Towards Converged Adjoint State for Large Industrial Cases by Improving the Discretization Schemes

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Motivation

Convergence of an adjoint solver is mainly affected by that of the primal flow solver, which in turn strongly depends on a) the chosen discretization scheme and b) the solution algorithm.

Classical FV schemes often employ numerical artifacts (e.g. Non-Orthogonal Correctors with limiters) and slow solution alghoritms. For large industrial cases this may affect convergence or generate results which, although "good enough" on their own, fail to produce a robust adjoint.

As an alternative we suggest here a *mimetic* discretization: **Mimetic Finite Differences**, a.k.a. **Mixed Virtual Elements**.

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As an alternative we suggest here a *mimetic* discretization: **Mimetic Finite Differences**, a.k.a. **Mixed Virtual Elements**.

Mixed Virtual Elements

- Is a consistent discretization (it *mimics* properties of continuous operators) → **can help converge adjoint by providing a more robust solution, as well as a more robust Jacobian**
- Does not depend on mesh orthogonality/quality → **very useful with shape optimization algorithms**
- Can deal with nonconforming meshes
- Can deal with discontinuous fields

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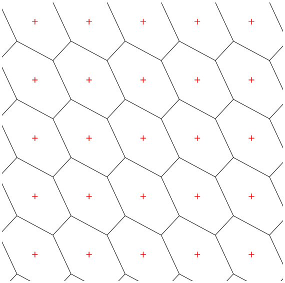
Discrete Spaces

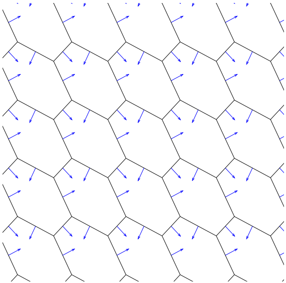
DOFs are defined as follows:

Space Q_h



Cell-averaged scalars:
$q_C := \frac{1}{|C|} \int_C q \, dV$

Space X_h



Face fluxes:
$W_{F \leftarrow C} := \int_F \vec{W} \cdot \vec{n}_F \, d\Sigma$

Conditions on DOFs

In addition, we also have face-averaged scalars:

$$q_F := \frac{1}{|F|} \int_F q \, d\Sigma$$

And we impose conservativity on the face fluxes:

$$W_{F \leftarrow C+} + W_{F \leftarrow C-} = 0$$

Thus on a mesh with n_C cells and n_F faces we have:

- $n_C + n_F$ unknowns for each scalar variable
- n_F unknowns for each vector variable

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Pure Anisotropic Diffusion Equation

At first we are going to discretize the **pure anisotropic diffusion** equation:

$$\nabla \cdot (-\mathbb{K} \nabla p) = f$$

re-written in mixed formulation:

$$\begin{cases} \vec{V} = -\mathbb{K} \nabla p \\ \nabla \cdot \vec{V} = f \end{cases}$$

We shall place p in Q_h and $\vec{V}$ in X_h; the variational form of the constitutional equation reads (on a cell):

$$\int_C \mathbb{K}^{-1} \vec{V} \cdot \vec{W} \, dV = - \int_C \nabla p \cdot \vec{W} \, dV$$

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The Finite Element Approach

$$\int_C \mathbb{K}^{-1} \vec{V} \cdot \vec{W} \, dV = -\int_C \nabla p \cdot \vec{W} \, dV$$

In classical FEM we would use a *lifting* $\mathcal{L}_C$ on X^h to reconstruct vector fields inside the cell based on the discrete fluxes V_F and W_F at the faces; then we would discretize the LHS as:

$$\int_C \mathbb{K}^{-1} \mathcal{L}_C(V_F)_{\partial C} \cdot \mathcal{L}_C(W_F)_{\partial C} \, dV$$

(here $(V_F)_{\partial C}$ stands for a vector holding values $V_{F \leftarrow C}$, i.e. fluxes through each face belonging to C).

