Mimetic finite difference methods for diffusion equations on AMR meshes

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Objectives

What are the perfect discretizations?

- they preserve and mimic mathematical properties of physical systems;
- they are accurate on adaptive smooth and non-smooth grids;
Objectives

What are the perfect discretizations?

- they preserve and mimic mathematical properties of physical systems;
- they are accurate on adaptive smooth and non-smooth grids;
- they can be used for a wide family of grids and operators.
Model diffusion problem

We consider the elliptic equation

$$-\text{div}(\mathbf{K} \nabla p) = b \quad \text{in} \quad \Omega$$

subject to the homogeneous Dirichlet b.c.

$$p = 0 \quad \text{on} \quad \partial\Omega.$$ 

The problem can be reformulated as a system of first order equations:

$$\text{div} \mathbf{f} = b,$$

$$\mathbf{f} = -\mathbf{K} \nabla p.$$

For simplicity we assume that $\mathbf{K} = I$. 
Support operator method (1/2)

Consider the mathematical identity:

$$\int_{\Omega} \text{grad} \, p \, f \, dx = - \int_{\Omega} \text{div} \, f \, p \, dx \quad \forall f \in H_{\text{div}}(\Omega), \ p \in H_0^1(\Omega).$$

Support-operators (SO) methodology (for div & grad):

1. define degrees of freedom for variables $p$ and $f$;
2. equip the discrete spaces for $p$ and $f$ with scalar products $[\cdot, \cdot]_Q$ and $[\cdot, \cdot]_X$, respectively;
3. choose a discrete approximation to the divergence operator, the *prime* operator $\text{DIV} : X_d \to Q_d$;
4. derive the discrete approximation of the gradient operator, the *derived* operator $\text{GRAD} : Q_d \to X_d$, from the discrete Green formula:

$$[f^d, \text{GRAD} \, p^d]_X = -[\text{DIV} \, f^d, p^d]_Q \quad \forall p^d \in Q_d, \ f^d \in X_d.$$
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Support operator method (2/2)

Applications of the SO methodology include:

- **Electromagnetics:** discrete operators \( \text{DIV}, \text{GRAD}, \text{CURL} \) and \( \text{CURL} \) mimic:

\[
\begin{align*}
\text{div} \; \text{curl} &= 0, \quad \text{curl} \; \text{grad} = 0 \\
\int_\Omega \text{curl} E \cdot H \, dx &= \int_\Omega \text{curl} H \cdot E \, dx + \oint_{\partial \Omega} (E \times H) \cdot n \, ds
\end{align*}
\]

- **CFD:** discrete operators \( \text{DIV} \) and \( \text{GRAD} \) mimic:

\[
\begin{align*}
\int_\Omega \text{grad} \; u : T \, dx &= -\int_\Omega \text{div} \; T \cdot u \, dx + \oint_{\partial \Omega} u \cdot (T \cdot n) \, ds
\end{align*}
\]

- **Gas dynamics, poroelasticity, magnetic diffusion, radiation diffusion, etc...**

http://www.sci.sdsu.edu/compscims/MIMETIC/index.htm
Mimetic discretizations (1/10)

Step 1 (degrees of freedom for $p$ and $f$).

- $p^d_i$ is defined at a center of cell $e_i$.
- $f^d_{i1}, \ldots, f^d_{i4}$ are defined at mid-points of cell edges. They approximate the normal components of $f$, e.g.

\[ f^d_{i1} \approx f \cdot n_{i1}. \]
Mimetic discretizations (2/10)

Step 2 (scalar products for $p^d$ and $f^d$).

