Mimetic Finite Difference Method for Elliptic Problems

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July 2014, Durham

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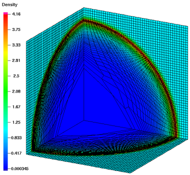
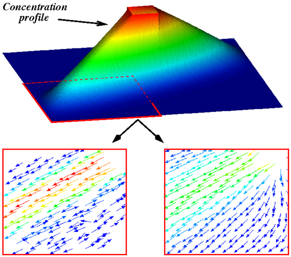
Objective

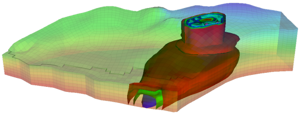
The mimetic finite difference method preserves or mimics critical mathematical and physical properties of systems of PDEs such as conservation laws, exact identities, solution symmetries, secondary equations, and maximum principles.

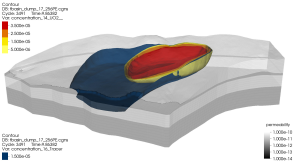
These properties are needed for multiphysics simulations.

The task of building mimetic schemes becomes more difficult on unstructured polygonal and polyhedral meshes.









Outline

Part I **Introduction to the MFD method**

1. **Motivation and requirements**
2. **Principles of mimetic discretizations**
3. **Family of mimetic schemes**

Part II **The MFD and other methods**

1. **Variational and finite volume viewpoints**
2. **Maximum and minimum principles**
3. **Discrete vector and tensor calculus**

Part I. Introduction to the MFD method

Duality property (1/2)

Let $q = 0$ **on** $\partial\Omega$**. We have the integration by part formula:**

$$\int_\Omega (\operatorname{div} \mathbf{u})\, q \,\mathrm{d}x = -\int_\Omega \mathbf{u} \cdot \nabla q \,\mathrm{d}x + \underbrace{\int_{\partial\Omega} q\mathbf{u} \cdot \mathbf{n} \mathrm{d}x}_{=0} = -\int_\Omega \mathbf{u} \cdot \nabla q \,\mathrm{d}x.$$

Duality property (1/2)

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Let $\mathrm{u}_h \in \mathcal{F}_h$ and $q_h \in \mathcal{C}_h$ be discrete fields (vectors of dofs), $q_h = 0$ on $\partial\Omega$, and

$$\mathrm{div}_h : \mathcal{F}_h \to \mathcal{C}_h, \qquad \nabla_h : \mathcal{C}_h \to \mathcal{F}_h$$

The discrete integration by parts formula mimics the continuous one:

$$\left[\mathrm{div}_h \mathbf{u}_h,\, q_h\right]_{\mathcal{C}_h} = -\left[\mathbf{u}_h,\, \nabla_h q_h\right]_{\mathcal{F}_h} \qquad \forall \mathbf{u}_h,\, q_h$$

where $[\cdot,\cdot]$ are inner products (approximation of integrals).

Duality property (2/2)

Requirement 1

$$\left[\mathrm{div}_h \mathbf{u}_h,\, q_h\right]_{\mathcal{C}_h} = -\left[\mathbf{u}_h,\, \nabla_h q_h\right]_{\mathcal{F}_h}$$

The discrete gradient and divergence operators cannot be discretized independently of one another.

Consequence of the duality property (1/2)

The equation of Lagrangian gasdynamic (density ρ, velocity $\mathbf{u}$, internal energy e, pressure p):

$$\begin{aligned} \frac{1}{\rho}\frac{d\rho}{dt} &= -\operatorname{div}\mathbf{u} \\ \rho\frac{d\mathbf{u}}{dt} &= -\nabla p \\ \rho\frac{de}{dt} &= -p\operatorname{div}\mathbf{u} \end{aligned}$$

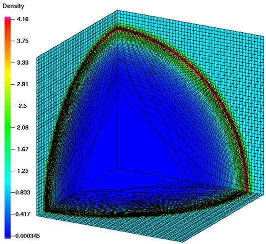
Let $p = 0$ of $\partial\Omega$. The integration by parts and continuity equation lead to conservation of the total energy E:

$$\frac{dE}{dt} = \int_{\Omega(t)} \rho\Big(\frac{d\mathbf{u}}{dt}\cdot\mathbf{u} + \frac{de}{dt}\Big)\,\mathrm{d}x = -\int_{\Omega(t)} (\mathbf{u}\cdot\nabla p + p\operatorname{div}\mathbf{u})\,\mathrm{d}x = 0.$$

Consequence of the duality property (2/2)

The semi-discrete equations read:

$$\begin{aligned} \frac{1}{\rho_h}\frac{d\rho_h}{dt} &= -\mathrm{div}_h \mathbf{u}_h \\ \rho_h \frac{d\mathbf{u}_h}{dt} &= -\nabla_h\, p_h \\ \rho_h \frac{de_h}{dt} &= -p_h\, \mathrm{div}_h \mathbf{u}_h \end{aligned}$$



The discrete integration by parts formula guarantees conservation of the total discrete energy E_h:

$$\frac{dE_h}{dt} = -[\mathbf{u}_h,\, \nabla_h\, p_h]_{\mathcal{F}_h} - [p_h,\, \mathrm{div}_h \mathbf{u}_h]_{\mathcal{C}_h} = 0.$$

Exact identities

For any $\mathbf{u}$ and p it holds:

$$\operatorname{div} \mathbf{curl}\, \mathbf{u} = 0, \qquad \mathbf{curl}\, \nabla p = 0.$$

Requirement 2

For any discrete fields $\mathbf{u}_h \in \mathcal{E}_h$ and $p_h \in \mathcal{N}_h$ it holds:

$$\operatorname{div}_h \mathbf{curl}_h\, \mathbf{u}_h = 0, \qquad \mathbf{curl}_h\, \nabla_h p_h = 0.$$

Consequence of the exact identities (1/2)

Maxwell's equations (magnetic field $\mathrm{H} = \mu\mathrm{B}$, magnetic flux density B, dielectric displacement $\mathbf{D} = \epsilon\mathbf{E}$, electric field $\mathbf{E}$):

$$\frac{\partial \mathbf{B}}{\partial t} = -\mathbf{curl}\,\mathbf{E}, \qquad \frac{\partial \mathbf{D}}{\partial t} = \mathbf{curl}\,\mathbf{H},$$

satisfy

$$\mathrm{div}\mathbf{B} = 0, \qquad \mathrm{div}\mathbf{D} = 0$$

for any time t.

Consequence of the exact identities (2/2)

The semi-discrete equations read:

$$\frac{\partial \mathbf{B}_h}{\partial t} = -\mathbf{curl}_h\, \mathbf{E}_h, \qquad \frac{\partial \mathbf{D}_h}{\partial t} = \widetilde{\mathbf{curl}}_h\, \mathbf{H}_h,$$

The exact discrete identities guarantee that the initial divergence-free condition is preserved:

$$\frac{\partial}{\partial t}\big(\mathrm{div}_h\, \mathbf{B}_h\big) = \mathrm{div}_h\, \frac{\partial \mathbf{B}_h}{\partial t} = -\mathrm{div}_h\, \mathbf{curl}_h\, \mathbf{E}_h = 0$$

and

$$\frac{\partial}{\partial t}\big(\widetilde{\mathrm{div}}_h\, \mathbf{D}_h\big) = \widetilde{\mathrm{div}}_h\, \frac{\partial \mathbf{D}_h}{\partial t} = -\widetilde{\mathrm{div}}_h\, \widetilde{\mathbf{curl}}_h\, \mathbf{H}_h = 0.$$

Requirements for the mimetic discretization

In this talk, we build discrete mimetic operators that

1. **satisfy the duality property for a pair of operators**
2. **satisfy exact identities**
3. **lead to conditional maximum and minimum principles**
4. **provide optimal approximation of PDEs**

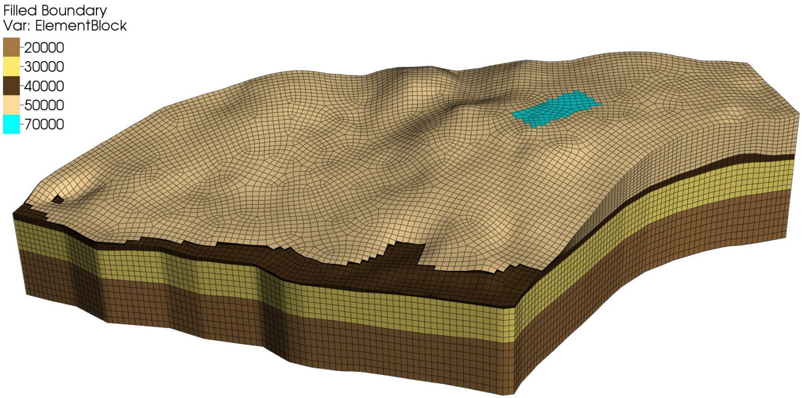
on unstructured polygonal and polyhedral meshes.

Incomplete list of related methods

- **Cell method**
- **Co-volume method**
- **Summation by parts**
- **Hybrid FV, mixed FV, discrete duality FV**
- **Mixed FE, VEM**
- **FE exterior calculus**

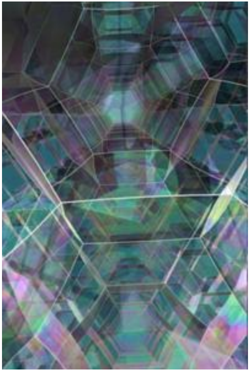
Mimetic method differs by constructive/practical approach to building discrete operators on general polyhedral meshes.

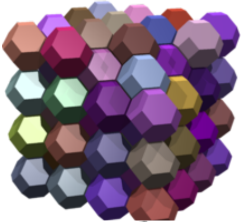
Unstructured polyhedral meshes in porous media

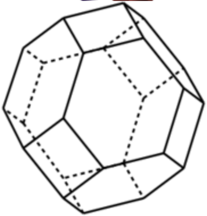


Polyhedral meshes provide enormous flexibility in mesh generation.

Kelvin's conjecture & Weaire-Phelan's structure







Polyhedral cell has more neighbors which leads to better transfer of information in expense of a higher stencil.

Overall, polyhedral meshes may lead to faster time to a solution compared to simplicial meshes.

Unstructured polyhedral meshes: engineering

The Weaire-Phelan structure inspired the design of the aquatic center for the 2008 Olympics Games in Beijing.

The design is ideally suited to absorbing energy from earthquakes.

