IMPROVED MIXED AND HYBRID DISCRETIZATION OF THE TRANSPORT EQUATION IN SLAB GEOMETRY

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• Mixed and Hybrid Finite Element Method (MHFEM) are very useful to solve 2nd order elliptic PDEs (see F. Brezzi, M. Fortin, *Springer-Verlag*, 1991),

• MHFEM applied to 2nd order (or mixed) form of the transport equation have a lot of advantages but suffers from some major drawbacks, even in slab geometry (J. Cartier, G. Samba, *NSE*, 2006),

• Ideas developed hereafter lead to circumvent these drawbacks in slab geometry,

• In an empirical way, we derive some desirable transport schemes from MHFEM.
Let us consider the following slab geometry transport problem

\[
\begin{align*}
\mu \frac{\partial u}{\partial x}(x, \mu) + \sigma_t(x)u(x, \mu) &= \sigma_s(x)\phi(x) + q(x), & \text{for } (x, \mu) \in [x_{\text{min}}, x_{\text{max}}] \times [-1, 1], \\
u(x_{\text{min}}, \mu) &= \alpha(\mu), & \text{for } \mu > 0, \\
u(x_{\text{max}}, \mu) &= \beta(\mu), & \text{for } \mu < 0,
\end{align*}
\]

where

\[
\phi(x) = \frac{1}{2} \int_{-1}^{1} u(x, \mu) d\mu.
\]
We introduce the **angular current density** $g = \mu u$ to get the **mixed transport formulation** in slab geometry:

\[
\begin{align*}
\frac{\partial g}{\partial x}(x, \mu) + \sigma_t(x) u(x, \mu) &= \sigma_s(x) \phi(x) + q(x), \\
\text{for } (x, \mu) &\in [x_{\text{min}}, x_{\text{max}}] \times [-1, 1],
\end{align*}
\]

\[
\begin{align*}
\mu^2 \frac{\partial u}{\partial x}(x, \mu) + \sigma_t(x) g(x, \mu) &= \mu \sigma_s(x) \phi(x) + \mu q(x), \\
\text{for } (x, \mu) &\in [x_{\text{min}}, x_{\text{max}}] \times [-1, 1],
\end{align*}
\]

\[
\begin{align*}
u(x_{\text{min}}, \mu) &= \alpha(\mu), & \text{for } \mu > 0, \\
u(x_{\text{max}}, \mu) &= \beta(\mu), & \text{for } \mu < 0,
\end{align*}
\]

\[
\begin{align*}g(x_{\text{max}}, \mu) &= \mu u(x_{\text{max}}, \mu), & \text{for } \mu > 0, \\
g(x_{\text{min}}, \mu) &= -\mu u(x_{\text{min}}, \mu), & \text{for } \mu < 0.
\end{align*}
\]
Spatial and angular discretization

Let us introduce a quadrature set \( Q_M = \{\mu_m, w_m; m = 1, \ldots, M\} \) for discretization in angle \( \mu \) in such a way that

\[
\sum_{m=1}^{M} w_m = 1, \quad \sum_{m=1}^{M} \mu_m w_m = 0, \quad \sum_{m=1}^{M} \mu_m^2 w_m = \frac{1}{3}.
\]

For example any standard symmetric quadrature set of even order \( M \) is a good candidate.

We cut the slab-geometry domain interval \( D = [x_{\text{min}}, x_{\text{max}}] \) in \( I \) intervals \([x_{i-1/2}, x_{i+1/2}]\) where \( x_{\text{min}} = x_{1/2} < \cdots < x_{i-1/2} < x_{i+1/2} < \cdots < x_{I+1/2} = x_{\text{max}} \).
MHFEM in slab geometry

\[
\begin{align*}
g_{i-\frac{1}{2}}^r & \quad & g_{i+\frac{1}{2}}^l & \quad & g_{i+\frac{1}{2}}^r & \quad & g_{i+\frac{3}{2}}^l \\
u_{i-\frac{1}{2}} & \quad & \nu_i & \quad & \nu_{i+\frac{1}{2}} & \quad & \nu_{i+1} & \quad & \nu_{i+\frac{3}{2}} \\
i-\frac{1}{2} & \quad & \text{Cell } i & \quad & i+\frac{1}{2} & \quad & \text{Cell } i+1 & \quad & i+\frac{3}{2}
\end{align*}
\]

