Mimetic Finite Difference Method for Nonlinear Parabolic Equations: Applications and Theory

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Outline

1. **Application driven requirements**
2. **Deficiency of conventional conservative schemes**
3. **Known solutions and their limitations**
4. **Mimetic finite difference method**
5. **Convergence analysis**
6. **Verification**

Nonlinear heat conduction

$$\frac{\partial(c_v\, u)}{\partial t} - \operatorname{div}\big(k(u)\nabla u\big) = b$$

where

u - **temperature**

c_v - **heat capacity**

$k(u)$ - **thermal conductivity**

Subsurface flow: Richards's equation

$$\frac{\partial(\phi\, s\, \eta)}{\partial t} - \mathrm{div}\Big(\frac{\eta\, k_r(p)}{\mu}\mathbb{K}(\nabla p - \rho \mathbf{g})\Big) = b$$

where

ϕ - **porosity**

η - **molar density of water**

ρ - **density of water**

μ - **viscosity of water**

$s = s(p)$ - **saturation**

$\mathbb{K}$ - **absolute permeability**

$k_r(p)$ - **relative permeability**

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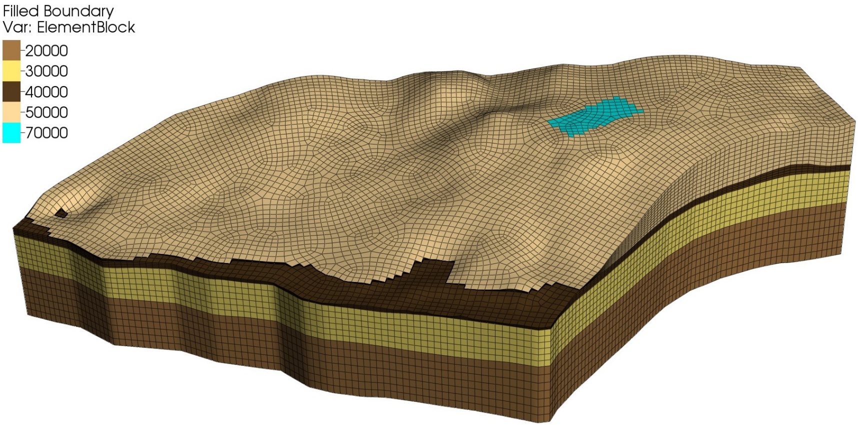
In terms of the hydraulic head $u = p/(\rho g) - z$**, we have**

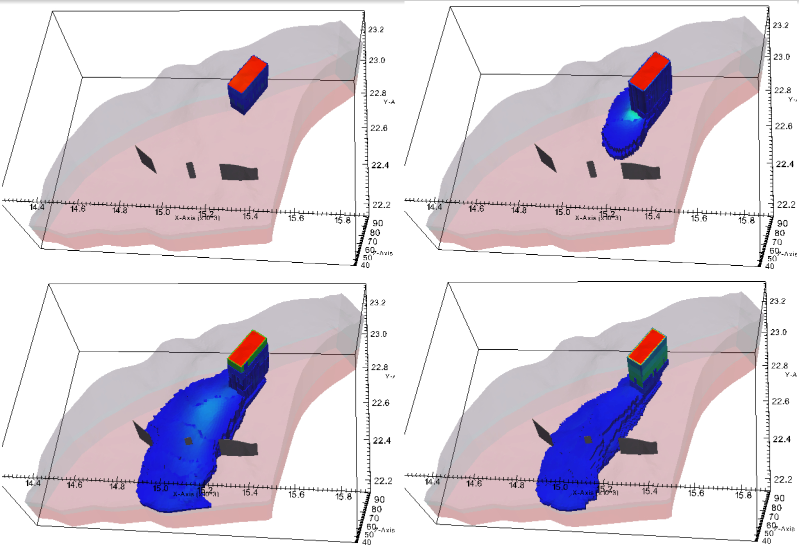
$$\frac{\partial\theta(u)}{\partial t} - \mathrm{div}\big(k(u)\nabla u\big) = b$$

Richards' equation: comments (1/2)



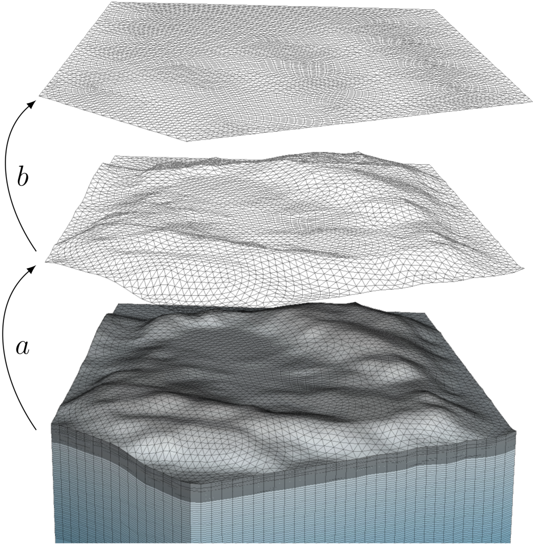
- **(coarse) polytopal meshes**
- **complex topography and stratigraphy**
- **heterogeneous coefficients**

Richards' equation: comments (2/2)



- **water conservation**
- **uncertainty quantification**

Surface flow (1/2)



Mesh is made by Rao Garimella from LANL.

