 & z_0 \\ 1 & x_1 & z_1 \\ 1 & x_3 & z_3 \end{vmatrix}, -\begin{vmatrix} 1 & x_0 & y_0 \\ 1 & x_1 & y_1 \\ 1 & x_3 & y_3 \end{vmatrix} \right)
\end{aligned} \tag{6}$$

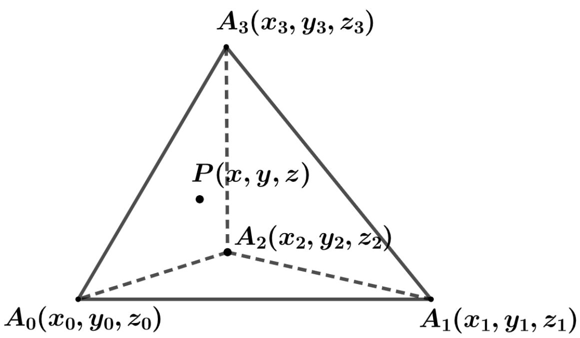

Figure 1: 四面体单元

通过体积坐标变换：

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \eta_0 \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} + \eta_1 \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} + \eta_2 \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix} + (1-\eta_0-\eta_1-\eta_2) \begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix} \tag{7}$$

可将单元 K 变换到标准四面体单元：

$$\hat{K} = \{\boldsymbol{\eta} = (\eta_0, \eta_1, \eta_2) \mid \eta_0 + \eta_1 + \eta_2 \leqslant 1, 0 \leqslant \eta_0, \eta_1, \eta_2 \leqslant 1\} \tag{8}$$

在参考单元 $\hat{K}$ 上考虑一次多项式空间，可以得到四个相互正交的基函数如下：

$$\begin{aligned} &\hat{\varphi}_0 = 1, \quad \hat{\varphi}_1 = -\frac{1}{4} + \eta_0, \quad \hat{\varphi}_2 = -\frac{1}{3} + \frac{1}{3}\eta_0 + \eta_1, \\ &\hat{\varphi}_3 = -\frac{1}{2} + \frac{1}{2}\eta_0 + \frac{1}{2}\eta_1 + \eta_2. \end{aligned} \tag{9}$$

在参考单元上定义 L^2 内积 $(\hat{\varphi}_i, \hat{\varphi}_j) = \int_{\hat{K}} \hat{\varphi}_i \hat{\varphi}_j d\boldsymbol{\eta}$，经过简单计算有：

$$\begin{aligned} &(\hat{\varphi}_i, \hat{\varphi}_j) = 0 \quad (i \neq j), \quad (\hat{\varphi}_0, \hat{\varphi}_0) = \frac{1}{6}, \quad (\hat{\varphi}_1, \hat{\varphi}_1) = \frac{1}{160}, \\ &(\hat{\varphi}_2, \hat{\varphi}_2) = \frac{1}{180}, \quad (\hat{\varphi}_3, \hat{\varphi}_3) = \frac{1}{240}. \end{aligned} \tag{10}$$

利用这些基函数，我们可以在单元 K 上定义 $\boldsymbol{u}$ 的近似

$$\boldsymbol{u}_h^K(\boldsymbol{X}, t) = \sum_{j=0}^{3} \boldsymbol{u}_j^K(t) \varphi_j^K(\boldsymbol{X}) \quad \boldsymbol{X} = (x, y, z) \in K \tag{11}$$

其中，$\varphi_j^K(\boldsymbol{X}) = \hat{\varphi}_j(\boldsymbol{\eta}(\boldsymbol{X}))$，因为

$$\int_K \left(\varphi_j^K\right)^2 d\boldsymbol{X} = \int_{\hat{K}} \hat{\varphi}_j{}^2 |J| d\boldsymbol{\eta} = |J| \left(\hat{\varphi}_j, \hat{\varphi}_j\right) \tag{12}$$

$|J| = 6|K|$ 为 Jacobian 矩阵行列式的绝对值，所以 $\varphi_j^K(\boldsymbol{X})$ 也是单元 K 上的正交基函数。