Figure: MHFEM degrees of freedom

- Spatial mesh such that \( h_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}} \) is the width of cell \( i \),
- Degrees of freedom:
  - \( u_{i,m} \) represents the value of the angular flux at cell \( i \) in the direction \( \mu_m \),
  - \( u_{i\pm\frac{1}{2},m} \) corresponds to the value of the angular flux at edge \( i \pm \frac{1}{2} \) in the direction \( \mu_m \),
  - \( g_{i\pm\frac{1}{2},m}^g \) is the value of the angular current density in the cell \( i \) at edge \( i \pm \frac{1}{2} \) in the direction \( \mu_m \).
MHFEM in slab geometry

- Internal and external sources:
  - $q_i$ is the external source at cell $i$,
  - $\phi_i = \sum_{m=1}^{M} w_m u_{i,m}$,
  - $\phi^l_{i+\frac{1}{2}} = \sum_{m=1}^{M} \frac{w_m}{\mu_m} g^l_{i+\frac{1}{2},m}$ and
  - $\phi^r_{i+\frac{1}{2}} = \sum_{m=1}^{M} \frac{w_m}{\mu_m} g^r_{i+\frac{1}{2},m}$.

\[
\begin{align*}
\text{i) } & \quad g^l_{i+\frac{1}{2},m} + g^r_{i-\frac{1}{2},m} + \sigma_{t,i} h_i u_i,m = h_i \sigma_s,i \phi_i + h_i q_i, \\
\text{ii) } & \quad \frac{\sigma_{t,i} h_i}{2} g^l_{i+\frac{1}{2},m} + \mu_m^2 \left( u_{i+\frac{1}{2},m} - u_i,m \right) = \frac{\mu_m \sigma_s,i h_i}{2} \phi^l_{i+\frac{1}{2}} + \frac{\mu_m h_i}{2} q_i, \\
\text{iii) } & \quad \frac{\sigma_{t,i} h_i}{2} g^r_{i-\frac{1}{2},m} + \mu_m^2 \left( u_{i-\frac{1}{2},m} - u_i,m \right) = -\frac{\mu_m \sigma_s,i h_i}{2} \phi^r_{i-\frac{1}{2}} - \frac{\mu_m h_i}{2} q_i, \\
\text{iv) } & \quad g^l_{i-\frac{1}{2},m} + g^r_{i-\frac{1}{2},m} = 0, \\
\text{v) } & \quad g^l_{i+\frac{1}{2},m} + g^r_{i+\frac{1}{2},m} = 0.
\end{align*}
\]

with boundary conditions

\[
\begin{align*}
\text{i) } & \quad u_{\frac{1}{2},m} = \alpha_m, \quad \mu_m > 0, \\
\text{ii) } & \quad u_{l+\frac{1}{2},m} = \beta_m, \quad \mu_m < 0, \\
\text{iii) } & \quad g^r_{\frac{1}{2},m} = -\mu_m u_{\frac{1}{2},m}, \quad \mu_m < 0, \\
\text{iv) } & \quad g^l_{l+\frac{1}{2},m} = \mu_m u_{l+\frac{1}{2},m}, \quad \mu_m > 0.
\end{align*}
\]
Main properties of MHFEM scheme

- **Advantages:**
  - Diffusion limit in entire diffusive domain,
  - Good behavior for boundary incoming flux in diffusive medium,
  - Linear system symmetric positive definite (SPD),
  - DSA scheme is the related MHFEM scheme for the correct diffusion equation,
  - 2nd order scheme,
  - Good scheme for multidimensional unstructured meshes,

- **Drawbacks:**
  - Poor behavior for internal interface problem,
  - Maximum principle not verified (matrix from linear system is not an M-matrix).
MHFEM $\varepsilon$-problem

Figure: $\varepsilon$-problem scalar flux for different values of $\varepsilon$
You can see in red MHFEM poor results with definition $\phi_{i+\frac{1}{2}} = \sum_{m=1}^{M} w_m u_{i+\frac{1}{2},m}$ (condition 1). Thanks to discrete Fredholm analysis with $\phi_{i+\frac{1}{2}} = \sum_{m=1}^{M} \frac{w_m}{\mu_m} g_{i+\frac{1}{2},m}$ (condition 2) (see Cartier, Samba, NSE 2006) we obtain the following excellent results:

**Figure:** Grazing problem scalar flux (on the left) and Normal problem scalar flux (on the right) for different schemes (tests from E.Larsen, J.Morel, *JCP*, 1989)
Figure: Larsen-Morel-like test case scalar flux (test case from E.Larsen, J.Morel, JCP, 1989 and M.Adams, C.Gesh, M&C, 2001)
Solution 1: MHFEM internal interface problem domain decomposition

To improve the behavior of the scheme for internal interface problems, we relax the continuity equations at the internal interface $i + \frac{1}{2}$ between diffusive and non-diffusive media:

\[
\begin{align*}
g_{i+\frac{1}{2},m}^l + g_{i+\frac{1}{2},m}^r &= 0, \\
g_{i+\frac{1}{2},m}^l + g_{i+\frac{1}{2},m}^r &= 0,
\end{align*}
\]

by applying the natural mixed transport outgoing conditions:

\[
\begin{align*}
g_{i+\frac{1}{2},m}^l &= \mu u_{i+\frac{1}{2},m}, \text{ for } \mu > 0, \\
g_{i+\frac{1}{2},m}^r &= -\mu u_{i+\frac{1}{2},m}, \text{ for } \mu < 0.
\end{align*}
\]

Then, we obtain excellent results for internal interface problems.
MHFEM internal interface problem with domain decomposition

Figure: Larsen-Morel-like test case scalar flux
We consider the discrete ordinates, lumped DMHFEM for mono-energetic transport problem:

\[
\begin{align*}
\text{i) } & \quad g_{i+\frac{1}{2},m}^l + g_{i-\frac{1}{2},m}^r + \sigma_{t,i} h_i u_i,m = h_i \sigma_{s,i} \phi_i + h_i q_i, \\
\text{ii) } & \quad \frac{\sigma_{t,i} h_i}{2} g_{i+\frac{1}{2},m}^l + \mu_m^2 (u_{i+\frac{1}{2},m} - u_{i,m}) = \frac{\mu_m \sigma_{s,i} h_i}{2} \phi_{i+\frac{1}{2}}^l + \frac{\mu_m h_i}{2} q_{i+\frac{1}{2}}, \\
\text{iii) } & \quad \frac{\sigma_{t,i} h_i}{2} g_{i-\frac{1}{2},m}^r + \mu_m^2 (u_{i-\frac{1}{2},m} - u_{i,m}) = -\frac{\mu_m \sigma_{s,i} h_i}{2} \phi_{i-\frac{1}{2}}^r - \frac{\mu_m h_i}{2} q_{i-\frac{1}{2}}, \\
\text{iv) } & \quad g_{i+\frac{1}{2},m}^l = \mu u_{i+\frac{1}{2}}, \text{ for } \mu > 0, \\
\text{v) } & \quad g_{i+\frac{1}{2},m}^r = -\mu u_{i+\frac{1}{2}}, \text{ for } \mu < 0.
\end{align*}
\]

with boundary conditions

\[
\begin{align*}
\text{i) } & \quad u_{\frac{1}{2},m} = \alpha_m, \quad \mu_m > 0, \\
\text{ii) } & \quad u_{l+\frac{1}{2},m} = \beta_m, \quad \mu_m < 0, \\
\text{iii) } & \quad g_{\frac{1}{2},m}^l = -\mu_m u_{\frac{1}{2},m}, \quad \mu_m < 0, \\
\text{iv) } & \quad g_{l+\frac{1}{2},m}^r = \mu_m u_{l+\frac{1}{2},m}, \quad \mu_m > 0.
\end{align*}
\]
Some remarks on DMHFEM

• Correct diffusion limit for DMHFEM under the condition:

\[ \phi_{i+\frac{1}{2}}^l = \phi_{i+\frac{1}{2}}^r = \sum_{m=1}^{M} w_m u_{i+\frac{1}{2},m}, \]

on the internal edges,

• Correct internal interface problem behavior under the condition:

\[ \phi_{i+\frac{1}{2}}^l = \sum_{m=1}^{M} \frac{w_m}{\mu_m} g_{i+\frac{1}{2},m}, \]

and

\[ \phi_{i+\frac{1}{2}}^r = \sum_{m=1}^{M} \frac{w_m}{\mu_m} g_{i+\frac{1}{2},m}, \]

which is the desirable condition to apply discrete Fredholm alternative.
Remark: Link between DMHFEM and SCB