Surface flow (2/2)

$$\frac{\partial(\eta\, h)}{\partial t} - \mathrm{div}\left(\eta\, \frac{h^{5/2}}{n_{mann}\sqrt{\|\nabla z_s\| + \epsilon}}\nabla(h + z_s)\right) = b$$

where

- h - **depth of ponded water(could be 0)**
- η - **molar density of water**
- z_s - **surface elevation**
- ϵ - **small regularization parameter**

Surface flow (2/2)

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where

- h - **depth of ponded water(could be 0)**
- η - **molar density of water**
- z_s - **surface elevation**
- ϵ - **small regularization parameter**

With this change of variables, $u = h + z_s$**, we have**

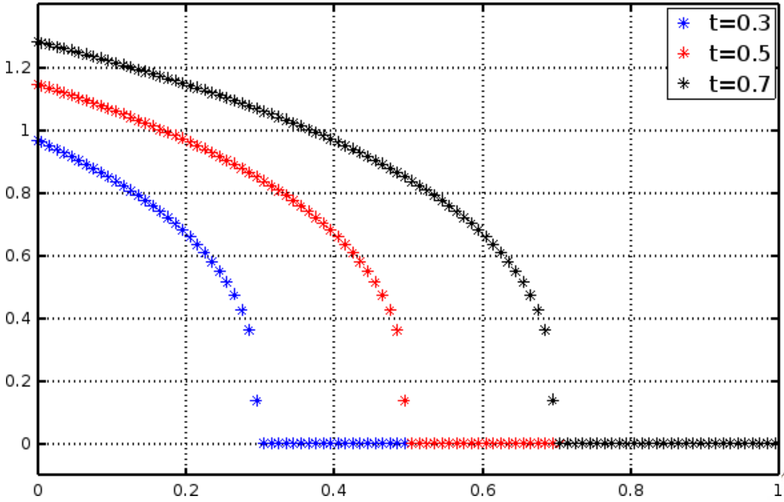
$$\frac{\partial\theta(u)}{\partial t} - \mathrm{div}(k(u)\nabla u) = b$$

Scheme requirements

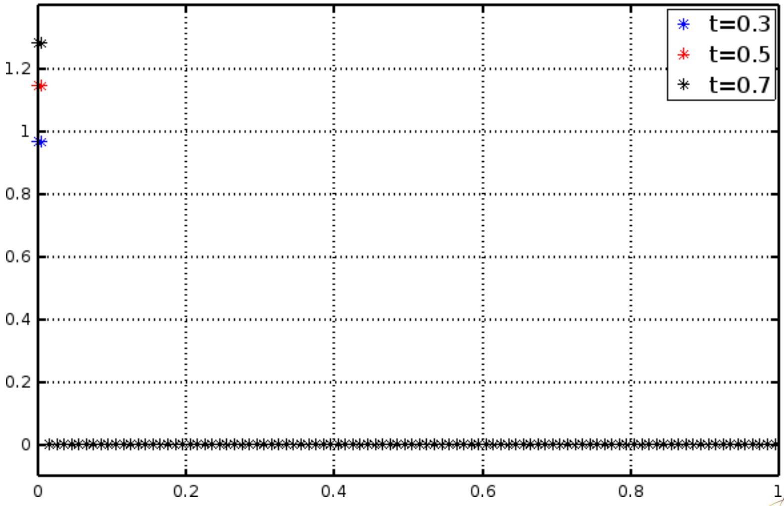
- **be conservative**
- **provide meaningful solution on coarse meshes**
- **be convergent on polytopal meshes**
- **handle degenerate and strongly varying coefficients**
- **lead to SPD matrix (stability and numerical efficiency)**

Numerical artifact (1/4)

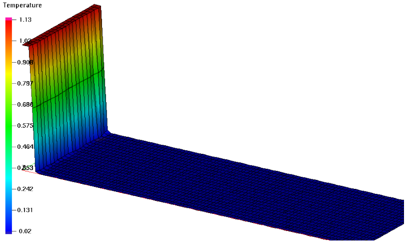
Consider 1D heat equation with $k(u) = u^3$ **and** $\theta(u) = u$**.**
Initial condition: $u(x,0) = 10^{-3}$
Boundary conditions: $u(0,t) = 1.4\sqrt[3]{t}$ **and** $u(1,t) = 10^{-3}$

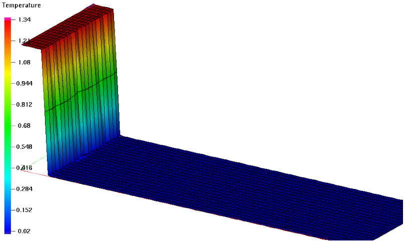


The classical conservative FV scheme underestimates extremely wave velocity:



The heat-barrier problem affects conventional conservative schemes (MFE, HFV, MFV, MFD) and schemes with similar properties:

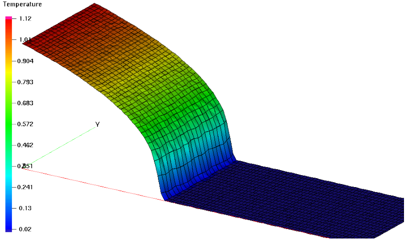


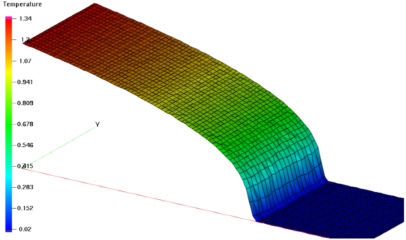


The problem remains after increasing the initial temperature to $u(x,0) = 0.02$, although wave speed has increased slightly.

Numerical artifacts (4/4)

Snapshots of the correct solution at the same time moments:



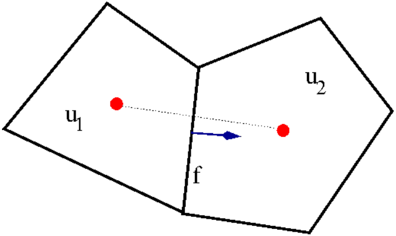


Consider the TPFA of the velocity $\mathrm{q} = -k(u)\nabla u$ on the interface between two cells:

$$q_f = -T_{12}\,(u_2 - u_1)$$

where

$$T_{12} = \frac{k_1\,k_2}{k_1\,d_{2f} + k_2\,d_{1f}}.$$



Thus, if $u_2 \ll u_1$, then $k_2 \ll k_1$ and

$$T_{12} \approx \frac{k_2}{d_{2f}}.$$

If $u_2 \approx 0$, the flux is almost zero and solution is incorrect even on a reasonably fine mesh.

Known solutions and their limitations (1/3)

- **Refine mesh around the moving front. This strategy should work for Richards's equation but should breaks down for other physical models that allow $k(u) = 0$ such as in the surface flow model. Cons:**
  - **strong mesh refinement may be needed**
  - **AMR data structure**

Known solutions and their limitations (2/3)

- **Two-velocity formulation (enhanced MFE (Arbogast, Dawson, Keenan, Wheeler, Yotov; SINUM, 1998)).**

$$
\begin{aligned}
\mathbf{v} &= -\nabla u, \\
\mathbf{q} &= k(u)\,\mathbf{v} \\
\frac{\partial \theta(u)}{\partial t} + \operatorname{div} \mathbf{q} &= b
\end{aligned}
$$

Known solutions and their limitations (3/3)

$$\begin{aligned} \mathbf{v}_h &= -\mathbb{M}_1^{-1}(\mathrm{div}_h)^T \mathbb{M}_2\, u_h \\ \mathbb{M}_3 \mathbf{q}_h &= \mathbb{M}_4\, \mathbf{v}_h \\ \frac{\partial \theta_h}{\partial t} + \mathrm{div}_h\, \mathbf{q}_h &= Q_h \end{aligned}$$

Eliminating velocities and multiplying by $\mathbb{M}_2$, we obtain

$$\mathbb{M}_2\, \frac{\partial \theta_h}{\partial t} + \mathbb{M}_2\, \mathrm{div}_h \underbrace{\mathbb{M}_3^{-1}\, \mathbb{M}_4\, \mathbb{M}_1^{-1}}_{symmetric\ ?} (\mathrm{div}_h)^T \mathbb{M}_2\, u_h = \mathbb{M}_2\, b_h$$

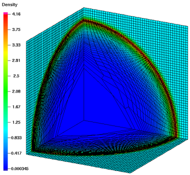
- $\mathbb{M}_3 = \mathbb{M}_1$. **Not clear how to enforce $q_f = k_f v_f$ on each mesh face f.**
- $\mathbb{M}_3 = \mathbb{I}$ **and** $\mathbb{M}_4 = \mathbb{D}_4$. **But $\mathbb{D}_4 \mathbb{M}_1^{-1}$ is not symmetric which leads to potential problems with multigrid solvers.**

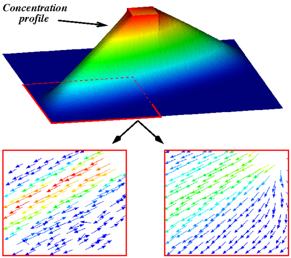
Objective of mimetic schemes

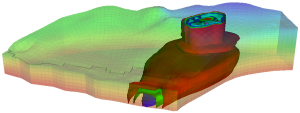
The mimetic finite difference method preserves or mimics critical mathematical and physical properties of systems of PDEs such as conservation laws, exact identities, solution symmetries, and maximum principles.

These properties are important for multiphysics simulations.

The mimetic schemes are designed to work on unstructured polygonal and polyhedral meshes.







