Outline of the 3D PPFV method used by Sayram: Yang et al., 2021

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The general quasilinear diffusion equation to be solved is

$$\frac{\partial f}{\partial t} = \frac{1}{G}\frac{\partial}{\partial Q_i}\left(G D_{ij}\frac{\partial f}{\partial Q_j}\right). \tag{1}$$

To solve is using a finite volume method, we rewrite it as

$$G\frac{\partial f}{\partial t} = \frac{\partial}{\partial Q_i}\left(G D_{ij}\frac{\partial f}{\partial Q_j}\right) \equiv \nabla\cdot\left(\Lambda\cdot\nabla f\right). \tag{2}$$

To simplify notation, we will let $\nabla \equiv \nabla_Q$ from now on. The equation has Dirichlet boundary conditions and Neumann boundary conditions on boundaries Γ_D and Γ_N, respectively. The Neumann boundary condition, or the flux at the boundary, must satisfy

$$(\Lambda\cdot\nabla f)\cdot\boldsymbol{n} \geq 0. \tag{3}$$

Applying the Gaussian divergence theorem to a control cell with center K, we have

$$\int_K G\frac{\partial f}{\partial t}\mathrm{d}V = \int_K \nabla\cdot\left(\Lambda\cdot\nabla f\right)\mathrm{d}V = \oint_{\partial K}\left(\Lambda\cdot\nabla f\right)\cdot\mathrm{d}\boldsymbol{A}. \tag{4}$$

Denoting the total flux $\tilde{F}$ as

$$\tilde{F} \equiv -\oint_{\partial K}\left(\Lambda\cdot\nabla f\right)\cdot\mathrm{d}\boldsymbol{A}. \tag{5}$$

Numerically, the boundary of the cell K is dividied into faces, σ, and $\tilde{F} = \sum_{\sigma\in\partial K}\tilde{F}_{K,\sigma}$. we rewrite the above equation as

$$\int_K G\frac{\partial f}{\partial t}\mathrm{d}V = -\sum_{\sigma\in\partial K}\tilde{F}_{K,\sigma}. \tag{6}$$

with

$$\tilde{F}_{K,\sigma} = -\int_\sigma \left(\Lambda\cdot\nabla f\right)\cdot\boldsymbol{n}_{K,\sigma}\mathrm{d}A. \tag{7}$$

Numerically, Equation (6) is approximated as

$$G_K V_K \frac{f_K^{t+\Delta t} - f_K^t}{\Delta t} \approx - \sum_{\sigma \in \partial K} \tilde{F}_{K,\sigma}, \tag{8}$$

with each flux across σ face as

$$\tilde{F}_{K,\sigma} \approx -|\sigma|[\Lambda_K \cdot (\nabla f)_K] \cdot \boldsymbol{n}_{K,\sigma} = -|\sigma| \boldsymbol{n}_{K,\sigma} \cdot \Lambda_K \cdot (\nabla f)_K. \tag{9}$$

According to Yang et al., 2021, and considering that we are dealing with a time dependent diffusion problem, we write the flux $\tilde{F}_{K,\sigma}$ in the following form if σ is not a boundary face constructed using the so-called one-sided flux $F_{K,\sigma}$ and $F_{L,\sigma}$ as

$$\tilde{F}_{K,\sigma} = \mu_{K,\sigma} F_{K,\sigma} - \mu_{L,\sigma} F_{L,\sigma}. \tag{10}$$

Here, L is the a neighboring cell of K, sharing the face σ. We will use the first type of one-sided flux in Yang et al., 2021. The one-sided flux is

$$F_{K,\sigma} = \sum_{i=1}^{N_{K,\sigma}} a_{K,\sigma,i} (f_K - f_{K,\sigma,i}) \tag{11}$$

Here $N_{K,\sigma}$ is the number of tetrahedrons constructed with one vertex in the center of K, and the face σ (see Figure 1 of Yang et al., 2021). For our case of regular mesh in 3D, $N_{K,\sigma} = 4$. The coefficient $a_{K,\sigma,i}$ is given by

$$\boxed{a_{K,\sigma,i} = |\sigma| \boldsymbol{n}_{K,\sigma} \cdot \Lambda_K \cdot \boldsymbol{\beta}_{K,\sigma,i},} \tag{12}$$

where

$$\boxed{\boldsymbol{\beta}_{K,\sigma,i} = \frac{1}{N_{K,\sigma}} \left(\boldsymbol{\alpha}^2_{K,\sigma,i} + \boldsymbol{\alpha}^3_{K,\sigma,i-1} + \frac{1}{N_{K,\sigma}} \sum_{i=1}^{N_{K,\sigma}} \boldsymbol{\alpha}^1_{K,\sigma,i} \right).} \tag{13}$$