- SCB scheme detailed in P. Lesaint, PhD, 1975, M. Adams, TTSP, 1997, T. Palmer, 1999,
- SCB degrees of freedom:

\[
\begin{array}{cccc}
  u_i^L & u_i^R & u_{i+1}^L & u_{i+1}^R \\
  u_{i-\frac{1}{2}} & u_i & u_{i+\frac{1}{2}} & u_{i+1} & u_{i+\frac{3}{2}} \\
  i-\frac{1}{2} & \text{Cell } i & i+\frac{1}{2} & \text{Cell } i+1 & i+\frac{3}{2}
\end{array}
\]

**Figure:** SCB discretization

- if we replace \( g_{i+\frac{1}{2},m}^l \) by \( \mu_m u_{i,m}^R \) and \( g_{i+\frac{1}{2},m}^r \) by \( -\mu_m u_{i,m}^L \) in DMHFEM scheme, we get the following schemes (DMHFEM in green, SCB in red):

\[
\begin{align*}
\mu_m \left( u_{i+\frac{1}{2},m}^L - u_{i,m} \right) + \frac{\sigma_t,i h_i}{2} u_{i,m}^L &= \frac{\sigma_s,i h_i}{2} \tilde{u}_{i,m}^R + \frac{q_i h_i}{2}, \\
\mu_m \left( u_{i,m} - u_{i-\frac{1}{2},m}^L \right) + \frac{\sigma_t,i h_i}{2} u_{i,m}^L &= \frac{\sigma_s,i h_i}{2} \tilde{u}_{i,m}^L + \frac{q_i h_i}{2}, \\
\mu_m u_{i,m} &= \frac{u_{i,m}^L + u_{i,m}^R}{2}, \quad \text{or} \quad \mu_m u_{i,m}^R - \mu_m u_{i,m}^L + \sigma_t,i h_i u_{i,m} = h_i \sigma_s,i \tilde{u}_{i,m} + h_i q_i,
\end{align*}
\]

\[
\begin{align*}
u_{i+\frac{1}{2},m} &= u_{i,m}^R \quad \text{for } \mu > 0, \\
u_{i-\frac{1}{2},m} &= u_{i,m}^L \quad \text{for } \mu < 0.
\end{align*}
\]
Internal interface problem with DMHFEM

Figure: Larsen-Morel-like test case scalar flux
DMHFEM properties

- **Advantages:**
  - **Diffusion limit** in entire diffusive domain under some specific conditions on discrete scalar flux,
  - Good behavior for *incoming flux* in diffusive medium,
  - Good behavior for *internal interface* problem under specific conditions on discrete scalar flux,

- **Drawbacks:**
  - Matrix from linear system *no more SPD*,
  - **Specific conditions** on discrete scalar flux to get the correct diffusion behavior.
Solution 2: weighted-MHFEM (WMHFEM) in slab geometry

We consider the discrete ordinates, lumped WMHFEM for mono-energetic transport problem:

\[
\begin{align*}
\text{i) } \quad g_{i+\frac{1}{2},m}^L + g_{i-\frac{1}{2},m}^R + \sigma_{t,i} h_i u_i,m &= h_i \sigma_s,i \phi_i + h_i q_i, \\
\text{ii) } \quad \frac{\sigma_{t,i} h_i}{2} g_{i+\frac{1}{2},m}^L + \mu_m^2 \left( u_{i+\frac{1}{2},m} - u_i,m \right) &= \frac{\mu_m \sigma_s,i h_i}{2} \phi_{i+\frac{1}{2}}^L + \frac{\mu_m h_i}{2} q_{i+\frac{1}{2}}, \\
\text{iii) } \quad \frac{\sigma_{t,i} h_i}{2} g_{i-\frac{1}{2},m}^R + \mu_m^2 \left( u_{i-\frac{1}{2},m} - u_i,m \right) &= -\frac{\mu_m \sigma_s,i h_i}{2} \phi_{i-\frac{1}{2}}^R - \frac{\mu_m h_i}{2} q_{i-\frac{1}{2}}, \\
\text{iv) } \quad g_{i+\frac{1}{2},m}^L + \beta_{i+\frac{1}{2},m} g_{i+\frac{1}{2},m}^R &= \mu (1 - \beta_{i+\frac{1}{2},m}) u_{i+\frac{1}{2},m}, \text{ for } \mu > 0, \\
\text{v) } \quad \beta_{i+\frac{1}{2},m} g_{i+\frac{1}{2},m}^L + g_{i+\frac{1}{2},m}^R &= -\mu (1 - \beta_{i+\frac{1}{2},m}) u_{i+\frac{1}{2},m}, \text{ for } \mu < 0.
\end{align*}
\]