New mimetic scheme for a linear problem

To resolve the heat-barrier problem, we first develop a new mimetic scheme for the Poisson equation written in the following mixed form:

$$\begin{aligned} \mathbf{q} &= -\nabla u \\ \mathrm{div}\,(k\,\mathbf{q}) &= b \end{aligned}$$

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

We will derive its mimetic discretization as

$$\begin{aligned} \mathbf{q}_h &= -\widetilde{\mathrm{GRAD}}\,u_h \\ \mathrm{DIV}^k\,\mathbf{q}_h &= b_h \end{aligned}$$

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DIV^k **approximates the combined operator** $\mathrm{div}\, k(.)$**.**
$\widetilde{\mathrm{GRAD}}$ **approximates the continuum operator** ∇**.**

Four-step discretization algorithm

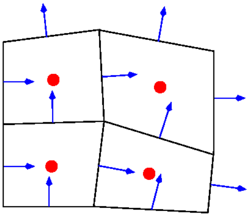
1. **Select degrees of freedom (for q and u).**
2. **Discretize the primary mimetic operator (DIV^k).**
3. **Construct local inner products that satisfy consistency and stability conditions. Assemble global inner products.**
4. **Formulate the discrete duality principle:**

$$\left[\mathrm{DIV}^k \mathbf{q}_h,\, u_h\right]_{\mathcal{C}_h} = -\left[\mathbf{q}_h,\, \widetilde{\mathrm{GRAD}}\, u_h\right]_{\mathcal{F}_h}$$

that mimics the continuum Green formula:

$$\int_\Omega \mathrm{div}(k\,\mathbf{q})\, u\,\mathrm{d}x = -\int_\Omega k\,\mathbf{q}\cdot\nabla u\,\mathrm{d}x$$

Step 1: Select degrees of freedom



Dofs for the velocity q are associated with mesh faces and represent average fluxes. Dofs for the potential u are associated with mesh cells and represent average values:

$$q_f^c \approx \frac{1}{|f|}\int_f \mathbf{q}\cdot\mathbf{n}_f \,\mathrm{d}x, \qquad u_c \approx \frac{1}{|c|}\int_c u \,\mathrm{d}x.$$

Define $\tilde{k}_f$ as some approximation of k on face f. Define spaces

$$\mathbf{q}_h = \begin{pmatrix} q_{f_1} \\ q_{f_2} \\ \vdots \\ q_{f_n} \end{pmatrix} \in \mathcal{F}_h, \qquad u_h = \begin{pmatrix} u_{c_1} \\ u_{c_2} \\ \vdots \\ u_{c_m} \end{pmatrix} \in \mathcal{C}_h,$$

Step 2: Discretize the primary mimetic operator

We use a coordinate-invariant definition of the divergence:

$$\int_c \operatorname{div}(k\mathbf{q})\,\mathrm{d}x = \int_{\partial c} k\mathbf{q}\cdot\mathbf{n}\,\mathrm{d}x = \sum_{f\in\partial c}\int_f k\,\mathbf{q}\cdot\mathbf{n}_f\,\mathrm{d}x$$

Replacing integrals by mid-point quadratures, we have

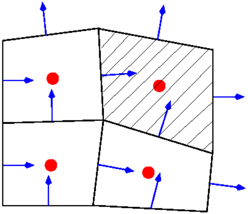
$$(\mathrm{DIV}^k\,\mathbf{q}_h)_{|c} = \frac{1}{|c|}\sum_{f\in\partial c}\alpha_{c,f}\,|f|\,\tilde{k}_f q_f$$

where $\alpha_{f,c} = \pm 1$**.**

Step 3: Construct local inner products

We need accurate approximations of cell-based integrals:

$$\left[v_h,\, u_h\right]_{c,\mathcal{C}_h} \approx \int_c v\, u\, \mathrm{d}x \qquad \left[\mathbf{w}_h,\, \mathbf{q}_h\right]_{c,\mathcal{F}_h} \approx \int_c k\, \mathbf{w}\cdot\mathbf{q}\, \mathrm{d}x$$



Inner products can be re-written as vector-matrix-vector products with SPD matrices:

$$\left[v_h,\, u_h\right]_{c,\mathcal{C}_h} = v_c\, \mathbb{M}_{c,\mathcal{C}_h}\, u_c$$

$$\left[\mathbf{w}_h,\, \mathbf{q}_h\right]_{c,\mathcal{F}_h} = \left(w^c_{f_1}, \ldots, w^c_{f_4}\right) \mathbb{M}_{c,\mathcal{F}_h} \begin{pmatrix} q_{f_1} \\ \vdots \\ q_{f_4} \end{pmatrix}$$

In this example, $\mathbb{M}_{c,\mathcal{C}_h}$ **is** 1×1 **matrix and** $\mathbb{M}_{c,\mathcal{F}_h}$ **is** 4×4 **matrix. Obvious choice is** $\mathbb{M}_{c,\mathcal{C}_h} = |c|$**.**

