Some remarks on Kershaw’s legacy diffusion scheme

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Introduction

One wants to discretize:

\[ \nabla \cdot (D(x) \nabla T) \]

on a 2D geometry \( \mathcal{D} \),
on any kind of combination mixing triangles and quadrangles
with arbitrary numbers of faces sharing a vertex.

T is any quantity submitted to Fourier, Fick or 1\textsuperscript{st} gradient closure,... relation \( D(x) \nabla T \), the coefficient \( D \) is positive on \( \mathcal{D} \).

Because one considers T and D as properties of matter itself, they are linked to hydro conservation laws and closure relations. In finite volume framework, T and D are constant \( (P_0) \) per cell \( \Omega_m \).
Kershaw’s scheme being

1. quite popular among ICF community - legacy scheme,
2. of low cost - numerous pde,
3. and of second order accuracy - laser instability,

but: it violates maximum principle and is sensitive to mesh shape (aspect ratio).

... but because grid regularisation exists and gains in reliability:

one tries to refresh (reshaping) that method.
Main principles described by Kershaw in 1981

Three constraints:

1. A spatial discretization giving birth to a suitable linear system:
   (a) Consistency
   (b) Positive definite matrix
   (c) Symmetric matrix with a 5-points stencil on an orthogonal grid "extensively tried and tested tradition for us",
   (d) M-matrix (maximum principle on a non smooth grid).

2. Respect of spherical symmetry,

3. Discontinuous diffusion coefficients.
An unfortunate conclusion

1. * (Second order .and. maximum principle) = .false.

**Tools** (numerical choices):

1. A quadratic weak formulation that ensures a symmetric matrix.
2. The flux continuity relation coupled to the discretization of only \( \nabla \).
3. A couple of chosen directions inside a cell for flow symmetry.

Nothing about unstructured grid (in 1981 !)... but negative about this scheme (Palmer (LLNL 1994), DRACO’s team (2003), etc...)

Kershaw’s scheme + *slight changes*

Weak form:

\[
\begin{align*}
I &= \int_{\mathcal{D}} S \nabla \cdot (D(\vec{x}) \vec{\nabla} T) dv \\
&= \int_{\mathcal{D}} \nabla \cdot (SD(\vec{x}) \vec{\nabla} T) dv \\
&\quad - \int_{\mathcal{D}} (D(\vec{x}) \vec{\nabla} T \cdot \vec{\nabla} S) dv \\
&= - \sum_{m} \int_{\Omega_m} (\sqrt{D} \vec{\nabla} T \cdot (\sqrt{D} \vec{\nabla} S)) dv
\end{align*}
\]
That also reads \((S = T)\):

\[
I = \sum_m \sum_{sm \in m} \int_{\Omega_{sm}} \left( \sqrt{D \nabla T} \right) \cdot \left( \sqrt{D \nabla T} \right) dv
\]

\[
= \sum_m \sum_{sm \in m} \left( p_{sm} \overrightarrow{G_{sm}} \cdot \overrightarrow{G_{sm}} \right) Aire_m
\]

Where: \(sm = s^{th}\) vertex of cell \(\Omega_m\), \(\overrightarrow{G_{sm}}\) a discretisation of \((\sqrt{D \nabla T})\), \(Aire_m = |\Omega_m|\), \(p_{sm}\) a weight per vertex per cell.

Figure 1: Subcell discretization.
Why \( \sum_{m} \sum_{s \in m} \)?

Let’s look in 1D.

Let \( \vec{G}_m \) be a natural second order cell-centered derivative:

\[
\vec{G}_m \simeq \frac{T_{m+1} - T_m}{2\Delta x} + \frac{T_m - T_{m-1}}{2\Delta x} = \frac{T_{m+1} - T_{m-1}}{2\Delta x}
\]

here \( D = 1 \) (simplified flux continuity condition).

So \( \vec{G}_m \cdot \vec{G}_m \simeq \) terms in \( \left\{ T_{m+1}^2, T_{m-1}^2, T_{m-1} \times T_{m+1} \right\} \) that induces decoupled temperature fields:

![Figure 2: 1D decoupled molecules.](image)

Factorization gives:

\[
T_{m-1} \times \left\{ T_{m-1}, \frac{T_{m+1}}{2} \right\}
\]

\[
T_{m+1} \times \left\{ T_{m+1}, \frac{T_{m-1}}{2} \right\}
\]

that ensures symmetry.
That gives a checkerboard pattern in 2D.