设 $\boldsymbol{n}_0$, $\boldsymbol{n}_1$, $\boldsymbol{n}_2$, $\boldsymbol{n}_3$ 分别表示为单元 K 四个顶点 A_0, A_1, A_2, A_3 所对的面上的单位外法向量，下面以 $\boldsymbol{n}_0$ 为例来说明它的计算方法：

$$\boldsymbol{A_1A_2} = (x_2 - x_1, y_2 - y_1, z_2 - z_1) \quad \boldsymbol{A_1A_3} = (x_3 - x_1, y_3 - y_1, z_3 - z_1)$$

$$\boldsymbol{A_1A_2} \times \boldsymbol{A_1A_3} = \left(\begin{vmatrix} y_2 - y_1 & z_2 - z_1 \\ y_3 - y_1 & z_3 - z_1 \end{vmatrix}, - \begin{vmatrix} x_2 - x_1 & z_2 - z_1 \\ x_3 - x_1 & z_3 - z_1 \end{vmatrix}, \begin{vmatrix} x_2 - x_1 & y_2 - y_1 \\ x_3 - x_1 & y_3 - y_1 \end{vmatrix} \right)$$

$$\boldsymbol{A_1A_0} = (x_0 - x_1, y_0 - y_1, z_0 - z_1)$$

$$\boldsymbol{n_0} = \begin{cases} \dfrac{\boldsymbol{A_1A_2} \times \boldsymbol{A_1A_3}}{|\boldsymbol{A_1A_2} \times \boldsymbol{A_1A_3}|} & (\boldsymbol{A_1A_2} \times \boldsymbol{A_1A_3}) \cdot \boldsymbol{A_1A_0} < 0, \\ -\dfrac{\boldsymbol{A_1A_2} \times \boldsymbol{A_1A_3}}{|\boldsymbol{A_1A_2} \times \boldsymbol{A_1A_3}|} & (\boldsymbol{A_1A_2} \times \boldsymbol{A_1A_3}) \cdot \boldsymbol{A_1A_0} > 0. \end{cases} \tag{13}$$

3 DG 格式的空间离散

为了求得在任意三角形单元 K 上的近似解

$$\boldsymbol{u}_h^K(\boldsymbol{X},t)=\sum_{j=0}^{3}\boldsymbol{u}_j^K(t)\varphi_j^K(\boldsymbol{X}) \tag{14}$$

我们要求近似解 $\boldsymbol{u}_h^K(\boldsymbol{X},t)$ 在 K 上满足方程

$$\int_K \frac{d}{dt}\boldsymbol{u}_h^K(\boldsymbol{X},t)\varphi_j^K d\boldsymbol{X}=\int_K \boldsymbol{f}(\boldsymbol{u}_h^K(\boldsymbol{X},t))\cdot\nabla\varphi_j^K d\boldsymbol{X}-\int_{\partial K}\hat{\boldsymbol{f}}(\boldsymbol{X},t)\varphi_j^K ds \tag{15}$$

其中 $j=0,1,2,3$, $\hat{\boldsymbol{f}}(\boldsymbol{X},t)$ 为人为定义的数值通量，将在后面给出具体的定义。将表达式(11)代入上式，并应用性质(12)得，系数 $\boldsymbol{u}_j^K(t)$ 满足常微分方程组：

$$\frac{d}{dt}\boldsymbol{u}_j^K(t)=\frac{1}{a_j}\left[\int_K \boldsymbol{f}\left(\boldsymbol{u}_h^K(\boldsymbol{X},t)\right)\cdot\nabla\varphi_j^K d\boldsymbol{X}-\int_{\partial K}\hat{\boldsymbol{f}}\left(\boldsymbol{X},t\right)\varphi_j^K ds\right] \tag{16}$$

其中，$a_j=\int_K\left(\varphi_j^K(\boldsymbol{X})\right)^2 d\boldsymbol{X}=\int_{\hat{K}}\hat{\varphi}_j{}^2(\boldsymbol{\eta})|J|d\boldsymbol{\eta}=|J|\left(\hat{\varphi}_j,\hat{\varphi}_j\right)$。

方程右端的积分项可以用数值求积公式来进行计算：

$$\int_K \boldsymbol{f}\left(\boldsymbol{u}_h^K(\boldsymbol{X},t)\right)\cdot\nabla\varphi_j^K(\boldsymbol{X})d\boldsymbol{X}\approx|K|\sum_{m=0}^{3}\frac{1}{4}\boldsymbol{f}\left(\boldsymbol{u}_h^K\left(\hat{\boldsymbol{X}}_m^K,t\right)\right)\cdot\nabla\varphi_j^K\left(\hat{\boldsymbol{X}}_m^K\right) \tag{17}$$

