

Local Discontinuous Galerkin Method for Thin Film Diffusion

We would like to solve the 1D thin film diffusion equation with a Discontinuous Galerkin Method. The equation is given as

$$q_t = -\left(q^3 q_{xxx}\right)_x.$$

Local Discontinuous Galerkin Method First rewrite the diffusion equation as a system of first order equations.

$$\begin{aligned} r &= q_x \\ s &= r_x = q_{xx} \\ u &= q^3 s_x = q^3 q_{xxx} \\ q_t &= -u_x = -\left(q^3 q_{xxx}\right)_x \end{aligned}$$

The LDG method becomes the process of finding $q_h, r_h, s_h, u_h \in V_h$ in the DG solution space, such that for all test functions $v_h, w_h, y_h, z_h \in V_h$ and for all j the following equations are satisfied

$$\begin{aligned} \int_{I_j} r_h w_h \, dx &= \int_{I_j} (q_h)_x w_h \, dx \\ \int_{I_j} s_h y_h \, dx &= \int_{I_j} (r_h)_x y_h \, dx \\ \int_{I_j} u_h z_h \, dx &= \int_{I_j} q_h^3 (s_h)_x z_h \, dx \\ \int_{I_j} (q_h)_t v_h \, dx &= - \int_{I_j} (u_h)_x v_h \, dx \end{aligned}$$

After integrating by parts, these equations are

$$\begin{aligned} \int_{I_j} r_h w_h \, dx &= \left((\hat{q}_h w_h^-)_{j+1/2} - (\hat{q}_j w_h^+)_{j-1/2} \right) - \int_{I_j} q_h (w_h)_x \, dx \\ \int_{I_j} s_h y_h \, dx &= \left((\hat{r}_h y_h^-)_{j+1/2} - (\hat{r}_j y_h^+)_{j-1/2} \right) - \int_{I_j} r_h (y_h)_x \, dx \\ \int_{I_j} (q_h)_t v_h \, dx &= - \left((\hat{u}_h v_h^-)_{j+1/2} - (\hat{u}_j v_h^+)_{j-1/2} \right) + \int_{I_j} u_h (v_h)_x \, dx \end{aligned}$$

The third equation is trickier and requires integrating by parts twice.

$$\begin{aligned} \int_{I_j} u_h z_h \, dx &= \int_{I_j} q_h^3 (r_h)_x z_h \, dx \\ \int_{I_j} u_h z_h \, dx &= \left((\hat{r}_h \hat{q}_h^3 z_h^-)_{j+1/2} - (\hat{r}_j \hat{q}_h^3 z_h^+)_{j-1/2} \right) - \int_{I_j} r_h (q_h^3 z_h)_x \, dx \\ \int_{I_j} u_h z_h \, dx &= \left((\hat{r}_h \hat{q}_h^3 z_h^-)_{j+1/2} - (\hat{r}_j \hat{q}_h^3 z_h^+)_{j-1/2} \right) \\ &\quad - \left(\left(\hat{r}_h (q_h^-)^3 z_h^- \right)_{j+1/2} - \left(\hat{r}_j (q_h^+)^3 z_h^+ \right)_{j-1/2} \right) + \int_{I_j} (r_h)_x q_h^3 z_h \, dx \end{aligned}$$

A common choice of numerical fluxes are the so-called alternating fluxes.

$$\begin{aligned} \hat{q}_h &= q_h^+ \\ \hat{r}_h &= r_h^- \\ \hat{s}_h &= s_h^+ \\ \hat{u}_h &= u_h^- \end{aligned}$$

or

$$\begin{aligned}\hat{q}_h &= q_h^- \\ \hat{r}_h &= r_h^+ \\ \hat{s}_h &= s_h^- \\ \hat{u}_h &= u_h^+\end{aligned}$$

Implementation If we consider a single cell I_j , do a linear transformation from $x \in [x_{j-1/2}, x_{j+1/2}]$ to $\xi \in [-1, 1]$, and consider specifically the Legendre polynomial basis $\{\phi^k(\xi)\}$ with the following orthogonality property

$$\frac{1}{2} \int_{-1}^1 \phi^j(\xi) \phi^k(\xi) d\xi = \delta_{jk}$$

we can form a more concrete LDG method for implementing. The linear transformation can be expressed as

$$x = \frac{\Delta x}{2} \xi + \frac{x_{j-1/2} + x_{j+1/2}}{2}$$

or

$$\xi = \frac{2}{\Delta x} \left(x - \frac{x_{j-1/2} + x_{j+1/2}}{2} \right)$$

After this tranformation the thin film diffusion equation become

$$u_t = -\frac{16}{\Delta x^4} (u^3 u_{\xi\xi\xi})_{\xi}$$

on the cell I_j . We can then write this as the following system of first order equations.