Step 4: Formulate the discrete duality principle

$$\big[\underbrace{\mathrm{DIV}^k\,\mathbf{q}_h}_{v_h},\, u_h\big]_{\mathcal{C}_h} = -\big[\mathbf{q}_h,\, \underbrace{\widetilde{\mathrm{GRAD}}\,u_h}_{\mathbf{w}_h}\big]_{\mathcal{F}_h} \quad \forall \mathbf{q}_h, \forall u_h$$

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

$$\begin{aligned}\big[v_h,\, u_h\big]_{\mathcal{C}_h} &= v_h^T\,\mathbb{M}_{\mathcal{C}_h}\,u_h \\ \big[\mathbf{w}_h,\, \mathbf{q}_h\big]_{\mathcal{F}_h} &= \mathbf{w}_h^T\,\mathbb{M}_{\mathcal{F}_h}\,\mathbf{q}_h\end{aligned}$$

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

Derived gradient operator

$$\widetilde{\mathrm{GRAD}} = -\mathbb{M}_{\mathcal{F}_h}^{-1}\,(\mathrm{DIV}^k)^T\,\mathbb{M}_{\mathcal{C}_h}$$

Final mimetic scheme

The algebraic form of the MFD scheme is

$$\begin{aligned} \mathbf{q}_h &= -\widetilde{\mathrm{GRAD}}\, u_h = \mathbb{M}_{\mathcal{F}_h}^{-1} (\mathrm{DIV}^k)^T \mathbb{M}_{\mathcal{C}_h}\, u_h \\ \mathrm{DIV}^k\, \mathbf{q}_h &= b_h \end{aligned}$$

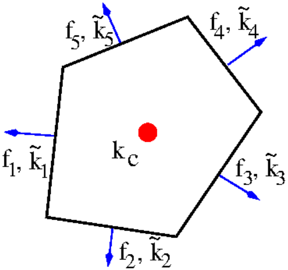
or in a symmetrized form:

$$\begin{pmatrix} \mathbb{M}_{\mathcal{F}_h} & -(\mathrm{DIV}^k)^T \mathbb{M}_{\mathcal{C}_h} \\ -\mathbb{M}_{\mathcal{C}_h} \mathrm{DIV}^k & 0 \end{pmatrix} \begin{pmatrix} \mathbf{q}_h \\ u_h \end{pmatrix} = \begin{pmatrix} 0 \\ -\mathbb{M}_{\mathcal{C}_h}\, b_h \end{pmatrix}$$

Consistency condition (1/4)

$$[\mathbf{w}_h,\, \mathbf{q}_h]_{c,\mathcal{F}_h} = (\mathbf{w}_h)^T \mathbb{M}_{c,\mathcal{F}_h} \mathbf{q}_h \approx \int_c k\, \mathbf{w} \cdot \mathbf{q}\, \mathrm{d}x$$

Derivation of the inner product matrix $\mathbb{M}_{c,\mathcal{F}_h}$ is based on the consistency and stability conditions. Consider a pentagonal cell for example:



Consistency condition (2/4)

The lowest-order scheme requires 1st-order approximation:

$$[\mathbf{w}_h,\, \mathbf{q}_h]_{c,\mathcal{F}_h} = \int_c k\, \mathbf{w} \cdot \mathbf{q}\, \mathrm{d}x + O(h)|c|$$

1. **Replace** w **with its best constant approximation** w^0
2. **Approximate** k **by a function** $k_c^1 \in P^1(c)$
3. **Restrict** q **to space** $\mathcal{S}_c$ **which contains constant functions:**

$$\mathcal{S}_c = \left\{\mathbf{q} :\ \mathbf{q} \cdot \mathbf{n}_f \in P^0(f),\ \mathrm{div}(k_c^1\, \mathbf{q}) \in P^0(c)\right\}$$

The consistency condition is

$$[\mathbf{w}_h^0,\, \mathbf{q}_h]_{c,\mathcal{F}_h} = \int_c k_c^1\, \mathbf{w}^0 \cdot \mathbf{q}\, \mathrm{d}x \qquad \forall \mathbf{w}^0 \in P^0(c),\ \forall \mathbf{q} \in \mathcal{S}_c.$$

For any w^0 there exists a linear polynomial v^1 such that

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

Using twice properties of space $\mathcal{S}_c$, we have:

$$[\mathbf{w}_h^0,\, \mathbf{q}_h]_{c,\mathcal{F}_h} = (\mathbf{w}_h^0)^T \mathbb{M}_{c,\mathcal{F}_h}\, \mathbf{q}_h = \int_c k_c^1\, \mathbf{w}^0 \cdot \mathbf{q}\, \mathrm{d}x$$

$$= -\int_c v^1 \underbrace{\mathrm{div}(k_c^1\, \mathbf{q})}_{=constant} \mathrm{d}x + \int_{\partial c} k_c^1\, v^1\, \mathbf{q}\cdot\mathbf{n}\, \mathrm{d}x = \sum_{i=1}^{5} \int_{f_i} k_c^1\, v^1\, \underbrace{\mathbf{q}\cdot\mathbf{n}_{f_i}}_{=constant}\, \mathrm{d}x$$

$$= \Big(\int_{f_1} k_c^1\, v^1\, \mathrm{d}x, \ldots, \int_{f_5} k_c^1\, v^1\, \mathrm{d}x \Big) \mathbf{q}_h \qquad \forall \mathbf{q} \in \mathcal{S}_c$$

Since q_h is arbitrary, we conclude $(\mathbf{w}_h^0)^T \mathbb{M}_{c,\mathcal{F}_h} = (\mathbf{r}_c)^T$.