其中，$\boldsymbol{u}_h^K\left(\hat{\boldsymbol{X}}_m^K,t\right)=\sum\limits_{j=0}^{3}\boldsymbol{u}_j^K(t)\varphi_j^K\left(\hat{\boldsymbol{X}}_m^K\right)=\sum\limits_{j=0}^{3}\boldsymbol{u}_j^K(t)\hat{\varphi}_j\left(\hat{\boldsymbol{\eta}}_m\right)$

$\hat{\boldsymbol{\eta}}_m$ 为标准单元内的求积节点，有 $\hat{\boldsymbol{\eta}}_0=(\alpha,\beta,\beta)$，$\hat{\boldsymbol{\eta}}_1=(\beta,\alpha,\beta)$，$\hat{\boldsymbol{\eta}}_2=(\beta,\beta,\alpha)$，$\hat{\boldsymbol{\eta}}_3=(\beta,\beta,\beta)$，参数 $\alpha=0.58541020$，$\beta=0.13819660$。

$$\nabla\varphi_j^K(\hat{\boldsymbol{X}}_m)=\left(\frac{\partial\varphi_j}{\partial x},\frac{\partial\varphi_j}{\partial y},\frac{\partial\varphi_j}{\partial z}\right)=\left(\frac{\partial\hat{\varphi}_j}{\partial\eta_0},\frac{\partial\hat{\varphi}_j}{\partial\eta_1},\frac{\partial\hat{\varphi}_j}{\partial\eta_2}\right)\begin{pmatrix}\frac{\partial\eta_0}{\partial x}&\frac{\partial\eta_0}{\partial y}&\frac{\partial\eta_0}{\partial z}\\\frac{\partial\eta_1}{\partial x}&\frac{\partial\eta_1}{\partial y}&\frac{\partial\eta_1}{\partial z}\\\frac{\partial\eta_2}{\partial x}&\frac{\partial\eta_2}{\partial y}&\frac{\partial\eta_2}{\partial z}\end{pmatrix} \tag{18}$$

$$\begin{aligned}&\int_{\partial K}\hat{\boldsymbol{f}}(\boldsymbol{X},t)\varphi_j^K(\boldsymbol{X})ds=\sum_{i=0}^{3}\int_{\partial K_i}\hat{\boldsymbol{f}}(\boldsymbol{X},t)\varphi_j^K(\boldsymbol{X})ds\\&\approx\sum_{i=0}^{3}\left(|\partial K_i|\sum_{m=0}^{2}\frac{1}{3}\hat{\boldsymbol{f}}\left(\bar{\boldsymbol{X}}_m^{\partial K_i},t\right)\varphi_j^K\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)\right)=\sum_{i=0}^{3}\left(|\partial K_i|\sum_{m=0}^{2}\frac{1}{3}\hat{\boldsymbol{f}}\left(\bar{\boldsymbol{X}}_m^{\partial K_i},t\right)\hat{\varphi}_j\left(\bar{\boldsymbol{\eta}}_m^{\partial K_i}\right)\right)\end{aligned} \tag{19}$$

其中，$\bar{\boldsymbol{\eta}}_m^{\partial K_i}$ 为标准单元边界 ∂K_i 上的求积节点，$|\partial K_i|$ 表示面积，如图2。

$$\begin{aligned}\bar{\boldsymbol{X}}_0^{\partial K_3}&=\frac{2}{3}\boldsymbol{X}_0+\frac{1}{6}\boldsymbol{X}_1+\frac{1}{6}\boldsymbol{X}_2 & \bar{\boldsymbol{\eta}}_0^{\partial K_3}&=\left(\frac{2}{3},\frac{1}{6},\frac{1}{6}\right)\\\bar{\boldsymbol{X}}_1^{\partial K_3}&=\frac{1}{6}\boldsymbol{X}_0+\frac{2}{3}\boldsymbol{X}_1+\frac{1}{6}\boldsymbol{X}_2 & \bar{\boldsymbol{\eta}}_1^{\partial K_3}&=\left(\frac{1}{6},\frac{2}{3},\frac{1}{6}\right)\\\bar{\boldsymbol{X}}_2^{\partial K_3}&=\frac{1}{6}\boldsymbol{X}_0+\frac{1}{6}\boldsymbol{X}_1+\frac{2}{3}\boldsymbol{X}_2 & \bar{\boldsymbol{\eta}}_2^{\partial K_3}&=\left(\frac{1}{6},\frac{1}{6},\frac{2}{3}\right)\end{aligned} \tag{20}$$