$$\begin{aligned}r &= \frac{2}{\Delta x} q_{\xi} \\ s &= \frac{2}{\Delta x} r_{\xi} = \frac{4}{\Delta x^2} q_{\xi\xi} \\ u &= \frac{2}{\Delta x} q^3 s_{\xi} = \frac{8}{\Delta x^3} q^3 q_{\xi\xi\xi} \\ q_t &= -\frac{2}{\Delta x} u_{\xi} = -\frac{16}{\Delta x^4} (q^3 q_{\xi\xi\xi})_{\xi}\end{aligned}$$

With the Legendre basis, the numerical solution on I_i can be written as

$$\begin{aligned}q|_{I_i} &\approx q_h|_{I_i} = \sum_{l=1}^M (Q_i^l \phi^l(\xi)) \\ r|_{I_i} &\approx r_h|_{I_i} = \sum_{l=1}^M (R_i^l \phi^l(\xi)) \\ s|_{I_i} &\approx s_h|_{I_i} = \sum_{l=1}^M (S_i^l \phi^l(\xi)) \\ u|_{I_i} &\approx u_h|_{I_i} = \sum_{l=1}^M (U_i^l \phi^l(\xi))\end{aligned}$$

Now plugging these into the system and multiplying by a Legendre basis and integrating over cell I_i gives. I will use the following shorthand for numerical fluxes using one of the alternating flux options.

$$\begin{aligned}
\hat{Q}_{i+1/2} &= \sum_{l=1}^M \left(Q_{i+1}^l \phi^l(-1) \right) \\
\hat{R}_{i+1/2} &= \sum_{l=1}^M \left(R_i^l \phi^l(1) \right) \\
\hat{S}_{i+1/2} &= \sum_{l=1}^M \left(S_{i+1}^l \phi^l(-1) \right) \\
\hat{U}_{i+1/2} &= \sum_{l=1}^M \left(U_i^l \phi^l(1) \right) \\
\\
r &= \frac{2}{\Delta x} q_\xi \\
\sum_{l=1}^M \left(R_i^l \phi^l(\xi) \right) &= \frac{2}{\Delta x} \sum_{l=1}^M \left(Q_i^l \phi_\xi^l(\xi) \right) \\
\frac{1}{2} \int_{-1}^1 \sum_{l=1}^M \left(R_i^l \phi^l(\xi) \right) \phi^k(\xi) d\xi &= \frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(Q_i^l \phi_\xi^l(\xi) \right) \phi^k(\xi) d\xi \\
R_i^k &= \frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(Q_i^l \phi_\xi^l(\xi) \right) \phi^k(\xi) d\xi \\
R_i^k &= -\frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(Q_i^l \phi^l(\xi) \right) \phi_\xi^k(\xi) d\xi + \frac{1}{\Delta x} \left(\phi^k(1) \hat{Q}_{i+1/2} - \phi^k(-1) \hat{Q}_{i-1/2} \right) \\
\\
s &= \frac{2}{\Delta x} r_\xi \\
\sum_{l=1}^M \left(S_i^l \phi^l(\xi) \right) &= \frac{2}{\Delta x} \sum_{l=1}^M \left(R_i^l \phi_\xi^l(\xi) \right) \\
\frac{1}{2} \int_{-1}^1 \sum_{l=1}^M \left(S_i^l \phi^l(\xi) \right) \phi^k(\xi) d\xi &= \frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(R_i^l \phi_\xi^l(\xi) \right) \phi^k(\xi) d\xi \\
S_i^k &= -\frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(R_i^l \phi^l(\xi) \right) \phi_\xi^k(\xi) d\xi + \frac{1}{\Delta x} \left(\phi^k(1) \hat{R}_{i+1/2} - \phi^k(-1) \hat{R}_{i-1/2} \right)
\end{aligned}$$