Consistency condition (4/4)

Algebraic equations w.r.t. unknown matrix $\mathbb{M}_{c,\mathcal{F}_h}$:

$$\mathbb{M}_{c,\mathcal{F}_h} \begin{pmatrix} w^0_{f_1} \\ \vdots \\ w^0_{f_5} \end{pmatrix} = \begin{pmatrix} \displaystyle\int_{f_1} k^1_c \, v^1 \, \mathrm{d}x \\ \vdots \\ \displaystyle\int_{f_5} k^1_c \, v^1 \, \mathrm{d}x \end{pmatrix} \qquad \forall \mathbf{w}^0 = \nabla v^1.$$

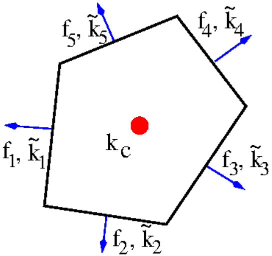
It is sufficient to consider only linearly independent functions v^1. In two-dimensions, we have $v^1_a = x - x_c$ and $v^1_b = y - y_c$:

Mimetic matrix equation

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

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

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

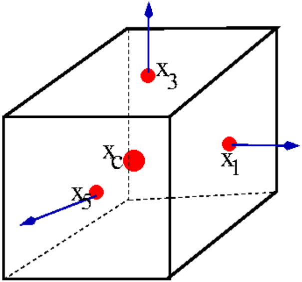


$$\mathbb{M}_{c,\mathcal{F}_h}\,\mathbb{N}_c = \mathbb{R}_c$$

Required information: normals to faces, centroid of cell, quadrature rule on faces:

$$\mathbb{N}_c = \begin{bmatrix} n_{1x} & n_{1y} \\ n_{2x} & n_{2y} \\ \vdots & \vdots \\ n_{5x} & n_{5y} \end{bmatrix} \qquad \mathbb{R}_c = \begin{bmatrix} \int_{f_1} k_c^1(x - x_c) & \int_{f_1} k_c^1(y - y_c) \\ \int_{f_2} k_c^1(x - x_c) & \int_{f_2} k_c^1(y - y_c) \\ \vdots & \vdots \\ \int_{f_5} k_c^1(x - x_c) & \int_{f_5} k_c^1(y - y_c) \end{bmatrix}$$

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



$$\mathbb{M}_{c,\mathcal{F}_h}\,\mathbb{N}_c = \mathbb{R}_c$$

Required information: normals to faces, centroid of cell, quadrature rule on faces:

$$\mathbb{N}_c = \begin{bmatrix} n_{1x} & n_{1y} & n_{1z} \\ n_{2x} & n_{2y} & n_{2z} \\ \vdots & \vdots & \vdots \\ n_{6x} & n_{6y} & n_{6z} \end{bmatrix} \qquad \mathbb{R}_c = \begin{bmatrix} \int_{f1} k_c^1(x-x_c) & \int_{f1} k_c^1(y-y_c) & \int_{f1} k_c^1(z-z_c) \\ \int_{f2} k_c^1(x-x_c) & \int_{f2} k_c^1(y-y_c) & \int_{f2} k_c^1(z-z_c) \\ \vdots & \vdots & \vdots \\ \int_{f6} k_c^1(x-x_c) & \int_{f6} k_c^1(y-y_c) & \int_{f6} k_c^1(z-z_c) \end{bmatrix}$$

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

Lemma

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

$$\mathbb{N}_c^T \, \mathbb{R}_c = \mathbb{R}_c^T \, \mathbb{N}_c = \mathbb{I} \int_c k_c^1 \, \mathrm{d}x$$

K.L., G.Manzini, D.Moulton, M.Shashkov, JCP, 305 (2016), 111-126

Solution of the mimetic matrix equation

Lemma

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

$$\mathbb{M}_{c,\mathcal{F}_h} = \mathbb{M}_{c,\mathcal{F}_h}^{consistency} + \mathbb{M}_{c,\mathcal{F}_h}^{stability}$$

where

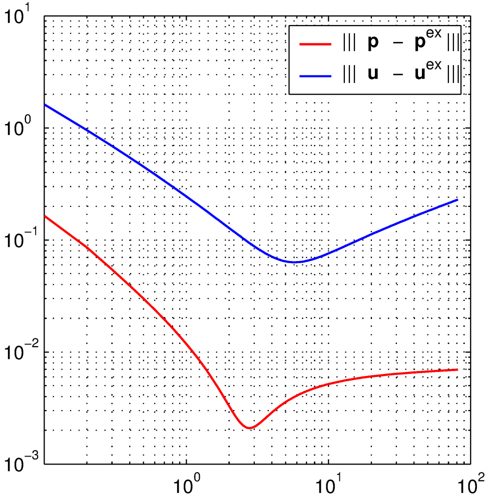
$$\mathbb{M}_{c,\mathcal{F}_h}^{consistency} = \mathbb{R}_c\,(\mathbb{R}_c^T\,\mathbb{N}_c)^{-1}\mathbb{R}_c^T$$

and

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

Stability condition (1/2)