Duality requirement (1/3)

Consider the one-dimensional Poisson equation

$$\begin{aligned} -\frac{d^2p}{dx^2} &= b \quad x \in (0,1) \\ p(0) = p(1) &= 0. \end{aligned}$$

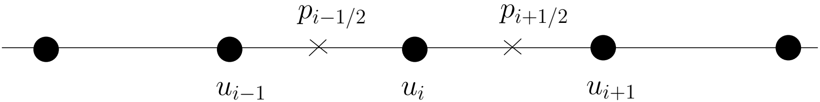
We write this second-order equation as a system of two first-order equations:

$$u = -\frac{dp}{dx}, \qquad \frac{du}{dx} = b.$$

Recall the integration by part property:

$$\int_0^1 \frac{dp}{dx} u \, dx = -\int_0^1 p \frac{du}{dx} dx.$$

Duality requirement (2/3)



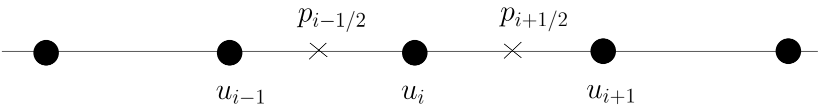
By the duality requirement, approximation $du/dx \approx \mathrm{div}_h u_h$ **and** $dp/dx \approx \nabla_h p_h$ **must satisfy the discrete integration by parts formula:**

$$\big[\underbrace{\mathrm{div}_h u_h}_{q_h},\, p_h\big]_{\mathcal{C}_h} = -\big[u_h,\, \underbrace{\nabla_h p_h}_{v_h}\big]_{\mathcal{F}_h} \quad \forall u_h, p_h,$$

where

- $\big[q_h,\, p_h\big]_{\mathcal{C}_h} = \sum_{i=1}^{n} \Delta x\, q_{i+1/2}\, p_{i+1/2} \approx \int_0^1 p\, q\, \mathrm{d}x$
- $\big[u_h,\, v_h\big]_{\mathcal{F}_h} = \sum_{i=1}^{n+1} \Delta x\, u_i\, v_i \approx \int_0^1 u\, v\, \mathrm{d}x$

Duality requirement (3/3)



$$(\mathrm{div}_h u_h)_{i+1/2} \equiv \frac{u_{i+1} - u_i}{\Delta x}$$

Inserting this in the discrete integration by parts formula:

$$\Delta x \sum_{i=1}^{n} \frac{u_{i+1} - u_i}{\Delta x} p_{i+1/2} = -\Delta x \sum_{i=1}^{n+1} (\nabla_h p_h)_i u_i \quad \forall u_h, p_h$$

Rearranging the left-hand side, we recover the natural FD formula for the gradient:

$$(\nabla_h p_h)_i = \frac{p_{i+1/2} - p_{i-1/2}}{\Delta x}$$

where $p_{1/2} = p_{n+3/2} = 0$**.**

Discretization principle

Commandment 1: Use duality

Select and discretize one the two adjoint operators. Derive the other discrete operator from the discrete duality formula.

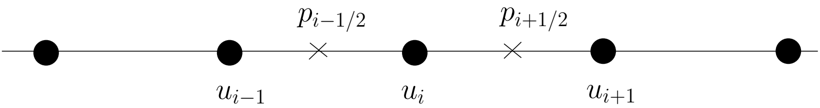
1. Divergence operator is discretized first. div_h is called the **primary mimetic operator**.
2. Discrete gradient operator ∇_h is called the **derived mimetic operator**.

The discrete integration by parts formula

$$\left[\mathrm{div}_h u_h,\, p_h\right]_{\mathcal{C}_h} = -\left[u_h,\, \nabla_h p_h\right]_{\mathcal{F}_h} \quad \forall u_h, p_h.$$

works the same way in two- and three-dimensions.

Accuracy requirement (1/4)



Accuracy of a mimetic scheme depends on properties of the inner products. For sufficiently smooth u and v:

$$\left[q_h,\, p_h\right]_{\mathcal{C}_h} = \sum_{i=1}^{n} \Delta x\, q_{i+1/2}\, p_{i+1/2} = \int_0^1 q\, p\, \mathrm{d}x + O(\Delta x)$$

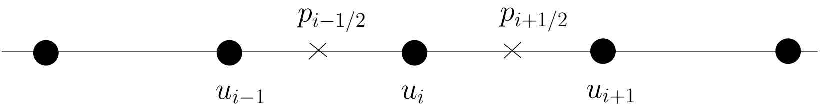
The construction of inner product can be done cell-by-cell:

$$\left[q_h,\, p_h\right]_{\mathcal{C}_h} = \sum_{i=1}^{n} \left[q_h,\, p_h\right]_{i,\mathcal{C}_h}$$

where

$$\left[q_h,\, p_h\right]_{i,\mathcal{C}_h} = \Delta x q_{i+1/2}\, p_{i+1/2} = \int_{x_i}^{x_{i+1}} q\, p\, \mathrm{d}x + O((\Delta x)^2)$$

Accuracy requirement (2/4)



Accuracy of a mimetic scheme depend on properties of the inner products. For sufficiently smooth u and v:

$$\left[v_h,\, u_h\right]_{\mathcal{F}_h} = \sum_{i=1}^{n+1} \Delta x\, v_i\, u_i = \int_0^1 vu\,\mathrm{d}x + O(\Delta x)$$

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where

$$\left[v_h,\, u_h\right]_{i,\mathcal{F}_h} = \frac{\Delta x}{2}(v_i\, u_i + v_{i+1}\, u_{i+1}) = \int_{x_i}^{x_{i+1}} vu\,\mathrm{d}x + O((\Delta x)^3)$$

By the definition of an inner-product, there exists a 2×2 SPD matrix $\mathbb{M}_i$ such that

$$\left[v_h,\, u_h\right]_{i,\mathcal{F}_h} = \left(v_i,\, v_{i+1}\right) \mathbb{M}_i \begin{pmatrix} u_i \\ u_{i+1} \end{pmatrix}.$$

In the considered case, $\mathbb{M}_i$ is the scalar matrix:

$$\mathbb{M}_i = \mathbb{M}_i^{FD} = \frac{\Delta x}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

It corresponds to trapezoidal integration rule:

$$\left(v_i,\, v_{i+1}\right)\mathbb{M}_i^{FD} \begin{pmatrix} u_i \\ u_{i+1} \end{pmatrix} = \frac{\Delta x}{2}(v_i u_i + v_{i+1} u_{i+1}) \approx \int_{x_i}^{x_{i+1}} v\, u\, \mathrm{d}x.$$

Accuracy requirement (3/4)

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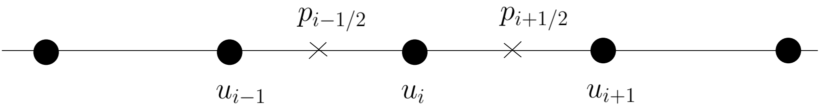
Another quadrature rule gives a new matrix $\mathbb{M}_i$; hence a different inner product and another mimetic scheme.

Accuracy requirement (4/4)



If we consider piecewise linear approximations to functions u and v, we obtain another good inner product matrix:

$$\mathbb{M}_i = \mathbb{M}_i^{RT} = \frac{\Delta x}{6} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

Direct calculation gives

$$\big(v_i,\, v_{i+1}\big)\mathbb{M}_i^{RT} \begin{pmatrix} u_i \\ u_{i+1} \end{pmatrix} = \int_{x_i}^{x_{i+1}} v\, u\, dx + O((\Delta x)^3)$$

In fact, we have a 1-parameter family of inner product matrices. We describe this family today and select the best scheme tomorrow.

Consistency condition

Let us approximate function v by a constant v^0 and function u by a linear function u^1. Then,

$$\int_{x_i}^{x_{i+1}} v^0\, u^1\, dx = \int_{x_i}^{x_{i+1}} v\, u\, dx + O((\Delta x)^2).$$

Note that both $\mathbb{M}_i^{FD}$ and $\mathbb{M}_i^{RT}$ satisfy

$$\int_{x_i}^{x_{i+1}} v^0\, u^1\, dx = \frac{\Delta x}{2} v^0 (u_i + u_{i+1}) = (v^0,\, v^0)\, \mathbb{M}_i \begin{pmatrix} u_i \\ u_{i+1} \end{pmatrix}$$

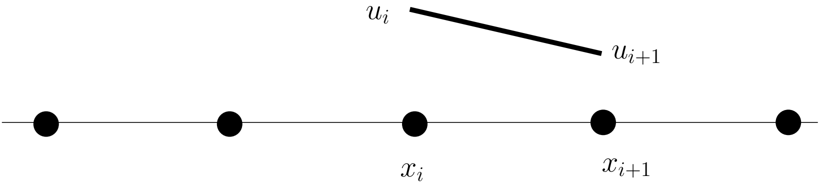
Commandment 2: Use a polynomial patch test

A consistent matrix $\mathbb{M}_i$ must satisfy

$$(v^0,\, v^0)\, \mathbb{M}_i \begin{pmatrix} u_i \\ u_{i+1} \end{pmatrix} = \int_{x_i}^{x_{i+1}} v^0\, u^1\, dx \qquad \forall v^0,\, \forall (u_i,\, u_{i+1})$$

where the integral is computable using dofs.

Bridge 1: to VEM



Consider a lifting operator from dofs to a functional space:

$$u^1 = \mathcal{L}\{\begin{pmatrix} u_i \\ u_{i+1} \end{pmatrix}\}$$

- **Interpolation returns back our dofs, i.e.** $u^1(x_i) = u_i$ **and** $u^1(x_{i+1}) = u_{i+1}$**.**
- **The lifted space contains constant functions.**
- **Divergence of** u^1 **is a constant.**

A lifting operator is introduced in many papers on mimetic schemes as a tool for their convergence analysis.

One-parameter family of inner product matrices

$$(v^0,\, v^0)\, \mathbb{M}_i \begin{pmatrix} u_i \\ u_{i+1} \end{pmatrix} = \int_{x_i}^{x_{i+1}} v^0\, u^1\, dx = \frac{\Delta x}{2} v^0 (u_i + u_{i+1})$$

It is each to verify that

$$\mathbb{M}_i = \frac{\Delta x}{2} \begin{pmatrix} 2a & 1-2a \\ 1-2a & 2a \end{pmatrix}.$$

Obviously, that we need to constraint the parameter a to get an SPD matrix $\mathbb{M}_i$.