The Finite Element Approach

Idea: we want to find a (SPD) matrix $\mathbb{M}_C$ such that the following holds:

$$\mathbb{M}_C (V_F)_{\partial C} \cdot (W_F)_{\partial C} = \int_C \mathbb{K}^{-1} \mathcal{L}_C (V_F)_{\partial C} \cdot \mathcal{L}_C (W_F)_{\partial C} \, dV$$

without having to explicitly compute the basis functions required by $\mathcal{L}_C$.

The $\mathbb{K}$-Scalar Product

$$\mathbb{M}_C(V_F)_{\partial C} \cdot (W_F)_{\partial C} = \int_C \mathbb{K}^{-1}\mathcal{L}_C(V_F)_{\partial C} \cdot \mathcal{L}_C(W_F)_{\partial C}\, dV$$

Clearly this means that $\mathbb{M}_C$ represents an inner product for space X^h; in fact, since it incorporates the (inverse) diffusivity tensor $\mathbb{K}^{-1}$, it is a material-dependent scalar product.

Theorem:[0] there is an admissible lifting satisfing the expression above as long as we introduce a large enough *stabilization term* when building $\mathbb{M}_C$ (explained later).

We introduce the following notation for such $\mathbb{K}$-scalar product:

$$[\vec{V}, \vec{W}]^{\mathbb{K}}_{C,X^h} := \mathbb{M}_C(V_F)_{\partial C} \cdot (W_F)_{\partial C}$$

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Properties of $\mathbb{M}_C$

1. **Consistency**: we want the Gauss-Green formula to be satisfied at a discrete level[1]; moreover, we want it to be exact for a linear function q^l:

$$[\mathbb{K}\nabla q^l, \vec{W}]^{\mathbb{K}}_{C,X^h} + \int_C q^l \mathcal{D}^h \vec{W}\, dV = \sum_{F\in\partial C} W_{F\leftarrow C} \frac{1}{|F|} \int_F q^l \, d\Sigma$$

[1]F.Brezzi *et al.*, *A Family of Mimetic Finite Difference Methods on Polygonal and Polyhedral Meshes*, Math.Mod.Met.Appl.Sci. 2005.

Properties of $\mathbb{M}_C$

2. **Stability**: the scalar product shall not vanish or become unbound[2]:

$$s_* \sum_{F \in \partial C} |C| W_F^2 \leq [\vec{W}, \vec{W}]^{\mathbb{K}}_{C, X^h} \leq S^* \sum_{F \in \partial C} |C| W_F^2$$

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[2]A.Cangiani *et al.*, *Flux Reconstruction and Solution Post-processing in Mimetic Finite Difference Methods*, Comp.Meth.App.Mech.Eng. 2008

Construction of $\mathbb{M}_C$

To construct $\mathbb{M}_C$, we found that using a *cell-average* operator for vector-valued functions:

$$[\vec{V}, \vec{W}]_{C,X^h}^{\mathbb{K},avg} = |C|(\mathbb{K}_C^{-1} < \vec{V} >_C, < \vec{W} >_C)$$

where:

$$< \vec{W} >_C = \sum_{F \in \partial C} \frac{W_{F \leftarrow C}(\vec{x}_F - \vec{x}_C)}{|C|}$$

with the addition of a *stabilization term*:

$$\mathcal{R}_C(\vec{V}, \vec{W}) = \sum_{F \in \partial C} \lambda_{F,C} \left(V_{F \leftarrow C} - |F|(< \vec{V} >_C, \vec{n}_F) \right) \left(W_{F \leftarrow C} - |F|(< \vec{W} >_C, \vec{n}_F) \right)$$

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Construction of $\mathbb{M}_C$

satisfies both conditions, thus yielding a family of admissible scalar products:

$$[\vec{V}, \vec{W}]^{\mathbb{K}}_{C,X^h} = [\vec{V}, \vec{W}]^{\mathbb{K},avg}_{C,X^h} + \alpha_C \mathcal{R}_C(\vec{V}, \vec{W})$$

Clarification

Evidently we have considerable freedom of choice on:

- the expression for the face weights $\lambda_{F,C}$
- the scaling factor α_C for the stabilization term

How is it possible? Remember: we are trying to mimic a dot product between two FEM-like reconstructions. **Reconstructions are not unique!**

Thus it is normal that there is no unique expression of $\mathbb{M}_C$. But as long as our $\mathbb{M}_C$ is SPD and satisfies consistency and stability, then we know that it comes from an admissible reconstruction; *we don't care "which one"*[3].