![Checkerboard Pattern](image)

Figure 3: 2D decoupled temperature fields.

Checkerboard $\Rightarrow$ underintegration $\Rightarrow$ additionnal unknowns.
→ a conclusion

Weak form $\Rightarrow$ Quadratic expression $\Rightarrow$ need to consider more than one ($\nabla$) per cell.

In order to get local connex stencil such as:

![Figure 4: Local molecules on distorted and orthogonal grids.](image)

Kershaw’s choice is:

one ($\nabla$) per subcell = one ($\nabla$) per node per cell $\Rightarrow \sum_{m} \sum_{sm \in m}$.
Gradient

**Problem:** define gradient on a volume associated to a vertex per cell and being coherent with flux continuity constraint.
Choice:

\[
\begin{align*}
\vec{G}_{sm} &= \sum_{i=\{a,a_+\}\ni sm} \vec{G}_i \\
\vec{G}_i &= d_i \times (T_{sm} - T_{sm_i}) \times \vec{n}_i \\
T_{sm} &= T_{sm_i} \forall sm \in m
\end{align*}
\]

(4)

"corresponding" to a 5-points operator with temperature equilibrium inside a cell

\[\implies \text{discretization on subcells without additional unknown.}\]

Figure 5: Local interaction
So: $\mathbf{G}_{sm} = (d_a(T_m - T_{ma})) \mathbf{n}_a + (d_{a+}(T_m - T_{ma+})) \mathbf{n}_{a+}$

Flux continuity condition gives

$$d_a = \sqrt{\left(\frac{e_{ma}}{D_m} + \frac{e_{am}}{D_{ma}}\right)^{-1}} \sqrt{\frac{1}{l_a}}$$

(5)

$e_{ma}$: width, $l_a$: half edge length.

Finally $\mathbf{G}_{sm} \cdot \mathbf{G}_{sm}$ gives birth to terms:

$T_m \times T_m, T_{ma} \times T_{ma}, T_{ma+} \times T_{ma+}, T_m \times T_{ma}, T_m \times T_{ma+}$

$T_{ma} \times T_{ma+}$

They define interactions between cells relatively to one vertex:

$m \leftrightarrow ma, m \leftrightarrow ma+, ma \leftrightarrow ma+$

The bold term express interaction of 2 corner cells ($ma$ and $ma+$) by way of cell $m$ depending on:

$\mathbf{n}_a \cdot \mathbf{n}_{a+}$ and $d_a \times d_{a+}$. 
Figure 6: Interaction between cells on a given node relatively to one cell and two cells.

Cross term of type:

\[ T_{ma} \times T_{ma^+} \]

is equally shared by cells \( ma \) and \( ma^+ \).

That allows the building of a symmetric diffusion matrix.
Remark: Div - Grad

Based on a gradient at vertices in each cell, these interactions allow to define a face centered gradient by way of a given divergence discretization.

With the standard finite volume relation:

\[
\int_{\Omega_m} \nabla \cdot \vec{V} \, dv = \int_{\partial\Omega_m} \vec{V} \cdot \vec{n} \, d\sigma = \sum_{\bar{a} \in \partial\Omega_m} \vec{V}_a \cdot L_a \vec{N}_a
\]

One obtains a two components gradient:

1. an "internal" (to the cell) part corresponding to interactions with neighbor cells,
2. an external part corresponding to interactions with corner cells and a contribution with neighbor cells.

Figure 7: Internal part (in red) and external part (in blue) for the face centered gradient.
Conclusion

1. Problem: $\nabla \cdot (D \nabla T)$,

2. Hypothesis: quadratic formulation in term of $\sqrt{D \nabla}$,

3. Necessary consequence: $\sqrt{D \nabla}$ discretized per vertex per cell as resulting from the summation of two vectors parallel to the edge normal,

4. Needed data: "$\sqrt{D \partial_n T}$" across faces including that vertex (module of those vectors),

5. Needed relation: $\sqrt{D}$ at face compatible to flux continuity condition.

As long as a vertex is the summit of two faces of a cell (great!), one can define the local gradient at node... and no need of a structured grid.
Figure 8: Kershaw test problem.
Figure 9: An unstructured grid.