Stability condition

Commandment 3: Limit a family of consistent matrices

An admissible matrix $\mathbb{M}_i$ is such that there exists two positive constants $\sigma_\star$ and $\sigma^\star$ independent of Δx such that

$$\sigma_\star \Delta x (u_i^2 + u_{i+1}^2) \leq (u_i,\, u_{i+1})\, \mathbb{M}_i \begin{pmatrix} u_i \\ u_{i+1} \end{pmatrix} \leq \sigma^\star \Delta x (u_i^2 + u_{i+1}^2)$$

for all vectors $(u_i,\, u_{i+1})^T$.

- **Matrix $\mathbb{M}_i^{FD}$ satisfies the stability condition with $\sigma\star = \sigma^\star = 1$.**
- **For matrix $\mathbb{M}_i^{RT}$ we have $\sigma\star = 1/6$ and $\sigma^\star = 1/2$.**

Five-step discretization algorithm

1. **Select degrees of freedom (for u and p).**
2. **Discretize the primary mimetic operator (e.g., div_h).**
3. **Construct local inner products that satisfy consistency and stability conditions.**
4. **Formulate the discrete duality principle:**

$$\left[\mathrm{div}_h u_h,\, p_h\right]_{\mathcal{C}_h} = -\left[u_h,\, \nabla_h p_h\right]_{\mathcal{F}_h} \quad \forall u_h, p_h.$$

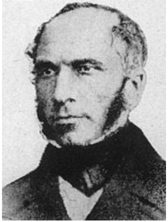
5. **Deduce the derived mimetic operator (resp., ∇_h) from it.**

Darcy flow in porous media

Consider a 2D or 3D Poisson equation:

$$\begin{aligned} \mathbf{u} &= -\nabla p \\ \operatorname{div} \mathbf{u} &= b \end{aligned}$$

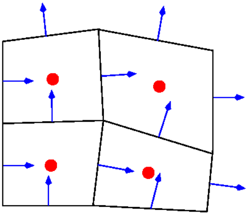
subject to $p = 0$ **on** $\partial\Omega$**.**



To derive its mimetic discretization

$$\begin{aligned} \mathbf{u}_h &= -\nabla_h \, p_h \\ \operatorname{div}_h \mathbf{u}_h &= b_h \end{aligned}$$

we apply the above five-step algorithm.



The discrete velocities are defined on mesh faces and represent average fluxes. The discrete pressures are defined in mesh cells and represent average pressures:

$$u_f \approx \frac{1}{|f|}\int_f \mathbf{u}\cdot\mathbf{n}_f\,\mathrm{d}x, \qquad p_c \approx \frac{1}{|c|}\int_c p\,\mathrm{d}x.$$

Define $\mathbf{u}_h = (u_{f_1}, u_{f_2}, \ldots, u_{f_n})^T$ **and** $p_h = (p_{c_1}, p_{c_2}, \ldots, p_{c_m})^T$**.**

We use a coordinate-invariant definition of the divergence:

$$\int_c \operatorname{div}\mathbf{u}\,\mathrm{d}x = \int_{\partial c} \mathbf{u}\cdot\mathbf{n}\,\mathrm{d}x = \sum_{f\in\partial c} \sigma_{c,f} \int_f \mathbf{u}\cdot\mathbf{n}_f\,\mathrm{d}x$$

Replacing integrals by mid-point quadratures, we have

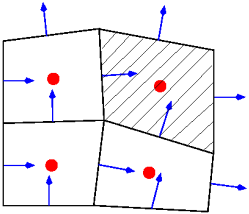
$$(\operatorname{div}_h \mathbf{u}_h)|_c = \frac{1}{|c|} \sum_{f\in\partial c} \sigma_{c,f}\,|f|\,u_f$$

The discrete divergence operator is like in the FV and MFE methods. The difference between methods is in the discretization of the constitutive equation.

Step 3: Local inner products

We need accurate approximations of cell-based integrals:

$$[q_h,\, p_h]_{c,\mathcal{C}_h} \approx \int_c q\, p\, \mathrm{d}x. \qquad [\mathbf{v}_h,\, \mathbf{u}_h]_{c,\mathcal{F}_h} \approx \int_c \mathbf{v}\cdot\mathbf{u}\, \mathrm{d}x$$



Recall that these inner products can be re-written as vector-matrix-vector products with SPD matrices:

$$[q_h,\, p_h]_{c,\mathcal{C}_h} = q_c\, \mathbb{M}_c^{\mathcal{C}}\, p_c$$

$$[\mathbf{v}_h,\, \mathbf{u}_h]_{c,\mathcal{F}_h} = (v_{f_1},\ldots,v_{f_4})\, \mathbb{M}_c^{\mathcal{F}} \begin{pmatrix} u_{f_1} \\ \vdots \\ u_{f_4} \end{pmatrix},$$

In this example, $\mathbb{M}_c^{\mathcal{C}}$ is 1×1 matrix and $\mathbb{M}_c^{\mathcal{F}}$ is 4×4 matrix. Obvious choice $\mathbb{M}_c^{\mathcal{C}} = |c|$ leads to the 1st-order approximation of the integral, i.e. it is the admissible matrix.

Step 3: Consistency condition (1/3)

A consistent matrix $\mathbb{M}_c^{\mathcal{F}}$ must satisfy

$$\left(v^0_{f_1}, \ldots, v^0_{f_4}\right) \mathbb{M}_c^{\mathcal{F}} \begin{pmatrix} u_{f_1} \\ \vdots \\ u_{f_4} \end{pmatrix} = \int_c \mathbf{v}^0 \cdot \mathbf{u}^1 \, \mathrm{d}x \qquad \forall \mathbf{v}^0, \, \mathbf{u}^1,$$

where $v^0_{f_i} = \mathbf{v}^0 \cdot \mathbf{n}_{f_i}$ **and** $\mathbf{u}^1 = \mathcal{L}((u_{f_1}, \ldots, u_{f_4})^T) \in \mathcal{S}_c$ **s.t.**

- $\mathbf{u}^1 \cdot \mathbf{n}_{f_i} = u_{f_i} \qquad i = 1, 2, 3, 4;$
- $\mathrm{div}\mathbf{u}^1 = \mathtt{constant} = (\mathrm{div}_h \, \mathbf{u}_h)_c$.

We need only existence result for u^1.

For any constant vector function v^0 there exists the linear polynomial q^1 such that

$$\mathbf{v}^0 = \nabla q^1 \qquad \text{and} \qquad \int_c q^1 \mathrm{d}x = 0.$$

Then,

$$\left(v^0_{f_1}, \ldots, v^0_{f_4}\right) \mathbb{M}^{\mathcal{F}}_c \begin{pmatrix} u_{f_1} \\ \vdots \\ u_{f_4} \end{pmatrix} = \int_c \mathbf{v}^0 \cdot \mathbf{u}^1 \,\mathrm{d}x$$

$$= -\int_c q_1 \underbrace{\mathrm{div}\mathbf{u}^1}_{=constant} \mathrm{d}x + \int_{\partial c} q_1 \,\mathbf{u}^1 \cdot \mathbf{n} \,\mathrm{d}x = \sum_{i=1}^4 \int_{f_i} q_1 \,\mathbf{u}^1 \cdot \mathbf{n}_{f_i} \,\mathrm{d}x$$

$$= \left(\int_{f_1} q_1 \,\mathrm{d}x, \ldots, \int_{f_4} q_1 \,\mathrm{d}x\right) \begin{pmatrix} u_{f_1} \\ \vdots \\ u_{f_4} \end{pmatrix} \qquad \forall \mathbf{v}^0, \,\mathbf{u}^1.$$

Step 3: Consistency condition (3/3)

Algebraic equations w.r.t. unknown matrix $\mathbb{M}_c^{\mathcal{F}}$:

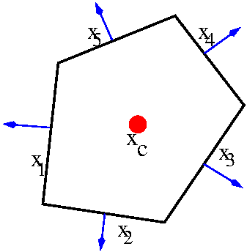
$$\mathbb{M}_c^{\mathcal{F}} \begin{pmatrix} v_{f_1}^0 \\ \vdots \\ v_{f_4}^0 \end{pmatrix} = \begin{pmatrix} \int_{f_1} q^1 \, \mathrm{d}x \\ \vdots \\ \int_{f_4} q^1 \, \mathrm{d}x \end{pmatrix} \qquad \forall \mathbf{v}^0 = \nabla q^1.$$

It is sufficient to consider only linearly independent functions q^1. In two-dimensions, we have $q_a^1 = x - x_c$ and $q_b^1 = y - y_c$:

Mimetic matrix equation

$$\underbrace{\mathbb{M}_c^{\mathcal{F}}}_{4\times 4} \underbrace{\mathbb{N}_c}_{4\times 2} = \underbrace{\mathbb{R}_c}_{4\times 2}.$$

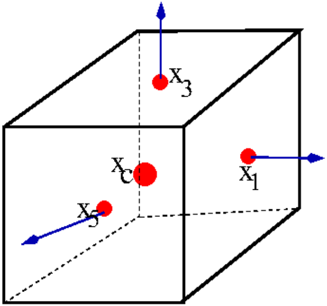
The problem is under-determined for any cell c (triangles: Shashkov, Hyman, Liska, Nicolaides, Trapp).



$$\mathbb{M}_c^{\mathcal{F}}\,\mathbb{N}_c = \mathbb{R}_c$$

Required geometric information: normals to faces, centroids of faces, areas of faces:

$$\mathbb{N}_c = \begin{bmatrix} n_{1x} & n_{1y} \\ n_{2x} & n_{2y} \\ \vdots & \vdots \\ n_{5x} & n_{5y} \end{bmatrix} \qquad \mathbb{R}_c = \begin{bmatrix} |f_1|(x_1 - x_c) & |f_1|(y_1 - y_c) \\ |f_2|(x_1 - x_c) & |f_2|(y_2 - y_c) \\ \vdots & \vdots \\ |f_5|(x_5 - x_c) & |f_5|(y_5 - y_c) \end{bmatrix}$$



$$\mathbb{M}_c^{\mathcal{F}}\,\mathbb{N}_c = \mathbb{R}_c$$

Required geometric information: normals to faces, centroids of faces, areas of faces:

$$\mathbb{N}_c = \begin{bmatrix} n_{1x} & n_{1y} & n_{1z} \\ n_{2x} & n_{2y} & n_{2z} \\ \vdots & \vdots & \vdots \\ n_{6x} & n_{6y} & n_{6z} \end{bmatrix} \qquad \mathbb{R}_c = \begin{bmatrix} |f_1|(x_1 - x_c) & |f_1|(y_1 - y_c) & |f_1|(z_1 - z_c) \\ |f_2|(x_1 - x_c) & |f_2|(y_2 - y_c) & |f_2|(z_2 - z_c) \\ \vdots & \vdots & \vdots \\ |f_6|(x_6 - x_c) & |f_6|(y_6 - y_c) & |f_6|(z_6 - z_c) \end{bmatrix}$$