Here the superscripts $1, 2, 3$ do not mean the power of 1,2, and 3. The corresponding variables are defined by

$$\boxed{\begin{aligned} \boldsymbol{\alpha}^1_{K,\sigma,i} &= \frac{(\boldsymbol{x}_{K,\sigma,i} - \boldsymbol{x}_K) \times (\boldsymbol{x}_{K,\sigma,i+1} - \boldsymbol{x}_K)}{6V_{T_i}}, \\ \boldsymbol{\alpha}^2_{K,\sigma,i} &= \frac{(\boldsymbol{x}_{K,\sigma,i+1} - \boldsymbol{x}_K) \times (\boldsymbol{x}_{K,\sigma,O} - \boldsymbol{x}_K)}{6V_{T_i}}, \\ \boldsymbol{\alpha}^3_{K,\sigma,i} &= \frac{(\boldsymbol{x}_{K,\sigma,O} - \boldsymbol{x}_K) \times (\boldsymbol{x}_{K,\sigma,i} - \boldsymbol{x}_K)}{6V_{T_i}}. \end{aligned}}$$

Yang et al proved that $\sum_i a_{K,\sigma,i} > 0$.

The definition of $\mu_{K,\sigma}$ and $\mu_{L,\sigma}$ are

$$\boxed{\begin{cases} \mu_{K,\sigma} = \mu_{L,\sigma} = 0.5, & a_{K,\sigma} = a_{L,\sigma} = 0. \\ \mu_{K,\sigma} = \dfrac{|a_{L,\sigma}|}{|a_{K,\sigma}| + |a_{L,\sigma}|}, \mu_{L,\sigma} = \dfrac{|a_{K,\sigma}|}{|a_{K,\sigma}| + |a_{L,\sigma}|}, & \text{otherwise.} \end{cases}} \tag{14}$$

Here $a_{K,\sigma}$ and $a_{L,\sigma}$ are given by

$$\boxed{\begin{aligned} a_{K,\sigma} &= \sum_{i=1}^{N_{K,\sigma}} a_{K,\sigma,i} f_{K,i}^t, \\ a_{L,\sigma} &= \sum_{i=1}^{N_{L,\sigma}} a_{L,\sigma,i} f_{L,i}^t. \end{aligned}}$$

Furthermore, define

$$\boxed{B_\sigma = \begin{cases} \mu_{L,\sigma} a_{L,\sigma} - \mu_{K,\sigma} a_{K,\sigma}, & \sigma \in \mathcal{E}_K \cap \mathcal{E}_K, \\ -a_{K,\sigma}, & \sigma \in \mathcal{E}_K \cap \Gamma_D, \end{cases}} \tag{15}$$

and

$$\boxed{\begin{aligned} B_\sigma^+ &= \frac{|B_\sigma| + B_\sigma}{2}, \\ B_\sigma^- &= \frac{|B_\sigma| - B_\sigma}{2}. \end{aligned}}$$

Clearly, $B_\sigma^\pm \geq 0$.

The final expression of $\tilde{F}_{K,\sigma}$ is

$$\tilde{F}_{K,\sigma} \approx A_{K,\sigma} f_K^{t+\Delta t} - A_{L,\sigma} f_L^{t+\Delta t} + \mathcal{O}(\epsilon). \tag{16}$$

We will ignore the $\mathcal{O}(\epsilon)$ term from now on. For flux conservation, naturally,

$$\tilde{F}_{L,\sigma} \approx A_{L,\sigma} f_L^{t+\Delta t} - A_{K,\sigma} f_K^{t+\Delta t}. \tag{17}$$

Here coefficients $A_{K,\sigma}$ and $A_{L,\sigma}$ are functions of f^t, so the above expresion is a nonlinear two point flux approximation (NLTPF).