This is the computation that requires integrating by parts twice. On the first integrating by parts I will treat the numerical fluxes normally, that is I will use the alternating fluxes for the flux of S and an average flux for the flux of q^3 . This allows for the propagation of information over cell interfaces. For the second integration by parts I will treat the integrand as existing solely within the cell and thus I will use interior fluxes for everything. For shorthand I will use

$$\hat{q}_{i+1/2}^3 = \left(\frac{\left(q_{i+1/2}^+ \right)^3 + \left(q_{i+1/2}^- \right)^3}{2} \right)$$

and I will explicitly write the interior fluxes as

$$\begin{aligned}
& \left(q_{i+1/2}^-\right)^3 \quad \left(q_{i-1/2}^+\right)^3 \\
& u = \frac{2}{\Delta x} q^3 s_\xi \\
& \sum_{l=1}^M \left(U_i^l \phi^l(\xi)\right) = \frac{2}{\Delta x} q^3 \sum_{l=1}^M \left(S_i^l \phi_\xi^l(\xi)\right) \\
& \frac{1}{2} \int_{-1}^1 \sum_{l=1}^M \left(U_i^l \phi^l(\xi)\right) \phi^k(\xi) d\xi = \frac{1}{\Delta x} \int_{-1}^1 q^3 \sum_{l=1}^M \left(S_i^l \phi_\xi^l(\xi)\right) \phi^k(\xi) d\xi \\
& U_i^k = -\frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(S_i^l \phi^l(\xi)\right) \left(q^3 \phi^k(\xi)\right)_\xi d\xi + \frac{1}{\Delta x} \left(\phi^k(1) \hat{q}_{i+1/2}^3 \hat{S}_{i+1/2} - \phi^k(-1) \hat{q}_{i-1/2}^3 \hat{S}_{i-1/2}\right) \\
& U_i^k = \frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(S_i^l \phi_\xi^l(\xi)\right) q^3 \phi^k(\xi) d\xi \\
& \quad - \frac{1}{\Delta x} \left(\phi^k(1) \left(q_{i+1/2}^-\right)^3 S_{i+1/2}^- - \phi^k(-1) \left(q_{i-1/2}^+\right)^3 S_{i-1/2}^+\right) \\
& \quad + \frac{1}{\Delta x} \left(\phi^k(1) \hat{q}_{i+1/2}^3 \hat{S}_{i+1/2} - \phi^k(-1) \hat{q}_{i-1/2}^3 \hat{S}_{i-1/2}\right) \\
& q_t = -\frac{2}{\Delta x} u_\xi \\
& \sum_{l=1}^M \left(\dot{Q}_i^l \phi^l(\xi)\right) = -\frac{2}{\Delta x} \sum_{l=1}^M \left(U_i^l \phi_\xi^l(\xi)\right) \\
& \frac{1}{2} \int_{-1}^1 \sum_{l=1}^M \left(\dot{Q}_i^l \phi^l(\xi)\right) \phi^k(\xi) d\xi = -\frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(U_i^l \phi_\xi^l(\xi)\right) \phi^k(\xi) d\xi \\
& \dot{Q}_i^k = \frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(U_i^l \phi_\xi^l(\xi)\right) \phi^k(\xi) d\xi - \frac{1}{\Delta x} \left(\phi^k(1) \hat{U}_{i+1/2} - \phi^k(-1) \hat{U}_{i-1/2}\right)
\end{aligned}$$

Now this is a system of ODEs, there are $M \times N$ ODEs if M is the spacial order and N is the number of cells.

Matrix Representation Some common matrices and vectors that appear in these equations are

$$\begin{aligned}
\mathbf{Q}_i &= \left[Q_i^l\right]_{l=1}^M \\
\phi(\xi) &= \left[\phi^k(\xi)\right]_{k=1}^M \\
\Phi(\xi_1, \xi_2) &= \phi(\xi_1) \phi^T(\xi_2) \\
A &= [a_{kl}]_{k,l=1}^M \\
a_{kl} &= \int_{-1}^1 \phi_\xi^k(\xi) \phi^l(\xi) d\xi \\
B_i &= [b_{kl}]_{k,l=1}^M \\
b_{kl} &= \int_{-1}^1 q_i^3(\xi) \phi^k(\xi) \phi_\xi^l(\xi) d\xi
\end{aligned}$$

For example if $M = 5$, then

$$\boldsymbol{\phi}(\xi) = \begin{bmatrix} \phi^1(\xi) \\ \phi^2(\xi) \\ \phi^3(\xi) \\ \phi^4(\xi) \\ \phi^5(\xi) \end{bmatrix}$$

and

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 2\sqrt{3} & 0 & 0 & 0 & 0 \\ 0 & 2\sqrt{3}\sqrt{5} & 0 & 0 & 0 \\ 2\sqrt{7} & 0 & 2\sqrt{5}\sqrt{7} & 0 & 0 \\ 0 & 6\sqrt{3} & 0 & 6\sqrt{7} & 0 \end{bmatrix}$$