类似的，可以得到 $\partial K_2, \partial K_1, \partial K_0$ 上求积节点的体积坐标：

$$
\begin{aligned}
&\bar{\boldsymbol{\eta}}_0^{\partial K_2}=\left(\frac{2}{3}, \frac{1}{6}, 0\right) \quad \bar{\boldsymbol{\eta}}_1^{\partial K_2}=\left(\frac{1}{6}, \frac{2}{3}, 0\right) \quad \bar{\boldsymbol{\eta}}_2^{\partial K_2}=\left(\frac{1}{6}, \frac{1}{6}, 0\right) \\
&\bar{\boldsymbol{\eta}}_0^{\partial K_1}=\left(\frac{2}{3}, 0, \frac{1}{6}\right) \quad \bar{\boldsymbol{\eta}}_1^{\partial K_1}=\left(\frac{1}{6}, 0, \frac{2}{3}\right) \quad \bar{\boldsymbol{\eta}}_2^{\partial K_1}=\left(\frac{1}{6}, 0, \frac{1}{6}\right) \\
&\bar{\boldsymbol{\eta}}_0^{\partial K_0}=\left(0, \frac{2}{3}, \frac{1}{6}\right) \quad \bar{\boldsymbol{\eta}}_1^{\partial K_0}=\left(0, \frac{1}{6}, \frac{2}{3}\right) \quad \bar{\boldsymbol{\eta}}_2^{\partial K_0}=\left(0, \frac{1}{6}, \frac{1}{6}\right)
\end{aligned} \tag{21}
$$

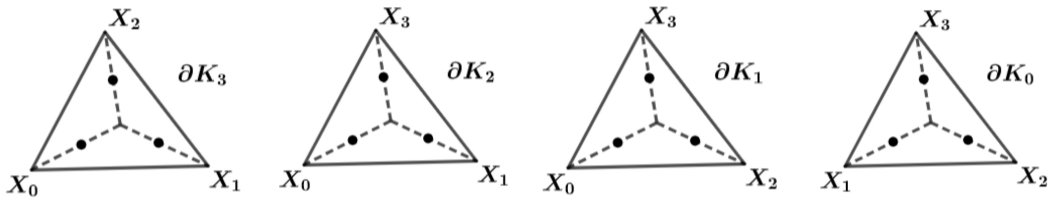

Figure 2: 边界处的求积节点

定义单元边界点 $\boldsymbol{X}$ 处的数值通量

$$
\hat{\boldsymbol{f}}(\boldsymbol{X}, t)=\hat{\boldsymbol{f}}\left(\boldsymbol{u}_h^K(\boldsymbol{X}, t), \boldsymbol{u}_h^{K'}(\boldsymbol{X}, t)\right) \tag{22}
$$

其中 $\boldsymbol{u}_h^K(\boldsymbol{X}, t)$ 与 $\boldsymbol{u}_h^{K'}(\boldsymbol{X}, t)$ 分别表示相邻单元 K 与 K' 上的数值解在 $\boldsymbol{X}$ 处的取值，有

$$
\boldsymbol{u}_h^K\left(\bar{\boldsymbol{X}}_m, t\right)=\sum_{j=0}^3 \boldsymbol{u}_j^K(t) \varphi_j^K\left(\bar{\boldsymbol{X}}_m\right)=\sum_{j=0}^3 \boldsymbol{u}_j^K(t) \hat{\varphi}_j\left(\bar{\boldsymbol{\eta}}_m\right) \tag{23}
$$

在计算 $\boldsymbol{u}_h^{K'}\left(\bar{\boldsymbol{X}}_m, t\right)$ 时，需要用到点 $\bar{\boldsymbol{X}}_m$ 在单元 K' 上对应的体积坐标。