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MVE Flux Operator

let's put everything together:

1. Applying our MVE inner product to the discrete variational form of our constitutional equation we get, after some manipulation:

$$\mathbb{M}_C (V_F)_{\partial C} \cdot (W_F)_{\partial C} = (p_C - p_F)_{\partial C} \cdot (W_F)_{\partial C}$$

2. Since $\vec{W}$ is an arbitrary test function, then the following must hold:

$$(V_F)_{\partial C} = \mathbb{M}_C^{-1} (p_C - p_F)_{\partial C}$$

3. This is the **flux operator** we were looking for.

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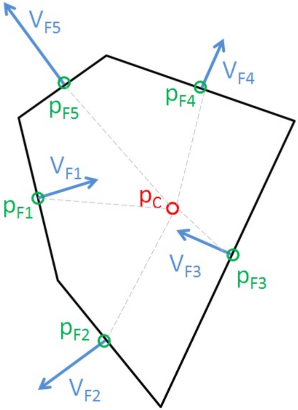

Relationship between MVE and FV

We managed to show that the operator:

$$(V_F)_{\partial C} = \mathbb{M}_C^{-1}(p_C - p_F)_{\partial C}$$

corresponds to a combination of two linearly consistent discrete gradients (Green-Gauss and least-squares) based on cell and face values of p.

Playing with different expressions of $\lambda_{F,C}$ we managed to show how our MVE scheme can be compared to a classical FV one with a fully implicit NOC $\rightarrow$ **solution stability becomes independent of mesh orthogonality; solution consistency holds at all times.**

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Convective Term

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$$\nabla \cdot (-\mathbb{K}\nabla p + \vec{U}p) = f$$

Again, we re-write in mixed formulation:

$$\begin{cases} \vec{V} = -\mathbb{K}\nabla p + \vec{U}p \\ \nabla \cdot \vec{V} = f \end{cases}$$

We already know how to discretize the diffusive flux. For the convective term, we just add it to each V_F:

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- **hybrid centering**: $p_{cnv} = p_F$ (which already exists as a DOF in our framework)
- **mixed centering**: $p_{cnv} = p_C$
- **hybrid upwinding**: $p_{cnv} = p_C$ if C is upwind, p_F otherwise
- **hybrid θ-scheme**: $p_{cnv} = \theta p_F + (1-\theta)p_C$ if C is upwind, p_F otherwise
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$$(V_F)_{\partial C} = \mathbb{M}_C^{-1}(p_C - p_F)_{\partial C} + (U_F p_{cnv})_{\partial C}$$

Stability will depend on how we choose p_{cnv}; we do so in analogy with traditional CFD schemes:

- **hybrid centering**: $p_{cnv} = p_F$ (which already exists as a DOF in our framework)
- **mixed centering**: $p_{cnv} = p_C$
- **hybrid upwinding**: $p_{cnv} = p_C$ if C is upwind, p_F otherwise
- **hybrid θ-scheme**: $p_{cnv} = \theta p_F + (1-\theta) p_C$ if C is upwind, p_F otherwise
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Contents

Pure Anisotropic Diffusion Test Case

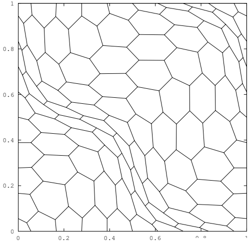
We validate with and h-convergece test for a benchmark pure anisotropic diffusion case, with diffusivity tensor:

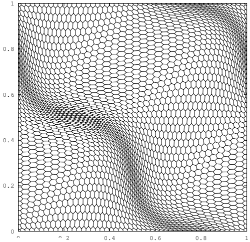
$$\mathbb{K} = \begin{pmatrix} (x+1)^2 + y^2 & -xy \\ -xy & (x+1)^2 \end{pmatrix}$$

and exact solution:

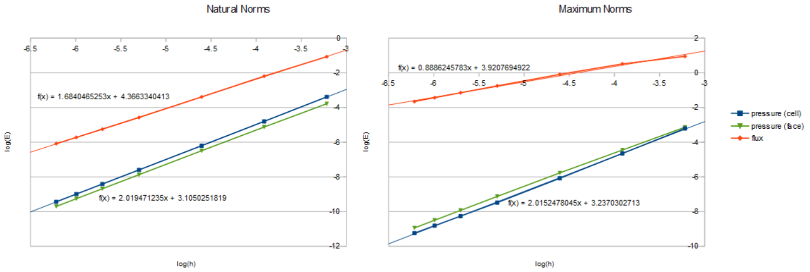
$$p_{ex}(x,y) = x^3 y^2 + x \sin(2\pi xy) \sin(2\pi y)$$

on highly distorted meshes:





Pure Anisotropic Diffusion Test Case



We observe second-order convergence for scalar variables and (roughly) first-order convergence for fluxes; this is in perfect agreement with predictions found in literature[4].

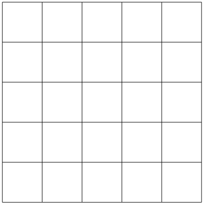
[4]F.Brezzi *et al.*, *Convergence of Mimetic Finite Difference Method for Diffusion Problems on Polyhedral Meshes*, SIAM Jour.Num.An. 2005.

Effects of Mesh Non-Orthogonality

We run a second pure diffusion test case with exact solution:

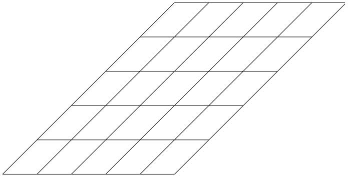
$$p_{ex}(x, y) = \cos(2\pi x) + 3y$$

On 4 progressively non-orthogonal meshes:



A

Effects of Mesh Non-Orthogonality



B

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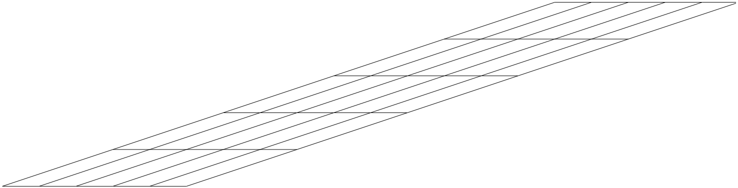
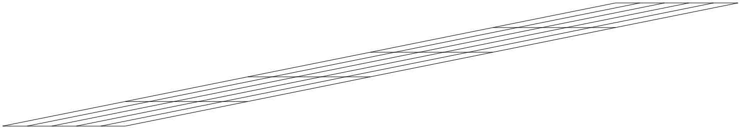


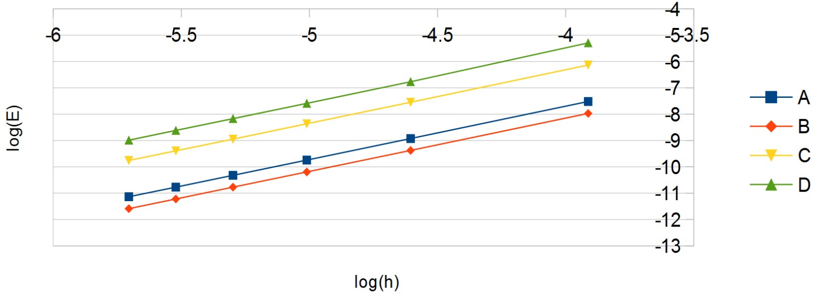
C

Effects of Mesh Non-Orthogonality



D

Effects of Mesh Non-Orthogonality



Convergence properties are identical on all four meshes.
Differences in error magnitude are due to the fact that, when distorting the mesh, we alter the average face area.