Also the numerical fluxes can be written as the following dot products

$$\begin{aligned} \hat{Q}_{i+1/2} &= \sum_{l=1}^M \left(Q_{i+1}^l \phi^l(-1) \right) \\ &= \boldsymbol{\phi}^T(-1) \mathbf{Q}_{i+1} \\ \hat{R}_{i+1/2} &= \sum_{l=1}^M \left(R_i^l \phi^l(1) \right) \\ &= \boldsymbol{\phi}^T(1) \mathbf{R}_i \\ \hat{S}_{i+1/2} &= \sum_{l=1}^M \left(S_{i+1}^l \phi^l(-1) \right) \\ &= \boldsymbol{\phi}^T(-1) \mathbf{S}_{i+1} \\ \hat{U}_{i+1/2} &= \sum_{l=1}^M \left(U_i^l \phi^l(1) \right) \\ &= \boldsymbol{\phi}^T(1) \mathbf{U}_i \end{aligned}$$

$$\begin{aligned} R_i^k &= -\frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(Q_i^l \phi^l(\xi) \right) \phi_\xi^k(\xi) d\xi + \frac{1}{\Delta x} \left(\phi^k(1) \hat{Q}_{i+1/2} - \phi^k(-1) \hat{Q}_{i-1/2} \right) \\ R_i^k &= -\frac{1}{\Delta x} \sum_{l=1}^M \left(Q_i^l \int_{-1}^1 \phi^l(\xi) \phi_\xi^k(\xi) d\xi \right) + \frac{1}{\Delta x} \left(\phi^k(1) \hat{Q}_{i+1/2} - \phi^k(-1) \hat{Q}_{i-1/2} \right) \\ R_i^k &= -\frac{1}{\Delta x} (A \mathbf{Q}_i)_k + \frac{1}{\Delta x} \left(\phi^k(1) \boldsymbol{\phi}^T(-1) \mathbf{Q}_{i+1} - \phi^k(-1) \boldsymbol{\phi}^T(-1) \mathbf{Q}_i \right) \\ \mathbf{R}_i &= -\frac{1}{\Delta x} A \mathbf{Q}_i + \frac{1}{\Delta x} \left(\boldsymbol{\phi}(1) \boldsymbol{\phi}^T(-1) \mathbf{Q}_{i+1} - \boldsymbol{\phi}(-1) \boldsymbol{\phi}^T(-1) \mathbf{Q}_i \right) \\ \mathbf{R}_i &= -\frac{1}{\Delta x} A \mathbf{Q}_i + \frac{1}{\Delta x} (\Phi(1, -1) \mathbf{Q}_{i+1} - \Phi(-1, -1) \mathbf{Q}_i) \\ \mathbf{R}_i &= -\frac{1}{\Delta x} (A + \Phi(-1, -1)) \mathbf{Q}_i + \frac{1}{\Delta x} \Phi(1, -1) \mathbf{Q}_{i+1} \end{aligned}$$

$$\begin{aligned}
S_i^k &= -\frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(R_i^l \phi^l(\xi) \right) \phi_\xi^k(\xi) d\xi + \frac{1}{\Delta x} \left(\phi^k(1) \hat{R}_{i+1/2} - \phi^k(-1) \hat{R}_{i-1/2} \right) \\
S_i^k &= -\frac{1}{\Delta x} (A \mathbf{R}_i)_k + \frac{1}{\Delta x} \left(\phi^k(1) \phi^T(1) \mathbf{R}_i - \phi^k(-1) \phi^T(1) \mathbf{R}_{i-1} \right) \\
\mathbf{S}_i &= -\frac{1}{\Delta x} (A - \Phi(1, 1)) \mathbf{R}_i - \frac{1}{\Delta x} \Phi(-1, 1) \mathbf{R}_{i-1}
\end{aligned}$$