实际计算中，常用 LF 通量：

$$
\hat{\boldsymbol{f}}(\boldsymbol{X}, t)=\frac{1}{2}\left[\boldsymbol{f}(\boldsymbol{u}_h^K(\boldsymbol{X}, t)) \cdot \boldsymbol{n}+\boldsymbol{f}(\boldsymbol{u}_h^{K'}(\boldsymbol{X}, t)) \cdot \boldsymbol{n}-\alpha_K(\boldsymbol{X}, t)(\boldsymbol{u}_h^{K'}(\boldsymbol{X}, t)-\boldsymbol{u}_h^K(\boldsymbol{X}, t))\right] \tag{24}
$$

其中 $\boldsymbol{n}=(n_x, n_y, n_z)$ 表示在四面体单元 K 的面上的单位外法向量

$$
\alpha_K(\boldsymbol{X}, t)=\max \left\{\lambda\left(\boldsymbol{u}_h^K(\boldsymbol{X}, t)\right), \lambda\left(\boldsymbol{u}_h^{K'}(\boldsymbol{X}, t)\right)\right\} \tag{25}
$$

$\lambda(\boldsymbol{u})$ 为 $\dfrac{\partial(\boldsymbol{f}(\boldsymbol{u}) \cdot \boldsymbol{n})}{\partial \boldsymbol{u}}$ 的谱半径，有

$$
\lambda(\boldsymbol{u})=|\boldsymbol{v} \cdot \boldsymbol{n}|+c_s=\left|\frac{u_1}{u_0} n_x+\frac{u_2}{u_0} n_y+\frac{u_3}{u_0} n_z\right|+c_s \tag{26}
$$

其中 $c_s=\sqrt{\dfrac{\gamma p}{\rho}}$ 为声速。

4 时间离散

关于系数函数 $\boldsymbol{u}_j^K(t), \forall K \in \mathcal{T}_h, j=0,1,2,3$ 的常微分方程组(16)可以将其简写为：

$$\frac{d\boldsymbol{u}_j^K(t)}{dt} = \boldsymbol{L}_j^K\left(\boldsymbol{u}_h^K(\boldsymbol{X},t), \boldsymbol{u}_h^{K'}(\boldsymbol{X},t), \boldsymbol{\beta}_h(\boldsymbol{X},t)\right) \quad j=0,1,2,3 \quad \forall K \in \mathcal{T}_h \tag{27}$$

其中，

$$\begin{aligned}
&\boldsymbol{L}_j^K\left(\boldsymbol{u}_h^K(\boldsymbol{X},t), \boldsymbol{u}_h^{K'}(\boldsymbol{X},t), \boldsymbol{\beta}_h(\boldsymbol{X},t)\right)\\
=&\frac{|K|}{4a_j}\sum_{m=0}^{3}\boldsymbol{f}\left(\boldsymbol{u}_h^K\left(\hat{\boldsymbol{X}}_m^K, t\right)\right)\cdot\nabla\varphi_j^K\left(\hat{\boldsymbol{X}}_m^K\right)\\
&-\sum_{i=0}^{3}\frac{|\partial K_i|}{3a_j}\sum_{m=0}^{2}\hat{\boldsymbol{f}}\left(\bar{\boldsymbol{X}}_m^{\partial K_i}, t\right)\varphi_j^K\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)
\end{aligned} \tag{28}$$

$\boldsymbol{\beta}_h(\boldsymbol{X},t)$ 表示数值解在计算区域的边界 $\partial\Omega$ 上的取值，由具体的边界条件给出，在紧邻边界的网格上计算数值通量时需要用到。

将要计算的时间区间 $[0,T]$ 划分成剖分 $0=t^0<t^1<\cdots<t^n<\cdots<t^N=T$, 记 $\boldsymbol{u}_j^{K,n}$ 为系数函数 $\boldsymbol{u}_j^K(t)$ 在任意 t^n 时刻的近似，结合空间离散近似(14)可得在 t^n 时刻解 $\boldsymbol{u}(\boldsymbol{X},t)$ 在单元 K 上的全离散近似为

$$\boldsymbol{u}(\boldsymbol{X},t^n) \approx \sum_{j=0}^{3}\boldsymbol{u}_j^{K,n}\varphi_j(\boldsymbol{X}) \tag{29}$$