- Let $Q_d$ be a vector space of discrete intensities with the scalar product

$$[p^d, q^d]_Q = \sum_{i=1}^{N} |e_i| p_i^d q_i^d \approx \int_{\Omega} p(x) q(x) \, dx.$$ 

- Let $X_d$ be a vector space of discrete fluxes with a scalar product

$$[f^d, g^d]_X \approx \int_{\Omega} f(x) \cdot g(x) \, dx.$$ 

The vectors can be recovered uniquely at four vertices of quadrilateral $e_i$. Let

$$[f^d_i, g^d_i]_{X_{e_i}} = \frac{1}{2} \sum_{j=1}^{4} |T_{ij}| f^d_{ij} \cdot g^d_{ij}$$

Then

$$[f^d, g^d]_X = \sum_{i=1}^{N} [f^d_i, g^d_i]_{X_{e_i}}.$$
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Then

$$[f^d, g^d]_X = \sum_{i=1}^{N} [f_i^d, g_i^d]_{X_{e_i}}.$$
Mimetic discretizations (3/10)

Steps 3 & 4 (prime and derived operators).

The prime operator $\text{DIV}$ follows from the Gauss theorem:

$$\text{div } f = \lim_{|e| \to 0} \frac{1}{|e|} \oint_{\partial e} f \cdot n \, dl.$$ 

Center-point quadrature gives

$$\left( \text{DIV } f^d \right)_i = \frac{1}{|e_i|} \left( f_{i1}^d |l_1| + f_{i2}^d |l_2| + f_{i3}^d |l_3| + f_{i4}^d |l_4| \right)$$

The derived operator $\text{GRAD}$ is implicitly given by

$$[f^d, \text{GRAD } p^d]_X = -[\text{DIV } f^d, p^d]_Q \quad \forall p^d \in Q_d, \ f^d \in X_d.$$
Mimetic discretizations (4/10)

Short summary.

The stationary diffusion problem

\[- \text{div } \mathbf{K} \nabla p = b \quad \text{in } \Omega\]

\[p = 0 \quad \text{on } \partial \Omega\]

is rewritten as the 1st order system

\[\mathbf{f} = -\mathbf{K} \nabla p, \quad \text{div } \mathbf{f} = b\]

and discretized as follows:

\[\mathbf{f}^d = -\text{GRAD } p^d, \quad \text{DIV } \mathbf{f}^d = b^d.\]
Mimetic discretizations (5/10)

By the definition,

\[ [f^d, \text{GRAD } p^d]_X = -[\text{DIV } f^d, p^d]_Q. \]

Let \( \langle \cdot, \cdot \rangle \) be the usual vector dot product. Then

\[ [p^d, q^d]_Q = \langle Dp^d, q^d \rangle, \quad [f^d, g^d]_X = \langle M f^d, g^d \rangle. \]

Combining the last two formulas, we get

\[
[f^d, \text{GRAD } p^d]_X = \langle M f^d, \text{GRAD } p^d \rangle \\
= -[\text{DIV } f^d, p^d]_Q = - \langle f^d, \text{DIV}^t D p^d \rangle.
\]

Therefore,

\[ \text{GRAD} = -M^{-1} \text{DIV}^t D. \]

is the non-local operator.
A local SO method mimics the mathematical identity

\[ \int_{e} f \cdot \text{grad} p \, dx + \int_{e} \text{div} f \, p \, dx = \int_{\partial e} p \, f \cdot n \, dl. \]

**Step 1 (degrees of freedom):**

- \( p^d \): at cell centers and edge centers
- \( f^d \): normal components at edge centers
Mimetic discretizations (7/10)

Steps 2 & 3 (discrete identity and prime operator).

The prime operator $\text{DIV}$ is derived from the Gauss theorem:

$$\text{DIV} \ f^d = \frac{1}{|e|} \left( f^d_R |l_R| + f^d_T |l_T| + f^d_L |l_L| + f^d_B |l_B| \right)$$

Derivation of the discrete identity:

- $\int_{e} \mathbf{f} \cdot \text{grad} p \, dx \approx \left[ f^d, \text{GRAD} \ p^d \right] x_e$

- $\int_{e} \text{div} \mathbf{f} \ p \, dx \approx (\text{DIV} \ f^d) p^d c |e|$

- $\int_{\partial e} p \ \mathbf{f} \cdot \mathbf{n} \, dl \approx p^d_R f^d_R |l_R| + p^d_T f^d_T |l_T| + p^d_L f^d_L |l_L| + p^d_B f^d_B |l_B|$
Mimetic discretizations (8/10)

Step 4 (derived operator).