Typical behavior of errors and function of the normalize parameter a_c/a_c^* where $a_c^* = \dfrac{1}{d}\displaystyle\int_c k^1 \, \mathrm{d}x$.



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

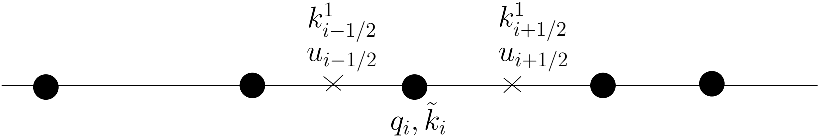
A reasonable choice for a_c leads to a more accurate mimetic scheme. Its value is controlled by the following inequalities:

$$\sigma_\star |c| \, \|\mathbf{q}_h\|^2 \leq \left[\mathbf{q}_h, \, \mathbf{q}_h\right]_{c,\mathcal{F}_h} \leq \sigma^\star |c| \, \|\mathbf{q}_h\|^2$$

where $\sigma_\star$ and $\sigma^\star$ are independent of mesh.

In practice, a good scaling is given by

$$a_c = a_c^* = \frac{1}{d} \int_c k^1 \; \mathrm{d}x.$$

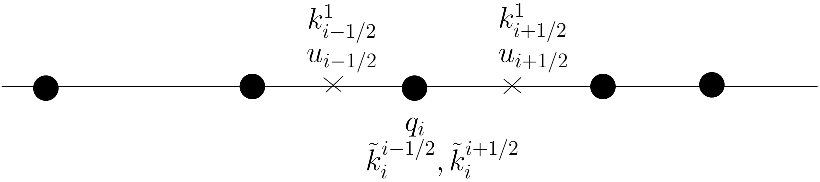


Flux formula is

$$\tilde{k}_i q_i = \frac{2\tilde{k}_i^2}{h_{i-1/2}k^1_{i-1/2} + h_{i+1/2}k^1_{i+1/2}} \left(u_{i-1/2} - u_{i+1/2}\right)$$

- **conventional FV scheme:** $\tilde{k}_i = \sqrt{k_i^H \, k_i^A}$
- **scheme with the arithmetic averaging:** $\tilde{k}_i = k_i^A$
- **"upwinded" scheme:** $\tilde{k}_i = k^1_{i-1/2}\, q_i^+ + k^1_{i+1/2}\, q_i^-$

The case of discontinuous coefficient k



New flux continuity conditions:

$$\tilde{k}_i^{i-1/2} q_i^{i-1/2} = \tilde{k}_i^{i+1/2} q_i^{i+1/2}$$

Flux formula is

$$\frac{2\big(\tilde{k}_i^{i-1/2}\,\tilde{k}_i^{i+1/2}\big)^2}{h_{i-1/2}\,k^1_{i-1/2}\big(\tilde{k}_i^{i+1/2}\big)^2 + h_{i+1/2}\,k^1_{i+1/2}\big(\tilde{k}_i^{i-1/2}\big)^2}\,(u_{i-1/2} - u_{i+1/2})$$

Convergence estimate

Theorem

Let

- $k \in W^{1,\infty}(\Omega)$
- $|k_c^1(x) - \tilde{k}_f| \leq Ch \qquad \forall x \in f$
- elliptic problem is H^2-regular

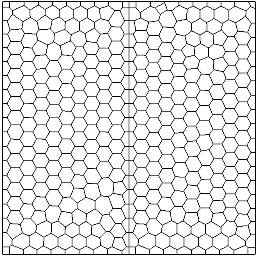
Then, in the mesh-dependent norms induced by the inner products, we have

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

Consider a 2D linear problem with $a_i b_i = 1$:

$$u(x,y) = \begin{cases} a_1 x^2 + y^2 & x < 0.5 \\ a_2 x^2 + y^2 + \frac{1}{4}(a_1 - a_2) & x > 0.5 \end{cases}$$

$$k(x,y) = \begin{cases} b_1(1 + x\sin(y)) & x < 0.5 \\ b_2(1 + 2x^2\sin(y)) & x > 0.5 \end{cases}$$



- **Conventional MFD scheme**
- **New MFD scheme with various choices for k_c^1 and $\tilde{k}_f^c$**

Numerical verification (2/4)

Continuous k **(**$b_1 = b_2 = 1$**)**
Linear approximation k_c^1
Arithmetic average value $\tilde{k}_f$ **on face** f
$\tilde{k}_f^c = \omega_f k_{c_1}^1(x_f) + (1-\omega_f) k_{c_2}^1(x_f)$