为了求得所有的系数 $\boldsymbol{u}_j^{K,n}$，我们采用二阶 TVD Runge-kutta 方法进行离散常微分方程组(27)，记第 n 步的时间步长 $\Delta t^n = t^{n+1}-t^n$，那么 $\boldsymbol{u}_j^{K,n}$ 的计算格式为

$$\begin{cases}
\boldsymbol{u}_j^{K,n+\frac{1}{2}} = \boldsymbol{u}_j^{K,n} + \Delta t^n \boldsymbol{L}_j^K\left(\boldsymbol{u}_h^{K,n}, \boldsymbol{u}_h^{K',n}, \boldsymbol{\beta}_h\left(t^n\right)\right) \quad j=0,1,2\\
\boldsymbol{u}_j^{K,n+1} = \frac{1}{2}\left(\boldsymbol{u}_j^{K,n} + \boldsymbol{u}_j^{K,n+\frac{1}{2}}\right) + \frac{1}{2}\Delta t^n \boldsymbol{L}_j^K\left(\boldsymbol{u}_h^{K,n+\frac{1}{2}}, \boldsymbol{u}_h^{K',n+\frac{1}{2}}, \boldsymbol{\beta}_h\left(t^{n+1}\right)\right)
\end{cases} \tag{30}$$

在上述推进计算中需给初始值 $\boldsymbol{u}_j^{K,0}$，根据初始条件 $\boldsymbol{u}(\boldsymbol{X},t=0)=\boldsymbol{u}_0(\boldsymbol{X})$，可设定初始值

$$\begin{aligned}
\boldsymbol{u}_j^{K,0} &= \frac{1}{a_j}\int_K \boldsymbol{u}_0(\boldsymbol{X})\varphi_j^K(\boldsymbol{X})d\boldsymbol{X}\\
&\approx \frac{|K|}{4a_j}\sum_{m=0}^{3}\boldsymbol{u}_0\left(\hat{\boldsymbol{X}}_m^K\right)\varphi_j^K\left(\hat{\boldsymbol{X}}_m^K\right)\\
&= \frac{|K|}{4a_j}\sum_{m=0}^{3}\boldsymbol{u}_0\left(\boldsymbol{X}(\hat{\boldsymbol{\eta}}_m)\right)\hat{\varphi}_j\left(\hat{\boldsymbol{\eta}}_m\right) \quad j=0,1,2,3
\end{aligned} \tag{31}$$

由于使用的是时间显格式，时间步长 $\Delta t^n = t^{n+1}-t^n$ 需满足限制条件

$$\Delta t^n = \frac{CFL}{\max\limits_{K\in\mathcal{T}_h}\left[(\|\boldsymbol{v}\|+c_s)\cdot\frac{\text{surfacearea }(K)}{|K|}\right]} \tag{32}$$

其中，$\dfrac{\text{surfacearea}\ (K)}{|K|}$ 为四面体单元 K 的表面积与体积之比，CFL 条件数取 0.3，

$$c_s+\|\boldsymbol{v}\| \triangleq \sqrt{v_1^2\left(\bar{\boldsymbol{u}}_h^{K,n}\right)+v_2^2\left(\bar{\boldsymbol{u}}_h^{K,n}\right)+v_3^2\left(\bar{\boldsymbol{u}}_h^{K,n}\right)}+c_s\left(\bar{\boldsymbol{u}}_h^{K,n}\right) \quad (v_1,v_2,v_3\ \text{表示速度}) \tag{33}$$

其中，$\bar{\boldsymbol{u}}_h^{K,n}=\frac{1}{|K|}\int_K \boldsymbol{u}_h^{K,n}(\boldsymbol{X})d\boldsymbol{X}=\boldsymbol{u}_0^{K,n}$ 为 t^n 时的单元均值。

下面我们将每个单元 K 上的计算进行向量化。为此，我们记

$$\boldsymbol{u}^{K,n}=\begin{bmatrix}\boldsymbol{u}_0^{K,n} & \boldsymbol{u}_1^{K,n} & \boldsymbol{u}_2^{K,n} & \boldsymbol{u}_3^{K,n}\end{bmatrix}_{4\times 4}, \quad \boldsymbol{L}^{K,n}=\begin{bmatrix}\boldsymbol{L}_0^{K,n} & \boldsymbol{L}_1^{K,n} & \boldsymbol{L}_2^{K,n} & \boldsymbol{L}_3^{K,n}\end{bmatrix}_{4\times 4} \tag{34}$$