Note that I am treating the q^3 fluxes as constants, they don't depend on the unknowns Q_i^l

$$\begin{aligned}
U_i^k &= \frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(S_i^l \phi_\xi^l(\xi) \right) q_i^3 \phi^k(\xi) d\xi \\
&\quad - \frac{1}{\Delta x} \left(\phi^k(1) (q_{i+1/2}^-)^3 S_{i+1/2}^- - \phi^k(-1) (q_{i-1/2}^+)^3 S_{i-1/2}^+ \right) \\
&\quad + \frac{1}{\Delta x} \left(\phi^k(1) \hat{q}_{i+1/2}^3 \hat{S}_{i+1/2} - \phi^k(-1) \hat{q}_{i-1/2}^3 \hat{S}_{i-1/2} \right) \\
U_i^k &= \frac{1}{\Delta x} \sum_{l=1}^M \left(S_i^l \int_{-1}^1 q_i^3 \phi^k(\xi) \phi_\xi^l(\xi) d\xi \right) \\
&\quad - \frac{1}{\Delta x} \left(\phi^k(1) (q_{i+1/2}^-)^3 \phi^T(1) \mathbf{S}_i - \phi^k(-1) (q_{i-1/2}^+)^3 \phi^T(-1) \mathbf{S}_i \right) \\
&\quad + \frac{1}{\Delta x} \left(\phi^k(1) \hat{q}_{i+1/2}^3 \phi^T(-1) \mathbf{S}_{i+1} - \phi^k(-1) \hat{q}_{i-1/2}^3 \phi^T(-1) \mathbf{S}_i \right) \\
U_i^k &= \frac{1}{\Delta x} (B_i \mathbf{S}_i)_k - \frac{1}{\Delta x} \left(\phi^k(1) (q_{i+1/2}^-)^3 \phi^T(1) \mathbf{S}_i - \phi^k(-1) (q_{i-1/2}^+)^3 \phi^T(-1) \mathbf{S}_i \right) \\
&\quad + \frac{1}{\Delta x} \left(\phi^k(1) \hat{q}_{i+1/2}^3 \phi^T(-1) \mathbf{S}_{i+1} - \phi^k(-1) \hat{q}_{i-1/2}^3 \phi^T(-1) \mathbf{S}_i \right) \\
\mathbf{U}_i &= \frac{1}{\Delta x} B_i \mathbf{S}_i - \frac{1}{\Delta x} \left(\phi(1) (q_{i+1/2}^-)^3 \phi^T(1) \mathbf{S}_i - \phi(-1) (q_{i-1/2}^+)^3 \phi^T(-1) \mathbf{S}_i \right) \\
&\quad + \frac{1}{\Delta x} \left(\phi(1) \hat{q}_{i+1/2}^3 \phi^T(-1) \mathbf{S}_{i+1} - \phi(-1) \hat{q}_{i-1/2}^3 \phi^T(-1) \mathbf{S}_i \right) \\
\mathbf{U}_i &= \frac{1}{\Delta x} B_i \mathbf{S}_i - \frac{1}{\Delta x} \left((q_{i+1/2}^-)^3 \Phi(1, 1) \mathbf{S}_i - (q_{i-1/2}^+)^3 \Phi(-1, -1) \mathbf{S}_i \right) \\
&\quad + \frac{1}{\Delta x} \left(\hat{q}_{i+1/2}^3 \Phi(1, -1) \mathbf{S}_{i+1} - \hat{q}_{i-1/2}^3 \Phi(-1, -1) \mathbf{S}_i \right) \\
\mathbf{U}_i &= \frac{1}{\Delta x} \left(B_i - (q_{i+1/2}^-)^3 \Phi(1, 1) + \left((q_{i-1/2}^+)^3 - \hat{q}_{i-1/2}^3 \right) \Phi(-1, -1) \right) \mathbf{S}_i \\
&\quad + \frac{1}{\Delta x} \left(\hat{q}_{i+1/2}^3 \Phi(1, -1) \mathbf{S}_{i+1} \right)
\end{aligned}$$

$$\begin{aligned}
\dot{Q}_i^k &= \frac{1}{\Delta x} \int_{-1}^1 \sum_{l=1}^M \left(U_i^l \phi_\xi^l(\xi) \right) \phi^k(\xi) d\xi - \frac{1}{\Delta x} \left(\phi^k(1) \hat{U}_{i+1/2} - \phi^k(-1) \hat{U}_{i-1/2} \right) \\
\dot{Q}_i^k &= \frac{1}{\Delta x} (A \mathbf{U}_i)_k - \frac{1}{\Delta x} \left(\phi^k(1) \phi^T(1) \mathbf{U}_i - \phi^k(-1) \phi^T(1) \mathbf{U}_{i-1} \right) \\
\dot{\mathbf{Q}}_i^k &= \frac{1}{\Delta x} (A - \Phi(1, 1)) \mathbf{U}_i + \frac{1}{\Delta x} \Phi(-1, 1) \mathbf{U}_{i-1}
\end{aligned}$$