# cells	New MFD		Standard MFD	
	$err(u)$	$err(\mathbf{q})$	$err(u)$	$err(\mathbf{q})$
412	2.674e-3	3.001e-3	1.892e-3	4.148e-3
1591	6.554e-4	9.612e-4	4.690e-4	1.248e-3
6433	1.572e-4	4.382e-4	1.135e-4	4.285e-4
25698	3.886e-5	1.289e-4	2.814e-5	1.227e-4
102772	9.693e-6	5.794e-5	6.984e-6	5.814e-5
rate	2.04	1.43	2.03	1.57

Discontinuous k ($b_1 = 1$ and $b_2 = 20$)
Linear approximation k_c^1
$\tilde{k}_f^c = k_c^1(x_f)$

# cells	New MFD		Standard MFD	
	$err(u)$	$err(\mathbf{q})$	$err(u)$	$err(\mathbf{q})$
412	2.480e-3	4.722e-3	2.762e-3	7.451e-3
1591	6.250e-4	1.567e-3	6.976e-4	2.370e-3
6433	1.729e-4	6.273e-4	1.650e-4	9.264e-4
25698	3.684e-5	1.956e-4	4.066e-5	2.581e-4
102772	9.142e-6	8.164e-5	1.007e-5	1.134e-4
rate	2.03	1.48	2.04	1.53

Smooth hexahedral mesh
Discontinuous k ($b_1 = 1$ and $b_2 = 20$)
Constant approximation k_c^1
$\tilde{k}_f^c = k_c^1(x_f)$

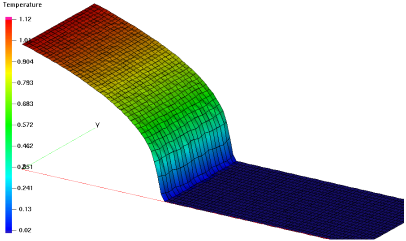
# $1/h$	New MFD		Standard MFD	
	$err(u)$	$err(\mathbf{q})$	$err(u)$	$err(\mathbf{q})$
10	**3.930e-3**	**2.291e-2**	**3.987e-3**	**2.547e-2**
20	**1.081e-3**	**6.751e-3**	**1.088e-3**	**7.618e-3**
40	**2.788e-4**	**1.805e-3**	**2.804e-4**	**2.023e-3**
80	**7.026e-5**	**4.816e-4**	**7.071e-5**	**5.197e-4**
rate	**1.94**	**1.87**	**1.94**	**1.86**

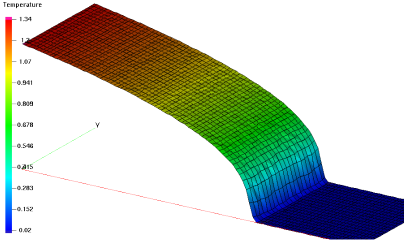
Examples: Marshak wave equation

Consider a nonlinear heat conduction equation:

$$\frac{\partial u}{\partial t} - \mathrm{div}(u^3 \nabla u) = 0.$$

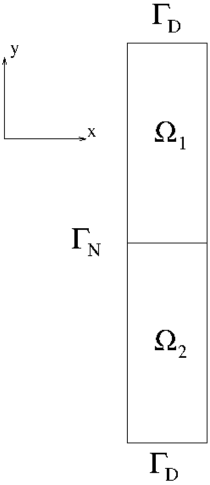
The initial value is $u(0) = 0.02$. Dirichlet BC on the left side is $u = 0.78\sqrt[3]{t}$, on the right side is $u = 0.02$, Neumann BC otherwise.

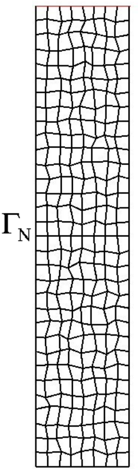


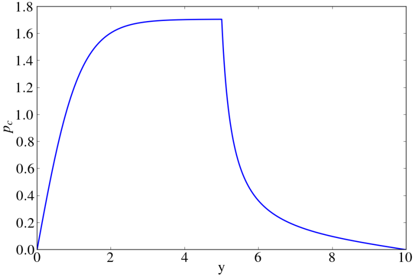


In a new MFD method the heat wave moves from left to right with the correct speed.

Constant approximation k_c^1
"Upwinded" value for $\tilde{k}_f^c$







# cells	New MFD	
	$err(u)$	$err(\mathbf{q})$
250	2.159e-01	1.754e-03
1000	9.893e-02	3.224e-04
4000	4.741e-02	8.353e-05
rate	1.09	2.19

Conclusion

- The new scheme solves the heat barrier problem.
- It preserves symmetry and positive-definiteness of the original operator on unstructured polyhedral meshes.
- First-order convergence estimates were derived for linear elliptic problems.
- On special meshes and for some choice of $\tilde{k}_f$, the new scheme reduces to the classical FV scheme.
- The new scheme can be extended easily to problems with zero diffusion coefficient.