Replacing integrals in the Green formula by their approximations, we get

\[
\text{GRAD } p^d = \mathcal{M}_e^{-1} \begin{pmatrix}
|l_R|(p_R^d - p_c^d) \\
|l_T|(p_T^d - p_c^d) \\
|l_L|(p_L^d - p_c^d) \\
|l_B|(p_B^d - p_c^d)
\end{pmatrix}
\]

where

\[
< \mathcal{M}_e f^d, g^d > = [f^d, g^d]_{X_e}
\]

and \( f^d = (f_R^d, f_T^d, f_L^d, f_B^d)^t \). The local discretization reads

\[
\text{DIV } f^d = b^d,
\]

\[
f^d = -\text{GRAD } p^d.
\]
Mimetic discretizations (9/10)

Short summary.

- matrix $M_e^{-1} \in \mathbb{R}^{4 \times 4}$;
- discrete divergence and gradient operators mimic essential properties of the continuous operators (local mass conservation, Green formula);
- discretization and continuity conditions are separated;
- we do not assume anything about a grid structure.
Mimetic discretizations (10/10)

\[ \int_{\partial e} p f \cdot n \, dl \approx p_R^d f_R^d |l_R| + p_T^d f_T^d |l_T| + p_L^d f_L^d |l_L| + p_B^d f_B^d |l_B|. \]

The global discretization is achieved by imposing the continuity of fluxes

\[ f_{iR}^d = -f_{jL}^d \]

and interface intensities

\[ p_{iR}^d = p_{jL}^d. \]
Locally refined meshes (1/6)

The global discretization is achieved by imposing the continuity of fluxes

\[ f_{iR}^d = -f_{jL}^d = -f_{kL}^d \]

and interface intensities

\[ |l_{iR}| p_{iR}^d = |l_{jL}| p_{jL}^d + |l_{kL}| p_{kL}^d. \]
Locally refined meshes (2/6)

Stencils of a stiffness matrix for interface intensities.
Locally refined meshes (3/6)

The derived mimetic discretizations are exact for linear solutions.
Locally refined meshes (4/6)

<table>
<thead>
<tr>
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<td>3.76e-3</td>
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<td>25.3</td>
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</table>

$$p(x, y) = 1 - \tanh \left( \frac{(x - 0.5)^2 + (y - 0.5)^2}{0.01} \right).$$
Spherically symmetric problem in $r - z$ coordinates with the exact solution:

$$p(R) = \frac{553}{640} - \frac{R^2}{6} - \frac{R^4}{20}$$

when $R < 0.5$ and

$$p(R) = \frac{101}{120} - \frac{R^2}{12} - \frac{R^4}{40}$$

when $0.5 < R < 1$. 
Locally refined meshes (6/6)

Let us consider the diffusion problem with strong material discontinuity

$$[K] = 100 \quad \text{at} \quad \sqrt{(x - 0.5)^2 + (y - 0.5)^2} = 0.25.$$
The system of mimetic finite difference equations

\[ f^d = -\text{GRAD} p^d, \quad \text{DIV} f^d = b^d \]

can be rewritten as

\[ [f^d, g^d]_x + [\text{GRAD} p^d, g^d]_x = 0, \]
\[ [\text{DIV} f^d, q^d]_Q = [b^d, q^d]_Q. \]

Recall that by the definition,

\[ [f^d, \text{GRAD} p^d]_x = -[\text{DIV} f^d, p^d]_Q. \]
SO and mixed FE methods (2/3)