Lemma

For any polygon (polyhedron in 3D), we have

$$\mathbb{N}_c^T\,\mathbb{R}_c = \mathbb{R}_c^T\,\mathbb{N}_c = |c|\mathbb{I}.$$

Sketch of the proof. **Direct calculations give**

$$\begin{aligned}
(\mathbb{N}_c^T\,\mathbb{R}_c)_{1,2} &= \sum_{i=1}^{k} n_{f_i,x}|f_i|(y_i - y_c) \\
&= \sum_{i=1}^{k} \int_{f_i} (\nabla x \cdot \mathbf{n}_{f_i})(y - y_c)\,\mathrm{d}x \\
&= \int_c (\nabla x)\cdot\nabla(y - y_c) = 0.
\end{aligned}$$

Other entries are verified similarly. □

Lemma

A one-parameter family of SPD solutions to $\mathbb{M}_c^{\mathcal{F}} \mathbb{N}_c = \mathbb{R}_c$ is

$$\mathbb{M}_c^{\mathcal{F}} = \mathbb{M}_c^{consistency} + \mathbb{M}_c^{stability}$$

where

$$\mathbb{M}_c^{consistency} = \frac{1}{|c|} \mathbb{R}_c \, \mathbb{R}_c^T$$

and

$$\mathbb{M}_c^{stability} = a_c \left(\mathbb{I} - \mathbb{N}_c \left(\mathbb{N}_c^T \mathbb{N}_c \right)^{-1} \mathbb{N}_c^T \right) \qquad a_c > 0.$$

A complete description of the family of solutions will be given tomorrow.

An admissible $k \times k$ matrix $\mathbb{M}_c^{\mathcal{F}}$ must satisfy

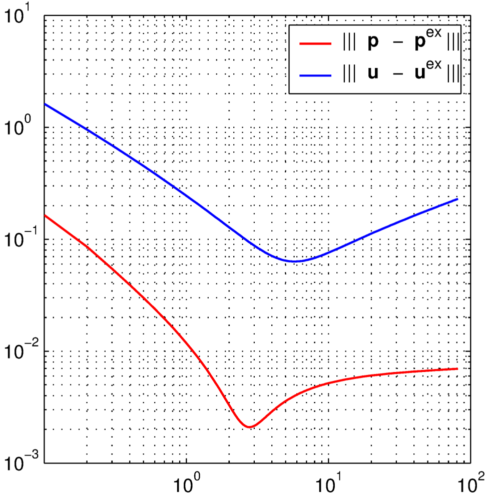
$$\sigma_\star |c| \sum_{i=1}^{k} |u_{f_i}|^2 \leq (u_{f_1}, \ldots, u_{f_k})\, \mathbb{M}_c^{\mathcal{F}} \begin{pmatrix} u_{f_1} \\ \vdots \\ u_{f_k} \end{pmatrix} \leq \sigma^\star |c| \sum_{i=1}^{k} |u_{f_i}|^2.$$

where $\sigma_\star$ and $\sigma^\star$ are positive constants independent of c.

In practice, a good scaling is given by

$$a_c = a_c^* \equiv |c|.$$

Consider a 2D elliptic problem and calculate Darcy flux and pressure errors as functions of the normalize parameter a_c/a_c^*.



The free parameter a_c can vary 2-orders in magnitude.

Step 4: Formulate the discrete duality principle

$$\left[\operatorname{div}_h \mathbf{u}_h,\, p_h\right]_{\mathcal{C}_h} = -\left[\mathbf{u}_h,\, \nabla_h p_h\right]_{\mathcal{F}_h} \quad \forall \mathbf{u}_h, p_h$$

Step 5: Deduce the derived mimetic operator

$$\big[\underbrace{\mathrm{div}_h \mathbf{u}_h}_{q_h},\, p_h\big]_{\mathcal{C}} = -\big[\mathbf{u}_h,\, \underbrace{\nabla_h p_h}_{\mathbf{v}_h}\big]_{\mathcal{F}} \quad \forall \mathbf{u}_h, p_h$$

By definition of the inner product, it can be associated with a symmetric positive definite matrix:

$$\begin{aligned}
\big[q_h,\, p_h\big]_{\mathcal{C}_h} &= q_h^T\, \mathbb{M}_{\mathcal{C}}\, p_h \\
\big[\mathbf{u}_h,\, \mathbf{v}_h\big]_{\mathcal{F}_h} &= \mathbf{u}_h^T\, \mathbb{M}_{\mathcal{F}}\, \mathbf{v}_h
\end{aligned}$$

Note that $\mathbb{M}_{\mathcal{C}} = \mathrm{diag}(|c_1|, \ldots, |c_n|)$ **and** $\mathbb{M}_{\mathcal{F}} = \sum_{c \in \Omega_h} \mathcal{N}_c\, \mathbb{M}_c^{\mathcal{F}}\, \mathcal{N}_c^T$.

Derived gradient operator

$$\nabla_h = -\mathbb{M}_{\mathcal{F}}^{-1}\, \mathrm{div}_h^T\, \mathbb{M}_{\mathcal{C}}.$$

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Final mimetic scheme

The algebraic form of the MFD scheme is

$$\begin{aligned} \mathbf{u}_h &= -\nabla_h\, p_h = \mathbb{M}_{\mathcal{F}}^{-1}\, \mathrm{div}_h^T\, \mathbb{M}_{\mathcal{C}}\, p_h \\ \mathrm{div}_h\, \mathbf{u}_h &= b_h \end{aligned}$$

or in a symmetrized form:

$$\begin{pmatrix} \mathbb{M}_{\mathcal{F}} & -\mathrm{div}_h^T\, \mathbb{M}_{\mathcal{C}} \\ -\mathbb{M}_{\mathcal{C}}\, \mathrm{div}_h & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u}_h \\ p_h \end{pmatrix} = \begin{pmatrix} 0 \\ -\mathbb{M}_{\mathcal{C}}\, b_h \end{pmatrix}$$

Derived gradient is not local on general meshes if $\mathbb{M}_{\mathcal{F}}^{-1}$ is dense.

Conclusion for Part I

- **The mimetic finite difference method is designed to mimic important properties of mathematical and physical systems on arbitrary polygonal or polyhedral meshes.**

- **The MFD method leads to a family of schemes that have the same stencil and formal accuracy order. Tomorrow I'll show how to find a member of this family that satisfies the maximum principle.**

- **The MFD method for diffusion problems is relative easy to implement on polyhedral meshes ($\mathbb{M}_c^{\mathcal{F}}\mathbb{N}_c = \mathbb{R}_c$). A similar equation holds for mimetic discretizations of other PDEs.**

Conclusion for Part I

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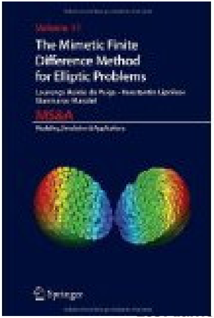


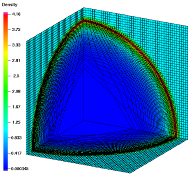
Part II. The MFD and other methods

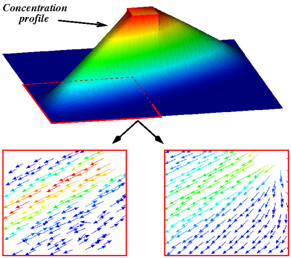
Objective

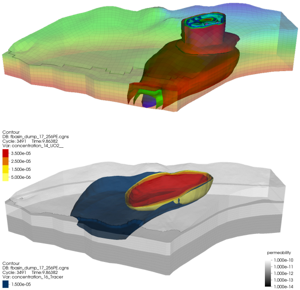
The mimetic finite difference method preserves or mimics critical mathematical and physical properties of systems of PDEs such as conservation laws, exact identities, solution symmetries, secondary equations, and maximum principles.

These properties are needed for multiphysics simulations.

The task of building mimetic schemes becomes more difficult on unstructured polygonal and polyhedral meshes.





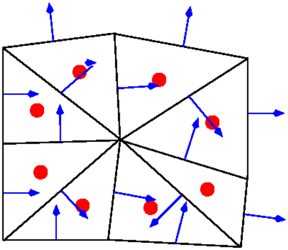


Five-step discretization algorithm

1. **Select degrees of freedom (for u and p).**
2. **Discretize the primary mimetic operator (e.g., div_h).**
3. **Construct local inner products that satisfy consistency and stability conditions.**
4. **Formulate the discrete duality principle:**

$$\left[\mathrm{div}_h \mathbf{u}_h,\, p_h\right]_{\mathcal{C}_h} = -\left[\mathbf{u}_h,\, \widetilde{\nabla}_h p_h\right]_{\mathcal{F}_h} \quad \forall \mathbf{u}_h, p_h.$$

5. **Deduce the derived mimetic operator (resp., $\widetilde{\nabla}_h$) from it.**



The MFD scheme for the Poisson equation with homogeneous b.c.:

$$\begin{aligned} \mathbf{u}_h &= -\widetilde{\nabla}_h\, p_h \\ \mathrm{div}_h\, \mathbf{u}_h &= b_h \end{aligned}$$

The primary divergence operator is

$$(\mathrm{div}_h\, \mathbf{u}_h)|_c = \frac{1}{|c|} \sum_{f \in \partial c} \sigma_{c,f}\, |f|\, u_f$$

Multiply the 1st equation by $\mathrm{v}_h^T \mathbb{M}_{\mathcal{F}}$, the 2nd one by $q_h^T \mathbb{M}_{\mathcal{C}}$, and apply the integration by part formula:

$$\big[\mathbf{v}_h,\, \mathbf{u}_h\big]_{\mathcal{F}_h} = -\big[\mathbf{v}_h,\, \widetilde{\nabla}_h\, p_h\big]_{\mathcal{F}_h} = \big[\mathrm{div}_h\, \mathbf{v}_h,\, p_h\big]_{\mathcal{C}_h}$$

$$\big[\mathrm{div}_h\, \mathbf{u}_h,\, q_h\big]_{\mathcal{C}_h} = [b_h,\, q_h]_{\mathcal{C}_h}$$