with boundary conditions

\[
\begin{align*}
\text{i) } \quad u_{\frac{1}{2},m} &= \alpha_m, \quad \mu_m > 0, \\
\text{ii) } \quad u_{l+\frac{1}{2},m} &= \beta_m, \quad \mu_m < 0, \\
\text{iii) } \quad g_{\frac{1}{2},m}^L &= -\mu_m u_{\frac{1}{2},m}, \quad \mu_m < 0, \\
\text{iv) } \quad g_{l+\frac{1}{2},m}^L &= \mu_m u_{l+\frac{1}{2},m}, \quad \mu_m > 0.
\end{align*}
\]
WMHFEM in slab geometry: some properties

- Parameter $\beta_{i+\frac{1}{2},m}$ depends on:
  - Optical length contrast between cell $i$ and cell $i+1$,
  - Direction $\mu_m$.

- If $\beta_{i+\frac{1}{2},m}$ goes to zero, we recover the same condition as DMHFEM one.

- Typically, one can write for $\mu_m > 0$ and $\sigma_{t,i+1} h_{i+1} >> \sigma_{t,i} h_i$:

  $$
  \beta_{i+\frac{1}{2},m} = \frac{\sigma_{t,i} h_i}{\sigma_{t,i+1} h_{i+1}}.
  $$

- Much more choices for $\beta_{i+\frac{1}{2},m}$ are available,

- Optimal values depending on mesh and medium characteristics should certainly be derived with a rigorous mathematical analysis,

- The definitions of $\phi^r_{i+\frac{1}{2}}$ and $\phi^l_{i+\frac{1}{2}}$ remain the same as the MHFEM ones.

- If $\beta_{i+\frac{1}{2},m} = 1$, WMHFEM reduces to MHFEM.

- We can easily symmetrize the system in order to get SPD matrix to inverse.
Internal interface problem with WMHFEM

\[ \beta_{i+\frac{1}{2},m} = \frac{\sigma_{t,i} h_i}{\sigma_{t,i+1} h_{i+1}} \]

**Figure:** Larsen-Morel-like test case scalar flux
Internal interface problem with WMHFEM compared to SCB

\[ \beta_{i+\frac{1}{2},m} = \frac{\sigma_{t,i} h_i}{\sigma_{t,i+1} h_{i+1}} \]

**Figure**: Larsen-Morel-like test case scalar flux
Alcouffe test problem: comparison of relative $L^2$ errors for different schemes R. Alcouffe, NSE, 1977

Figure: Alcouffe test case scalar flux

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Relative $L^2$ error ($n = 10$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MHFEM</td>
<td>$1.18 \times 10^{-5}$</td>
</tr>
<tr>
<td>DMHFEM</td>
<td>$9.51 \times 10^{-8}$</td>
</tr>
<tr>
<td>WMHFEM</td>
<td>$1.11 \times 10^{-7}$</td>
</tr>
<tr>
<td>SCB</td>
<td>$2.47 \times 10^{-6}$</td>
</tr>
</tbody>
</table>
WMHFEM properties

- **Advantages:**
  - Diffusion limit in entire diffusive domain under some specific conditions on discrete scalar flux,
  - Good behavior for incoming flux in diffusive medium,
  - Good behavior for internal interface problem under specific conditions on discrete scalar flux,
  - Matrix from linear system symmetric positive definite,

- **Drawbacks:**
  - Principle Maximum not verified,
  - No more conservative?
Conclusions and prospects

• Conclusions:
  • Empirical derivation of natural schemes from MHFEM,
  • Improvement of behavior for internal interface problems,
  • Keep good properties of initial MHFEM scheme (diffusion limit, correct behavior at the boundaries, SPD matrix for linear system, etc...),

• Prospects:
  • Convergence and error analysis of the schemes, conservative schemes?,
  • Convergence analysis for DSA,
  • Multi-dimensional: lost of SPD property ...