Combining above equations, we can find that expressions of $A_{K,\sigma}$ and $A_{L,\sigma}$ are given by

$$\boxed{\begin{aligned} A_{K,\sigma} &= \mu_{K,\sigma} \sum_{i=1}^{N_{K,\sigma}} a_{K,\sigma,i} + \frac{B_\sigma^+}{f_K^t + \epsilon}, \\ A_{L,\sigma} &= \mu_{L,\sigma} \sum_{i=1}^{N_{L,\sigma}} a_{L,\sigma,i} + \frac{B_\sigma^-}{f_L^t + \epsilon}. \end{aligned}}$$

If $\sigma \in \Gamma_D$, we denote it as σ_D, the face with Dirichlet boundary condition, then

$$\tilde{F}_{K,\sigma_D} \approx F_{K,\sigma_D} = \left(\sum_{i=1}^{N_{K,\sigma_D}} a_{K,\sigma_D,i} + \frac{B^+_{\sigma_D}}{f^t_K + \epsilon} \right) f^{t+\Delta t}_K - B^-_{\sigma_D}. \tag{18}$$

Note that the coefficient of $f^{t+\Delta t}_K$ is similar to $A_{K,\sigma}$ but with $\mu_{K,\sigma} = 1$, so we define

$$\boxed{A_{K,\sigma_D} = \sum_{i=1}^{N_{K,\sigma_D}} a_{K,\sigma_D,i} + \frac{B^+_{\sigma_D}}{f^t_K + \epsilon}.} \tag{19}$$

If $\sigma \in \Gamma_N$, we denote it as σ_N, the face with Neumann boundary condition, then the flux is given directly by the boundary condition; i.e.,

$$\tilde{F}_{K,\sigma_N} \approx -|\sigma_N| \boldsymbol{n}_{K,\sigma_N} \cdot \Lambda_K \cdot (\nabla f)_K. \tag{20}$$

Putting things together, we have Equation (8) as

$$\begin{aligned}
\frac{G_K V_K}{\Delta t} \left(f^{t+\Delta t}_K - f^t_K \right) = &- \sum_\sigma \left(A_{K,\sigma} f^{t+\Delta t}_K - A_{L,\sigma} f^{t+\Delta t}_L \right) && (21)\\
&- \left(\sum_{\sigma_D} A_{K,\sigma_D} \right) f^{t+\Delta t}_K && (22)\\
&+ \sum_{\sigma_D} B^-_{\sigma_D} + \sum_{\sigma_N} \left[\boldsymbol{n}_{K,\sigma_N} \cdot \Lambda_K \cdot \nabla f_K \right]. && (23)
\end{aligned}$$

Denoting $U_{KK} \equiv G_K V_K / \Delta t$, we rewrite the above equation

$$\begin{aligned}
&\left[U_{KK} + \sum_\sigma A_{K,\sigma} + \sum_{\sigma_D} A_{K,\sigma_D} \right] f^{t+\Delta t}_K - \sum_\sigma A_{L,\sigma} f^{t+\Delta t}_{L,\sigma} \\
&= \sum_{\sigma_D} B^-_{\sigma_D} + \sum_{\sigma_N} \left(\boldsymbol{n}_{K,\sigma_N} \cdot \Lambda_K \cdot \nabla f_K \right) + U_{KK} f^t_K.
\end{aligned}$$

The above equation can be written in the matrix form as

$$\mathsf{M} \cdot \boldsymbol{f}^{t+\Delta t} = \boldsymbol{R}. \tag{24}$$

where the right hand side vector $\boldsymbol{R}$ is given by

$$\boxed{R_K = \sum_{\sigma_D} B^-_{\sigma_D} + \sum_{\sigma_N} \left(\boldsymbol{n}_{K,\sigma_N} \cdot \Lambda_K \cdot \nabla f_K \right) + U_{KK} f^t_K.} \tag{25}$$

The matrix M has the following components:

$$\boxed{\begin{aligned}
M_{KK} &= U_{KK} + \sum_\sigma A_{K,\sigma} + \sum_{\sigma_D} A_{K,\sigma_D}, \\
M_{KL} &= -A_{L,\sigma}.
\end{aligned}}$$

where L is the neighboring cell of K sharing the face σ. By construction, $R_K > 0$, and M has the following properties $M_{KK} > 0$, and $M_{KL} < 0$, and the summation along the K_{th} column is nonnegative; i.e.,

$$\sum_L M_{LK} \geq 0. \tag{26}$$

To see this, we note that $M_{LK} = -A_{K,\sigma}$; therefore,

$$\sum_L M_{LK} = U_{KK} + \sum_{\sigma_D} A_{K,\sigma_D} \geq 0. \tag{27}$$

These properties of M makes it an M-matrix.