Bridge 2: to MFE (2/3)

Let $\mathcal{F}_h \times \mathcal{C}_h$ correspond to a MFE space $RT_0 \times P_0$. Then, we can define the inner products using the FE functions:

$$\begin{aligned} \left[\mathbf{v}_h,\, \mathbf{u}_h\right]_{\mathcal{F}_h} &= \int_\Omega \mathbf{v}_h^{RT} \cdot \mathbf{u}_h^{RT}\,\mathrm{d}x \\ \left[q_h,\, p_h\right]_{\mathcal{C}_h} &= \int_\Omega q_h^{P0} p_h^{P0}\,\mathrm{d}x \end{aligned}$$

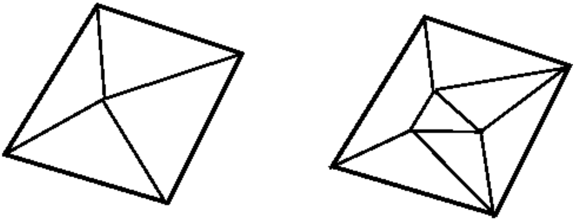
We can verify that this leads to admissible matrices $\mathbb{M}_\mathcal{F}$ and $\mathbb{M}_\mathcal{C}$. With such inner products, the MFD scheme becomes a MFE formulation:

$$\int_\Omega \mathbf{v}_h^{RT} \cdot \mathbf{u}_h^{RT}\,\mathrm{d}x = \int_\Omega \mathrm{div}\,\mathbf{v}_h^{RT}\, p_h^{P0}\,\mathrm{d}x$$

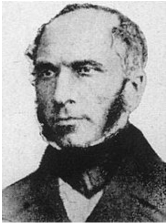
$$\int_\Omega \mathrm{div}\,\mathbf{u}_h^{RT}\, q_h^{P0}\,\mathrm{d}x = \int_\Omega b_h^{P0}\, q_h^{P0}\,\mathrm{d}x$$

Hence, the MFE method on simplices is a member of the MFD family of schemes.

A few mimetic schemes (not all) can be related to a triangular sub-partition of a polygon and the Raviart-Thomas FE function $\mathbf{u}_h^{RT}$



$\mathbf{u}_h^{RT}$ **is an example of a lifting operator** $\mathcal{L}((u_{f_1}, \ldots, u_{f_4}))$ **and must satisfy the above properties, e.g.** $\mathrm{div}\mathbf{u}_h^{RT} = constant$**.**



Consider a 2D or 3D Poisson equation:

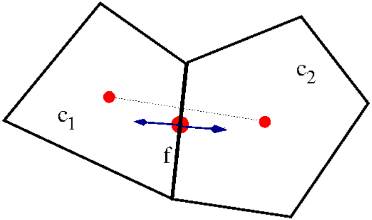
$$\begin{aligned} \mathbf{u} &= -\mathbb{K}\nabla p \\ \operatorname{div} \mathbf{u} &= b \end{aligned}$$

subject to $p = 0$ on $\partial\Omega$.

We derive its mimetic discretization

$$\begin{aligned} \mathbf{u}_h &= -\widetilde{\nabla}_h \, p_h \\ \operatorname{div}_h \mathbf{u}_h &= b_h \end{aligned}$$

using a FV framework. The material properties will be absorbed in the derived gradient operator $\widetilde{\nabla}_h$.



To explain difference between the FV and MFD schemes, we write both in a hybrid form using edge-based pressures p_f:

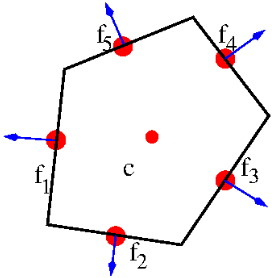
$$u_{c_1,f} = -K_{c_1}\frac{p_f - p_{c_1}}{d_{1f}}, \qquad u_{c_2,f} = -K_{c_2}\frac{p_f - p_{c_2}}{d_{2f}}$$

subject to the flux continuity condition:

$$u_{c_1,f} + u_{c_2,f} = 0.$$

The mass balance equation is common for both methods:

$$\mathrm{div}_h\, \mathbf{u}_h = b_h$$



$$\mathbb{M}_c^{\mathcal{F}} \begin{bmatrix} u_{c,f_1} \\ u_{c,f_2} \\ \vdots \\ u_{c,f_5} \end{bmatrix} = - \begin{bmatrix} |f_1|(p_{f_1} - p_c) \\ |f_2|(p_{f_2} - p_c) \\ \vdots \\ |f_5|(p_{f_5} - p_c) \end{bmatrix}$$

subject to flux continuity conditions:

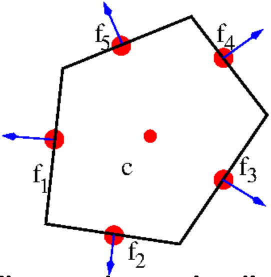
$$u_{c,f_i} + u_{c',f_j} = 0.$$

Multiplying these equations by v_{c,f_i} and summing over cells:

$$\underbrace{\sum_{c\in\Omega^h} \mathbf{v}_{c,h}^T \mathbb{M}_c^{\mathcal{F}} \mathbf{u}_{c,h}}_{\left[\mathbf{v}_h,\, \mathbf{u}_h\right]_{\mathcal{F}_h} = -[\mathbf{v}_h,\, \widetilde{\nabla} p_h]_{\mathcal{F}_h}} = - \sum_{f\in\Omega_h^{int}} |f| p_f \underbrace{(v_{c,f} + v_{c',f})}_{=0} + \underbrace{\sum_{c\in\Omega^h} |c| (\mathrm{div}_{c,h} \mathbf{v}_{c,h}) p_c}_{\left[\mathrm{div}_h \mathbf{v}_h,\, p_h\right]_{\mathcal{C}_h}}$$

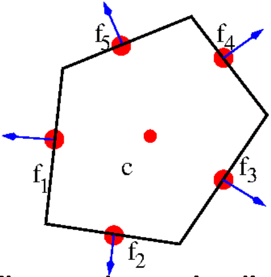
Duality requirement is satisfied.

Bridge 3: to FV (3/3)



$$\mathbb{M}_c^{\mathcal{F}} \begin{bmatrix} u_{c,f_1} \\ u_{c,f_2} \\ \vdots \\ u_{c,f_5} \end{bmatrix} = - \begin{bmatrix} |f_1|(p_{f_1} - p_c) \\ |f_2|(p_{f_2} - p_c) \\ \vdots \\ |f_5|(p_{f_5} - p_c) \end{bmatrix}$$

The patch test implies that this flux-pressure relationship must be exact for any solution p that is linear on cell c and the corresponding constant velocity $\mathbf{u} = -\mathbb{K}_c \nabla p$.



$$\mathbb{M}_c^{\mathcal{F}} \begin{bmatrix} u_{c,f_1} \\ u_{c,f_2} \\ \vdots \\ u_{c,f_5} \end{bmatrix} = - \begin{bmatrix} |f_1|(p_{f_1} - p_c) \\ |f_2|(p_{f_2} - p_c) \\ \vdots \\ |f_5|(p_{f_5} - p_c) \end{bmatrix}$$

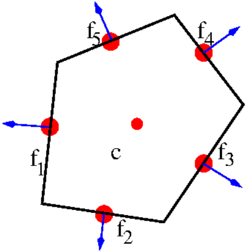
The patch test implies that this flux-pressure relationship must be exact for any solution p that is linear on cell c and the corresponding constant velocity $\mathbf{u} = -\mathbb{K}_c \nabla p$.

On a Voronoi mesh, we can obviously take a diagonal matrix $\mathbb{M}_c^{\mathcal{F}}$ with diagonal entries provided by the FV scheme:

$$(\mathbb{M}_c^{\mathcal{F}})_{f_i,f_i} = \frac{K_c}{d_{f_i}}$$

This matrix will be admissible and the resulting scheme will be mimetic.

General mesh or full permeability tensor



$$\mathbb{M}_c^{\mathcal{F}} \begin{bmatrix} u_{c,f_1} \\ u_{c,f_2} \\ \vdots \\ u_{c,f_5} \end{bmatrix} = - \begin{bmatrix} |f_1|(p_{f_1} - p_c) \\ |f_2|(p_{f_2} - p_c) \\ \vdots \\ |f_5|(p_{f_5} - p_c) \end{bmatrix}$$

On a general polygonal cell, we have to consider three linearly independent linear functions:

$$p_1 = 1, \quad p_2 = x, \quad p_3 = y.$$

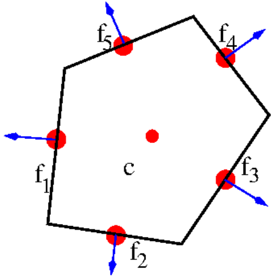
The corresponding Darcy velocity $\mathbf{u}$ is

$$\mathbf{u}_1 = 0, \quad \mathbf{u}_2 = -\mathbb{K}_c \nabla x, \quad \mathbf{u}_3 = -\mathbb{K}_c \nabla y.$$

Mimetic matrix equation

$$\underbrace{\mathbb{M}_c^{\mathcal{F}}}_{5\times 5} \underbrace{\mathbb{N}_c}_{5\times 2} = \underbrace{\mathbb{R}_c}_{5\times 2}.$$

Construction of $\mathbb{N}_c$ and $\mathbb{R}_c$ for a pentagon



$$\mathbb{M}_c^{\mathcal{F}} \begin{bmatrix} u_{c,f_1} \\ u_{c,f_2} \\ \vdots \\ u_{c,f_5} \end{bmatrix} = - \begin{bmatrix} |f_1|(p_{f_1} - p_c) \\ |f_2|(p_{f_2} - p_c) \\ \vdots \\ |f_5|(p_{f_5} - p_c) \end{bmatrix}$$

Required geometric information: normals to faces, centroids of faces, areas of faces, constant diffusion tensor:

$$\mathbb{N}_c = \begin{bmatrix} n_{1x} & n_{1y} \\ n_{2x} & n_{2y} \\ \vdots & \vdots \\ n_{5x} & n_{5y} \end{bmatrix} \mathbb{K}_c, \qquad \mathbb{R}_c = \begin{bmatrix} |f_1|(x_1 - x_c) & |f_1|(y_1 - y_c) \\ |f_2|(x_1 - x_c) & |f_2|(y_2 - y_c) \\ \vdots & \vdots \\ |f_5|(x_5 - x_c) & |f_5|(y_5 - y_c) \end{bmatrix}$$