Thus, the mimetic discretizations are equivalent to

\[
[f^d, g^d]_X - [\text{DIV } f^d, p^d]_Q = 0,
\]

\[
-[\text{DIV } f^d, q^d]_Q = -[b^d, q^d]_Q, \quad \forall p^d \in Q_d, \; g^d \in X_d.
\]

On the other hand, the MFE method with the *Raviart-Thomas* elements gives

\[
(f^h, g^h) - (\text{div } f^h, p^h) = 0,
\]

\[
-(\text{div } f^h, q^h) = -(b, q^h) \quad \forall q^h \in Q_h, \; g^h \in X_h.
\]

\[p^d: \quad \text{at cell centers} \quad \text{one per cell}\]

Degrees of freedom: \[f^d: \quad \text{normal components} \quad \text{normal components,}\]

\[\text{at edge centers} \quad \text{one per edge}\]
SO and mixed FE methods (3/3)

<table>
<thead>
<tr>
<th>$h^{-1}$</th>
<th>modified RT FE</th>
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<tr>
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<td>512</td>
<td>4.98e-5</td>
<td>8.32e-4</td>
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|          | $\varepsilon_p$ | $\varepsilon_f$ | $\varepsilon_p$ | $\varepsilon_f$ |
| 16       | 1.42e-3         | 2.24e-2 | 1.43e-3         | 2.25e-2         |
| 32       | 7.15e-4         | 1.17e-2 | 7.18e-4         | 1.17e-2         |
| 64       | 3.59e-4         | 5.96e-3 | 3.59e-4         | 5.98e-3         |
| 128      | 1.80e-4         | 3.06e-3 | 1.80e-4         | 3.07e-3         |
| 256      | 9.00e-5         | 1.56e-3 | 9.00e-5         | 1.56e-3         |
| 512      | 4.50e-5         | 7.93e-4 | 4.50e-5         | 7.93e-4         |
In collaboration with M. Pernice (CCS-3), the SO method was compared with the FD method by R. Ewing, R. Lazarov, and P. Vassilevski (1991):

- the FD method works on rectangular locally refined grids;
- in the case of smooth solutions, the FD method results in larger error (left picture) on irregular grid interfaces:
The control-volume mixed FE method by T.Russell (2001):
- the method does not preserve the uniform flow on irregular grids;
- the principle difficulty is the scalar product in a space of fluxes.

The control-volume method on general polygonal meshes by T.Palmer (2001):
- the method is exact for linear solutions;
- the method results in non-symmetric matrices.

The SO method on general polygonal meshes (2003):
- the method is exact for linear solutions;
- the method results in symmetric positive definite matrices.
Recent developments (1/3)

Exact solution is $p(x, y) = x + y$. A new scalar product in the space of fluxes results in mimetic discretizations which are exact for linear solutions.

The polygonal grids were generated by Raphael Loubere (T-7).
Recent developments (2/3)

Convergence test for exact solution $p(x, y) = \sin(2\pi x) \sin(2\pi y)$.

<table>
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<tr>
<th>$m$</th>
<th>New scalar product</th>
<th>Old scalar product</th>
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</table>

![Diagram of convergence test](image1.png)

![Diagram of convergence test](image2.png)
Recent developments (3/3)

Examples of bad-shaped elements which are common for locally refined and non-matching meshes:

We believe that the new methodology can be extended to all the above elements.
Conclusion

- the convergence of mimetic discretizations for the linear diffusion equation is optimal on locally refined meshes in both Cartesian and $r-z$ geometries (2nd order on smooth meshes but only 1st order for fluxes on random grids);
- the mimetic discretizations are comparable with mixed FE discretizations but more preferable than the discretizations based on CV or FD methods;
- a reduced system for interface intensities has SPD coefficient matrix and can be efficiently solved with a PCG method;
- the preliminary numerical experiments on general polygonal meshes show the optimal convergence rate for mimetic discretizations (2nd order for intensities and 1st order for fluxes).