我们考虑 $\boldsymbol{L}_j^K\left(\boldsymbol{u}_h^{K,n},\boldsymbol{u}_h^{K',n},\boldsymbol{\beta}_h\left(t^n\right)\right)$ 的计算。我们有

$$\boldsymbol{u}_h^{K,n}\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)=\sum_{j=0}^{3}\boldsymbol{u}_j^{K,n}\varphi_j^K\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)=\boldsymbol{u}^{K,n}\begin{bmatrix}\varphi_0^K\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)\\ \varphi_1^K\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)\\ \varphi_2^K\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)\\ \varphi_3^K\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)\end{bmatrix}=\boldsymbol{u}^{K,n}\begin{bmatrix}\hat{\varphi}_0\left(\bar{\boldsymbol{\eta}}_m^{\partial K_i}\right)\\ \hat{\varphi}_1\left(\bar{\boldsymbol{\eta}}_m^{\partial K_i}\right)\\ \hat{\varphi}_2\left(\bar{\boldsymbol{\eta}}_m^{\partial K_i}\right)\\ \hat{\varphi}_3\left(\bar{\boldsymbol{\eta}}_m^{\partial K_i}\right)\end{bmatrix} \tag{35}$$

$$\begin{aligned}\hat{\boldsymbol{f}}\left(\bar{\boldsymbol{X}}_m^{\partial K_i},t^n\right)=&\frac{1}{2}\left[\boldsymbol{f}\left(\boldsymbol{u}_h^{K,n}\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)\right)+\boldsymbol{f}\left(\boldsymbol{u}_h^{K',n}\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)\right)\right]\cdot\boldsymbol{n}\\ &-\frac{\alpha_K(\bar{\boldsymbol{X}}_m^{\partial K_i},t^n)}{2}\left[\boldsymbol{u}_h^{K',n}\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)-\boldsymbol{u}_h^{K,n}\left(\bar{\boldsymbol{X}}_m^{\partial K_i}\right)\right]\end{aligned} \tag{36}$$

且根据定义(25)以及谱半径表达式(26)可得

$$\alpha_K(\bar{\boldsymbol{X}}_m^{\partial K_i},t^n)=\max\left\{\lambda\left(\boldsymbol{u}_h^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})\right),\lambda\left(\boldsymbol{u}_h^{K',n}(\bar{\boldsymbol{X}}_m^{\partial K_i})\right)\right\} \tag{37}$$

$$\begin{aligned}\lambda(\boldsymbol{u}_h^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i}))=&\left|\frac{u_1^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})}{u_0^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})}n_x+\frac{u_2^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})}{u_0^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})}n_y+\frac{u_3^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})}{u_0^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})}n_z\right|\\ &+\sqrt{\frac{\gamma(\gamma-1)\left(u_4^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})-\frac{1}{2u_0^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})}\left((u_1^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i}))^2+(u_2^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i}))^2+(u_3^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i}))^2\right)\right)}{u_0^{K,n}(\bar{\boldsymbol{X}}_m^{\partial K_i})}}\end{aligned} \tag{38}$$

5 边界条件处理

边界条件处理流体力学方程计算中边界条件通常有如下四种:

1. 周期边界：在我们的数值例子中，当计算边界上的数值流时，对应单元直接赋值即可;
2. 入流边界：密度、速度、压力这些物理量都已经指定好，直接使用这些物理量计算;
3. 出流边界：令边界外部的物理量值等于边界内部的值;

4. 反射边界，我们把边界内部的法向速度改变符号后赋给边界外部，而其他方向的速度、密度与压力复制给边界外部.

在处理边界条件时有两种方法：

- 将靠近 $\partial\Omega$ 的单元 K 沿着边界处翻转过来，设置一个虚拟单元 K'，进行编号。跟区域 Ω 内部的单元 K 一样，在 K' 上定义数值解。这样做的好处是：计算数值通量时，在区域 Ω 的内部单元与边界单元处可以统一处理。
- 不设置虚拟单元，在区域边界 $\partial\Omega$ 处计算数值通量时需用到数值解在边界外侧的极限值，它可以由边界条件直接给出。