Properties of $\mathbb{N}_c$ and $\mathbb{R}_c$

Lemma

For any polygon (polyhedron in 3D), we have

$$\mathbb{N}_c^T\,\mathbb{R}_c = \mathbb{R}_c^T\,\mathbb{N}_c = |c|\,\mathbb{K}_c.$$

Convergence results

Let

- Ω **have a Lipschitz continuous boundary;**
- **Every cell** c **be shape regular;**
- $p_h^I \in \mathcal{C}_h$ **and** $\mathbf{u}_h^I \in \mathcal{F}_h$ **be interpolants of exact solution.**

Then,

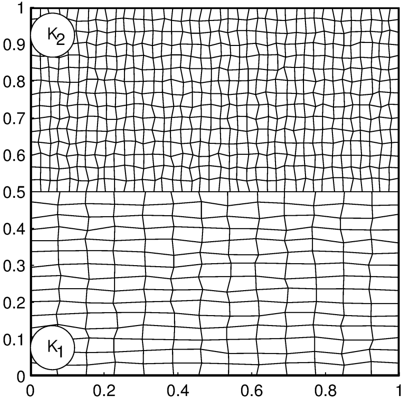
$$|||p_h^I - p_h|||_{\mathcal{C}_h} + |||\mathbf{u}_h^I - \mathbf{u}_h|||_{\mathcal{F}_h} \leq C\,h$$

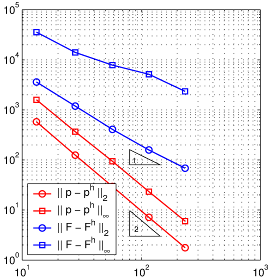
If Ω **is convex and** a_c^* **is sufficiently large, then**

$$|||p_h^I - p_h|||_{\mathcal{C}_h} \leq C\,h^2$$

where h **is the mesh parameter.**

Non-matching randomly perturbed meshes





- $K_1 = 1, K_2 = 10^6$
- **aspect ratio variations:**

$$167 < \max_{cells} \frac{\max_k |f_k|}{\min_k |f_k|} < 2024$$

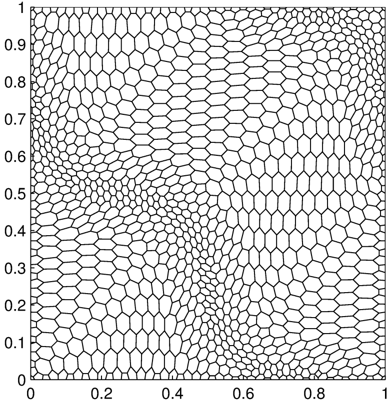
- **exact solution is**

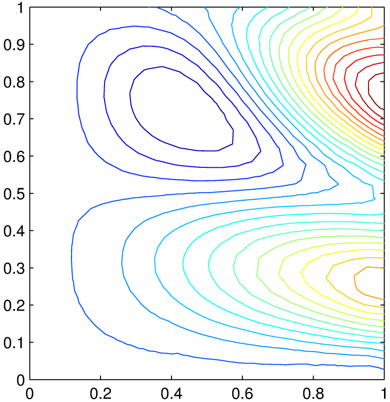
$$\color{red}{p}(x,\ y) = \begin{cases} \frac{7}{16} - \frac{K_2}{12K_1} + \frac{2K_2}{3K_1}\, y^3, & y < 0.5, \\ y - y^4, & y \geq 0.5. \end{cases}$$

Polygonal meshes (1/2)

$$p(x,\,y) = x^3y^2 + x\sin(2\pi xy)\sin(2\pi y)$$

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





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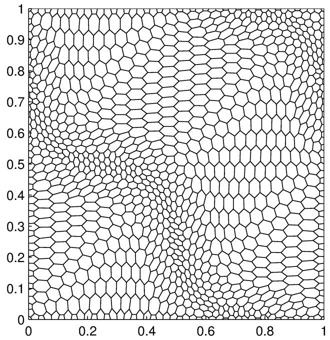
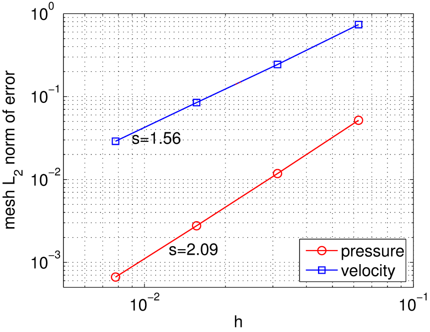
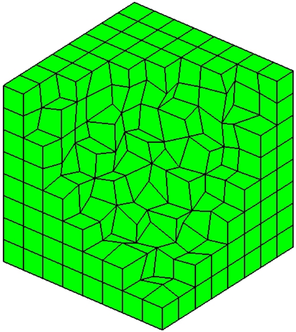
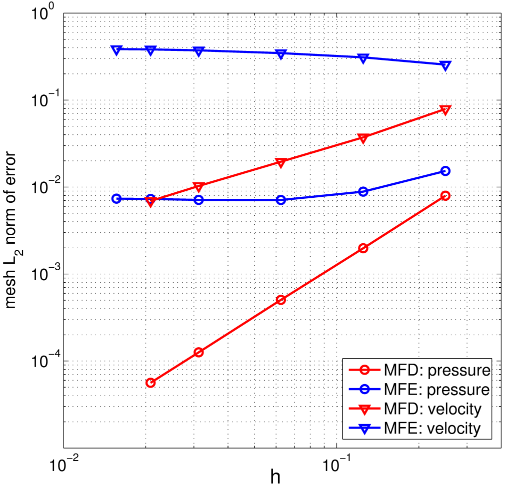
$$
\begin{aligned}
p(x,\,y) &= x^3y^2 + x\sin(2\pi xy)\sin(2\pi y) \\
\mathbb{K}(x,\,y) &= \begin{bmatrix} (x+1)^2 + y^2 & -xy \\ -xy & (x+1)^2 \end{bmatrix}
\end{aligned}
$$





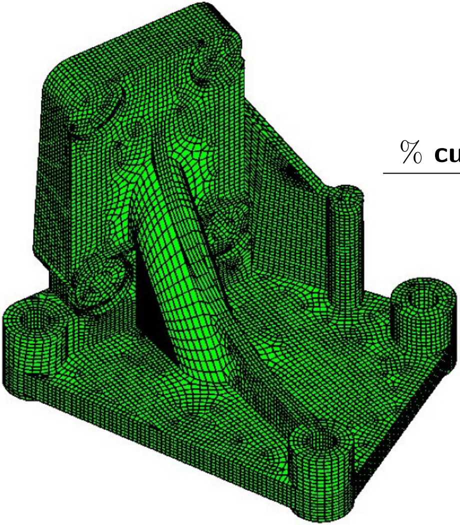
Hexahedral meshes with curved faces (1/2)





Methods with one velocity unknown per curved mesh face do not converge. MFD technology allows to use 3 unknowns (F.Brezzi,K.L.,M.Shashkov, M3AS, 2006).

Hexahedral meshes with curved faces (2/2)



$$K = 1, \quad p = x^3 + y^2 + 2z^2$$

% curved	$\|\mathbf{u}_h^I - \mathbf{u}_h\|_{\mathcal{F}_h}$	$\|\mathbf{u}_h^I - \mathbf{u}_h\|_\infty$
0.00	7.86e+4	1.79e+4
0.05	7.80e+4	1.62e+4
0.44	6.69e+4	1.54e+4
2.25	3.54e+4	1.59e+3
9.45	3.25e+4	7.37e+2

Discrete maximum principle (1/2)

$$\begin{bmatrix} u_{c,f_1} \\ u_{c,f_2} \\ \vdots \\ u_{c,f_5} \end{bmatrix} = -\left(\mathbb{M}_c^{\mathcal{F}}\right)^{-1} \begin{bmatrix} |f_1|(p_{f_1} - p_c) \\ |f_2|(p_{f_2} - p_c) \\ \vdots \\ |f_5|(p_{f_5} - p_c) \end{bmatrix}, \qquad \mathbb{W}_c = \left(\mathbb{M}_c^{\mathcal{F}}\right)^{-1}.$$

Inserting this into the mass balance ($\mathrm{div}_h \mathbf{u}_h = b_h$) and flux continuity ($u_{c,f} + u_{c',f} = 0$) equations, and imposing boundary conditions, we obtain an algebraic problem for only pressure unknowns:

$$\mathbb{A} p_h = b_h, \qquad \mathbb{A} = \sum_{c \in \Omega_h} \mathcal{N}_c \, \mathbb{A}_c \, \mathcal{N}_c^T.$$

Discrete maximum principle (2/2)

Define matrix $\mathbb{B}_c^T$ as a shorter notation for $(\mathrm{div}_h)_c$ and define a square diagonal matrix $\mathbb{C}_c$ such that $\mathbb{C}_c 1 = \mathbb{B}_c$. Then, for most matrices, we have

$$\mathbb{A}_c = \left[\begin{array}{cc} \mathbb{C}_c^T \, \mathbb{W}_c \, \mathbb{C}_c & -\mathbb{C}_c^T \, \mathbb{W}_c \, \mathbb{B}_c \\ -\mathbb{B}_c^T \, \mathbb{W}_c \, \mathbb{C}_c & \mathbb{B}_c^T \, \mathbb{W}_c \, \mathbb{B}_c \end{array} \right].$$

Discrete maximum principle (2/2)

Define matrix $\mathbb{B}_c^T$ as a shorter notation for $(\mathrm{div}_h)_c$ and define a square diagonal matrix $\mathbb{C}_c$ such that $\mathbb{C}_c 1 = \mathbb{B}_c$. Then, for most matrices, we have

$$\mathbb{A}_c = \begin{bmatrix} \mathbb{C}_c^T \, \mathbb{W}_c \, \mathbb{C}_c & -\mathbb{C}_c^T \, \mathbb{W}_c \, \mathbb{B}_c \\ -\mathbb{B}_c^T \, \mathbb{W}_c \, \mathbb{C}_c & \mathbb{B}_c^T \, \mathbb{W}_c \, \mathbb{B}_c \end{bmatrix}.$$

Lemma

(i) Let $\mathbb{W}_c$ be an M-matrix. (ii) Let vector $\mathbb{W}_c \, \mathbb{B}_c$ have non-negative entries.
Then matrix $\mathbb{A}_c$ is a singular M-matrix with the null space consisting of constant vectors.