Convective Term: Patch Test

Patch test: in case of linear scalar field p, hybrid centered scheme produces the exact solution (at least for reasonable Pe):

Pe	hyb. centered	mix. centered	hyb. 1st upwinding	hyb. θ-scheme (0.49)
1.41E+000	5.73E-015	3.72E-005	1.95E-004	9.98E-005
1.41E+001	3.91E-014	3.56E-004	1.68E-003	8.88E-004
1.41E+002	1.44E-015	2.52E-003	5.84E-003	3.71E-003
1.41E+003	2.09E-012	5.77E-003	9.88E-003	8.87E-003
1.41E+004	3.57E-010	6.50E+000	1.10E-002	1.10E-002

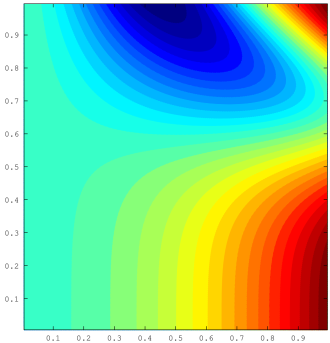
Convective Term: Different Strategies

For a nonlinear case, each scheme behaves similarily to its classical FV counterpart:

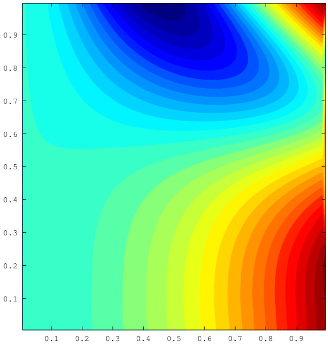
Pe	hyb. centered	mix. centered	hyb. 1st upwinding	hyb. θ-scheme (0.49)
8.53E+002	1.89E-004	3.73E+002	1.72E-002	1.37E-002
8.53E+003	4.22E+000	3.25E+002	2.05E-002	2.00E-002
8.53E+004	1.81E+000	3.34E+000	2.11E-002	2.14E-002
8.53E+005	5.16E+000	4.61E+000	2.11E-002	2.16E-002
8.53E+006	1.33E+001	1.29E+001	2.11E-002	2.16E-002

Stability of the θ-Scheme

Theoretical findings show that when applying the θ-scheme to the convective term, is always stable for $0 \leq \theta \leq 0.5$.



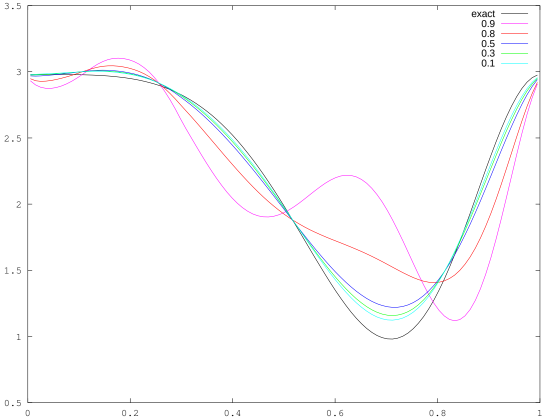
exact solution



MVE solution, θ=0.9

Stability of the θ-Scheme

Cross-section of critical area for different values of θ (high Pe):



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What We Did...

- Introduced the discrete spaces Q^h and X^h;
- Derived a set of *consistent* and *stable* discrete operators acting on them;
- "bridged the gap" between MVE and FV
- Used these operators to discretize the *pure anisotropic diffusion* equation in mixed-formulation;
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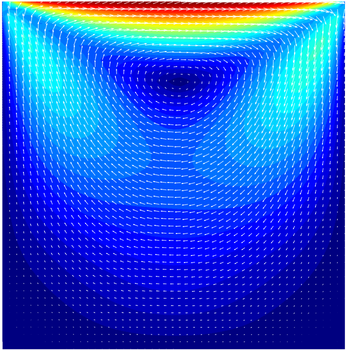

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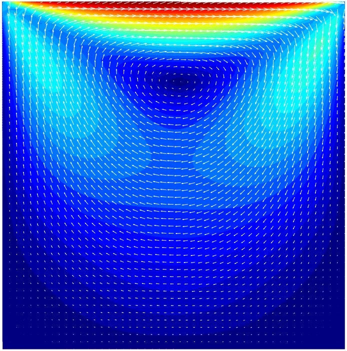

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Acknowledgements

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http://aboutflow.sems.qmul.ac.uk

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