Parameterizations of $\mathbb{W}_c$

The matrix equation $\mathbb{M}_c^{\mathcal{F}}\,\mathbb{N}_c = \mathbb{R}_c$ can be written as

$$\mathbb{N}_c = \mathbb{W}_c\,\mathbb{R}_c.$$

The solution to this matrix equation is

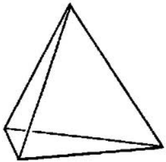
$$\mathbb{W}_c = \frac{1}{|c|}\mathbb{N}_c\,\mathbb{K}_c^{-1}\,\mathbb{N}_c^T + \mathbb{D}_c\,\mathbb{P}_c\,\mathbb{D}_c^T$$

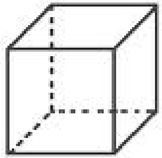
where $\mathbb{D}_c^T\,\mathbb{R}_c = 0$ and $\mathbb{P}_c$ is an arbitrary SPD matrix. Recall that $\mathbb{N}_c^T\,\mathbb{R}_c = \mathbb{K}_c\,|c|$.

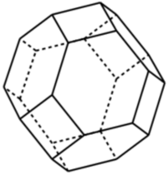
The goal is to find a mimetic scheme where all matrices $\mathbb{W}_c$ are M-matrices.

How rich is the family of MFD schemes?

Cell	$\mathbb{P}_c$	# parameters
triangle/tetrahedron	1×1	**1**
quadrilateral	2×2	**3**
hexahedron	3×3	**6**
tetradecahedron	11×11	**66**







Control of positive definiteness of $\mathbb{W}_c$ (1/2)

$$\mathbb{W}_c = \frac{1}{|c|}\mathbb{N}_c\,\mathbb{K}_c^{-1}\,\mathbb{N}_c^T + \mathbb{D}_c\,\mathbb{P}_c\,\mathbb{D}_c^T, \qquad \mathbb{A}_c = \begin{bmatrix} \mathbb{C}_c^T\,\mathbb{W}_c\,\mathbb{C}_c & -\mathbb{C}_c^T\,\mathbb{W}_c\,\mathbb{B}_c \\ -\mathbb{B}_c^T\,\mathbb{W}_c\,\mathbb{C}_c & \mathbb{B}_c^T\,\mathbb{W}_c\,\mathbb{B}_c \end{bmatrix}$$

Direct control of a Z-matrix structure and spectral properties of $\mathbb{W}_c$ is not practical. We introduce a stronger requirement.

Lemma

(i) Let $\mathbb{W}_c$ be a Z-matrix. (ii) Let vector $\mathbb{W}_c\,\mathbb{B}_c$ have positive entries.
Then matrix $\mathbb{A}_c$ is a singular M-matrix with the null space consisting of constant vectors.

Control of positive definiteness of $\mathbb{W}_c$ (2/2)

A general symmetric square matrix $\mathbb{P}_c$ of size m can be described by $s = m(m+1)/2$ parameters, e.g.

$$\mathbb{P}_c = \begin{pmatrix} a_1 & a_3 \\ a_3 & a_2 \end{pmatrix}.$$

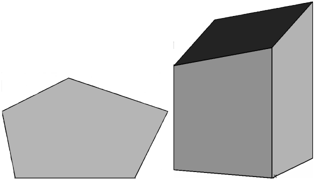
- **Since $\mathbb{W}_c$ depends linearly on $\mathbb{P}_c$, the Z-matrix property $(\mathbb{W}_c)_{ij} \leq 0$ for $i \neq j$ leads to linear inequality constraints.**
- **$(\mathbb{W}_c \mathbb{B}_c)_i \geq \epsilon > 0$ are also linear inequality constraints.**

A linear programming tools (simplex or interior point methods) can be used to find an M-matrix $\mathbb{W}_c$. To enforce its diagonal dominance, we maximize

$$\Phi(a_1, \ldots, a_s) = \sum_{i,j=1}^{k} (\mathbb{W}_c)_{ij}.$$

Cost of the simplex method

cell type	Experiment I		Experiment II	
	monotone MFD	base MFD	monotone MFD	base MFD
quad	15.3 μs	5.05μs	14.7μs	4.91μs
pentagon	28.0 μs	6.62μs	29.3μs	6.64μs
hexahedron	—	—	48.7μs	8.92μs

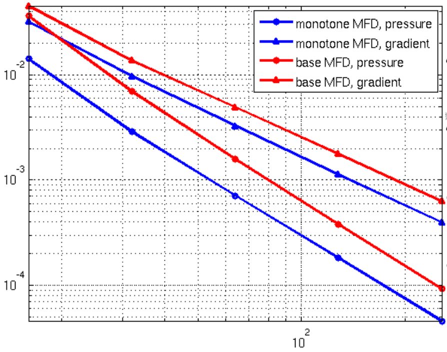


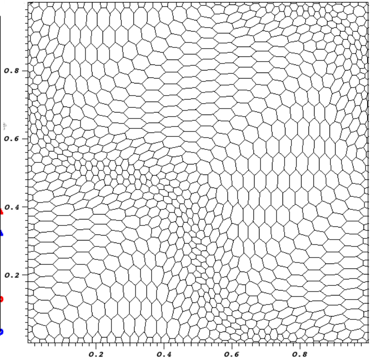
- **The monotone MFD method is 3-6 times more expensive than the base MFD with** $\mathbb{W}_c^{stability} = \alpha_c \mathbb{D}_c \mathbb{D}_c^T$.
- **The simplex method returns diagonal matrices** $\mathbb{W}_c$ **on a Voronoi mesh.**
- **It can be used in other MFD schemes.**

Monotone MFD method (1/2)

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

$$p(x,y) = x^3y^2 + x\sin(2\pi x)\sin(2\pi y).$$



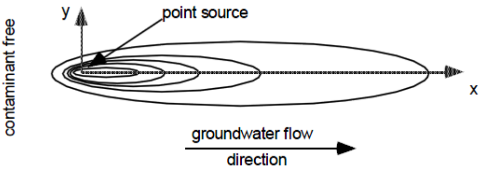


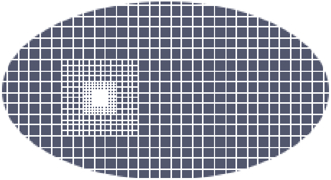
Optimization improves errors on non-Voronoi meshes.

Monotone MFD method (2/2)

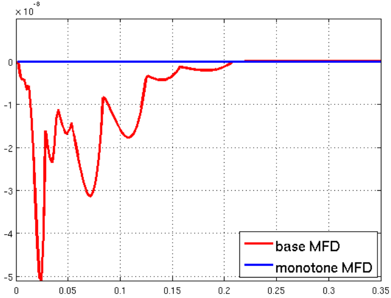
$$\frac{\partial C}{\partial t} + \mathrm{div}(\mathbf{u}C) = -\mathrm{div}(\mathbb{K}\nabla C), \qquad \mathbb{K} = \alpha_L \frac{\mathbf{u}\mathbf{u}}{\|\mathbf{u}\|^2} + \alpha_T\left(\mathbb{I} - \frac{\mathbf{u}\mathbf{u}}{\|\mathbf{u}\|^2}\right) + \phi\tau D_m$$

$\mathbf{u}$ makes angle 30° with the primary mesh orientation.





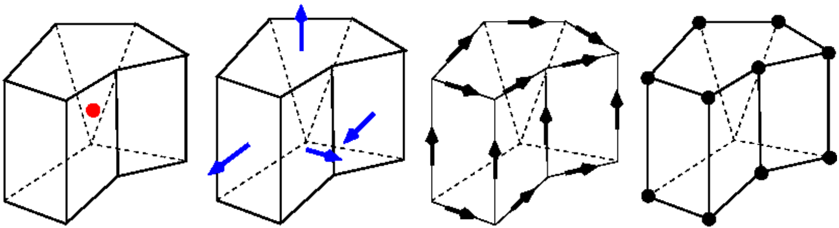
Undershoots in the base MFD method are small enough and go to zero as the contamination front moves away from the source. Inclusion of chemical reactions may lead to significant amplification of the undershoots (C.Steefel and K.MacQuarrie, Reactive transport in porous media, 34).



Discrete spaces

Exact discrete identities are enforced using staggered discretization. Discrete fields associated with various geometric objects:

- $\mathcal{C}_h$ - **cell-centered values**
- $\mathcal{F}_h$ - **face-centered values**
- $\mathcal{E}_h$ - **edge-centered values**
- $\mathcal{N}_h$ - **node-centered values**

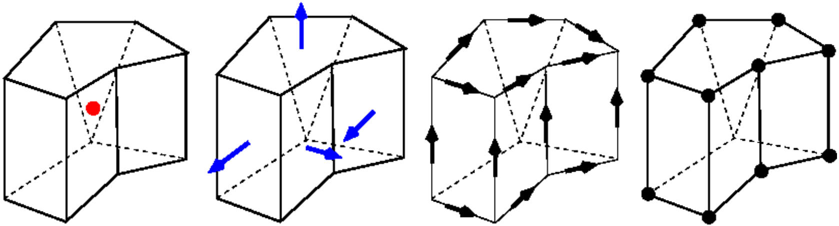


De Rham complex

The three primary and three derived operators fit in to the following diagram:

$$\mathcal{N}_h \;\underset{\nabla_h}{\longrightarrow}\; \mathcal{E}_h \;\underset{\mathrm{curl}_h}{\longrightarrow}\; \mathcal{F}_h \;\underset{\mathrm{div}_h}{\longrightarrow}\; \mathcal{C}_h$$

$$\mathcal{N}_h \;\underset{\widetilde{\mathrm{div}}_h}{\longleftarrow}\; \mathcal{E}_h \;\underset{\widetilde{\mathrm{curl}}_h}{\longleftarrow}\; \mathcal{F}_h \;\underset{\widetilde{\nabla}_h}{\longleftarrow}\; \mathcal{C}_h$$



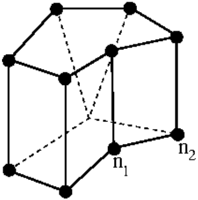
Coordinate-invariant definition of operators

We start with coordinate invariant definitions of discrete operators. Such approach is important for curvilinear coordinate systems.

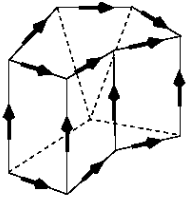
$$\int_{\mathbf{x}_a}^{\mathbf{x}_b} (\nabla\, p) \cdot \boldsymbol{\tau}\, \mathrm{d}x = p(\mathbf{x}_a) - p(\mathbf{x}_b)$$

$$\int_S (\mathbf{curl}\, \mathbf{u}) \cdot \mathbf{n}\, \mathrm{d}x = \oint_{\partial S} \mathbf{u} \cdot \boldsymbol{\tau}\, \mathrm{d}x,$$

$$\int_V \mathrm{div}\, \mathbf{u}\; \mathrm{d}x = \oint_{\partial V} \mathbf{u} \cdot \mathbf{n}\, \mathrm{d}x$$



$$\nabla_h : \ \mathcal{N}_h \to \mathcal{E}_h$$



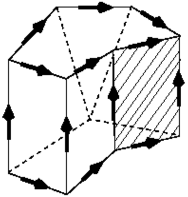
The continuum coordinate-invariant definition is

$$\int_e (\nabla p) \cdot \boldsymbol{\tau}_e \, \mathrm{d}x = p(\mathbf{x}_{n_2}) - p(\mathbf{x}_{n_1}).$$

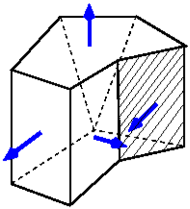
Using mid-point quadratures, we get the primary gradient operator:

$$\big(\nabla_h \, p_h\big)_e = \frac{p_{n_2} - p_{n_1}}{|e|}.$$

Primary discrete curl operator



$$\mathrm{curl}_h : \ \mathcal{E}_h \to \mathcal{F}_h$$



The continuum coordinate-invariant definition is

$$\int_f (\mathbf{curl}\,\mathbf{u}) \cdot \mathbf{n}_f \, \mathrm{d}x = \oint_{\partial f} \mathbf{u} \cdot \boldsymbol{\tau} \, \mathrm{d}x.$$

Using mid-point quadratures, we get the primary curl operator:

$$\left(\mathrm{curl}_h \, \mathbf{u}_h\right)_f = \frac{1}{|f|} \sum_{e \in \partial f} \sigma_{f,e} \, |e| \, u_e, \qquad u_e \approx \frac{1}{|e|} \int_e \mathbf{u} \cdot \boldsymbol{\tau}_e \, \mathrm{d}x.$$

Exact discrete identities: primary operators

Lemma

Let domain Ω and its mesh partition Ω_h be simply connected. Then,

$$\operatorname{curl}_h \mathbf{u}_h = 0 \quad \textbf{if and only if} \quad \mathbf{u}_h = \nabla_h p_h$$

for some $p_h \in \mathcal{N}_h$ and

$$\operatorname{div}_h \mathbf{v}_h = 0 \quad \textbf{if and only if} \quad \mathbf{v}_h = \operatorname{curl}_h \mathbf{u}_h$$

for some $\mathbf{u}_h \in \mathcal{E}_h$.

Derived divergence operator

Consider homogeneous boundary conditions and continuum relationship

$$\int_\Omega p \operatorname{div} \mathbf{u} \, \mathrm{d}x = -\int_\Omega (\nabla p) \cdot \mathbf{u} \, \mathrm{d}x.$$

Its discrete analog

$$[p_h, \widetilde{\operatorname{div}}_h \, \mathbf{u}_h]_\mathcal{N} = -[\nabla_h \, p_h, \mathbf{u}_h]_\mathcal{E} \qquad \forall p_h, \ \mathbf{u}_h.$$

Using definition of inner products, we obtain explicit formula for the derived gradient operator:

$$\widetilde{\operatorname{div}}_h = -\mathbb{M}_\mathcal{N}^{-1} \, \nabla_h^T \, \mathbb{M}_\mathcal{E}.$$

Derived curl operator

Consider homogeneous boundary conditions and continuum relationship

$$\int_\Omega \mathbf{v} \cdot (\mathbf{curl}\,\mathbf{u})\,\mathrm{d}x = \int_\Omega (\mathbf{curl}\,\mathbf{v}) \cdot \mathbf{u}\,\mathrm{d}x.$$

Its discrete analog

$$[\mathbf{v}_h, \widetilde{\mathrm{curl}}_h\,\mathbf{u}_h]_{\mathcal{E}} = [\mathrm{curl}_h\,\mathbf{v}_h, \mathbf{u}_h]_{\mathcal{F}} \qquad \forall \mathbf{u}_h,\ \mathbf{v}_h.$$

Using definition of inner products, we obtain explicit formula for the derived gradient operator:

$$\widetilde{\mathrm{curl}}_h = \mathbb{M}_{\mathcal{E}}^{-1}\,\mathrm{curl}_h^T\,\mathbb{M}_{\mathcal{F}}.$$

Exact discrete identities: derived operators

Lemma

The derived discrete gradient, divergence, and curl operators satisfy the following exact relationship:

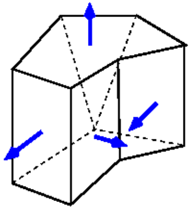
$$\widetilde{\mathrm{curl}}_h \, \mathbf{u}_h = 0 \quad \textbf{if and only if} \quad \mathbf{u}_h = \widetilde{\nabla}_h \, p_h$$

for some $p_h \in \mathcal{C}_h$ **and**

$$\widetilde{\mathrm{div}}_h \, \mathbf{v}_h = 0 \quad \textbf{if and only if} \quad \mathbf{v}_h = \widetilde{\mathrm{curl}}_h \, \mathbf{u}_h$$

for some $\mathbf{u}_h \in \mathcal{F}_h$**.**

Helmholtz decomposition theorems (1/3)

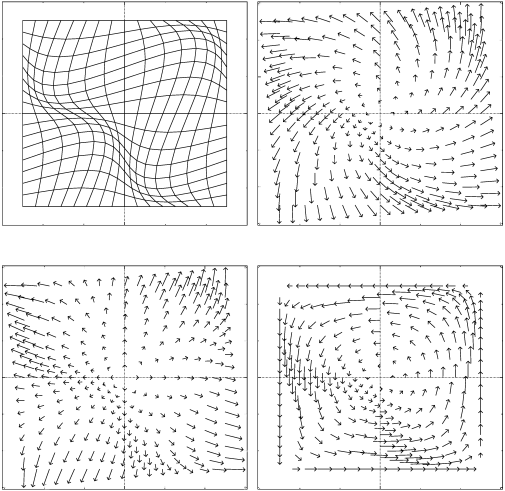


Theorem

Let domain Ω and mesh Ω_h be simply-connected. Then, for any $\mathbf{u}_h \in \mathcal{F}_h$ there exists a unique $p_h \in \mathcal{C}_h$ and a unique $\mathbf{v}_h \in \mathcal{E}_h$ with $\widetilde{\mathrm{div}}_h \, \mathbf{v}_h = 0$ such that

$$\mathbf{u}_h = \widetilde{\nabla}_h \, p_h + \mathrm{curl}_h \, \mathbf{v}_h$$

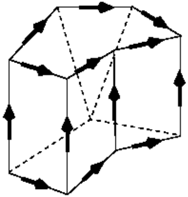
Helmholtz decomposition theorems (2/3)



mesh and $\mathbf{u}_h$

Fields $\widetilde{\nabla}_h\, p_h$ **and** $\mathrm{curl}_h\, \mathbf{v}_h$

Helmholtz decomposition theorems (3/3)

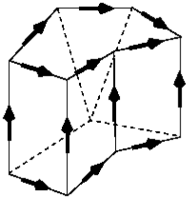


Theorem

Let domain Ω and mesh Ω_h be simply-connected. Then, for any $\mathbf{u}_h \in \mathcal{E}_h$ there exist a discrete field $p_h \in \mathcal{N}_h$, which is defined up to a constant field, and a unique discrete field $\mathbf{u}_h \in \mathcal{F}_h$ with $\operatorname{div}_h \mathbf{v}_h = 0$ such that

$$\mathbf{u}_h = \nabla_h \, p_h + \widetilde{\operatorname{curl}}_h \, \mathbf{v}_h.$$

Mimetic inner product in $\mathcal{E}_h$ (1/2)



$$\left[\mathbf{v}_h,\, \mathbf{u}_h\right]_{c,\mathcal{E}_h} = \int_c \mathbf{v}^0 \cdot \mathbf{u}^1 \, \mathrm{d}x,$$

where v^0 is a constant vector function and and $\mathbf{u}^1 = \mathcal{L}(\mathbf{u}_{c,h})$ is a lifted function such that

- **Interpolation returns back our dofs, i.e. $\mathbf{u}^1 \cdot \boldsymbol{\tau}_{e_i} = u_{e_i}$.**
- **The lifted space contains constant vector functions.**
- **Curl of u^1 is bounded and its trace is constant on each face f.**

We need only existence result for such an approximation.

Mimetic inner product in $\mathcal{E}_h$ (2/2)

Any constant vector function $\mathbf{v}^0$ can be written as

$$\mathbf{v}^0 = \frac{1}{2}\,\mathbf{curl}(\mathbf{v}^0 \times (\mathbf{x} - \mathbf{x}_c))$$

Then,

$$\left(v^0_{e_1}, \ldots, v^0_{e_{17}}\right) \mathbb{M}_c^{\mathcal{E}} \begin{pmatrix} u_{e_1} \\ \vdots \\ u_{e_{12}} \end{pmatrix} = \int_c \mathbf{v}^0 \cdot \mathbf{u}^1 \,\mathrm{d}x$$

$$= \left(R_{e_1}, \ldots, R_{e_{17}}\right) \begin{pmatrix} u_{e_1} \\ \vdots \\ u_{e_{17}} \end{pmatrix} + \underbrace{hO(|P|)}_{\textbf{drop out}}$$

where R_{e_i} depends on cell geometry and $\mathbf{v}^0$. Result is the mimetic matrix equation $\mathbb{M}_c^{\mathcal{E}} = \mathbb{N}_c = \mathbb{R}_c$.

Conclusion for Part II

- **We established connection of the MFD method with a few other methods.**
- **Essential difference with other compatible discretization methods is the constructive approach to building inner products. Material properties are embedded there.**
- **MFD is a family of schemes may contain a monotone sub-family. Simplex method is efficient tool to find it.**
- **Rigorous convergence theory does exists (2013 JCP review paper with 200+ references, book).**