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Mimetic finite difference methods: theory and applications

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Abstract

The talk is about development and analysis of advanced numerical methods that preserve or mimic important properties of underlying PDEs, such as conservation laws, symmetry and positivity of a solution, and fundamental indentities of vector and tensor calculus. This talk will summarize our progress in development and analysis of mimetic finite difference (MFD) methods.

The MFD method lies between finite volume and finite element methods. Like finite volume methods, the MFD method works on arbitrary polygonal, polyhedral and generalized polyhedral meshes. Like finite element methods, it readily handles tensorial coefficients and enforces duality relationships between discrete operators (e.g. divergence and gradient). Combining best of two worlds, the MFD method has a few unique features. For instance, a parametric family of MFD methods is used to enlarge the monotonicity region. The developed convergence analysis is now used by other researchers to prove convergence of finite volume methods such as the multi-point flux approximation (MPFA) methods.

We present a general framework for development of MFD methods for PDEs and illustrate their performance with diffusion, advection-diffusion, Stokes, and magnetostatic problems. The mimetic discretization methods is the core of the M^3 methods, our effort in development of multilevel multiscale methods for efficient simulation of two-phase flows in porous media. Another application of the MFD methodology, that will be mentioned in the talk, is development of artificial viscosity methods for Lagrangian shock calculations.

We also present research results on non-linear monotone finite volume methods that preserves positivity of solutions of advection diffusion equations, and therefore are also mimetic methods. All aforementioned methods are considered for use in the Advanced Simulation Capability for Environmental Management (ASCEM) project.

Some of the mentioned results is the join research with D.Svyatskiy, D.Moulton (LANL), Yu.Vassilevski (INM, RUSSIA), F.Brezzi,A.Buffa,L.Beirao da Veiga, M.Manzini (IMATI, ITALY), and I.Yotov (Univ. of Pittsburgh).

Mimetic Finite Difference (MFD) Methods: Theory and Applications

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- The research was supported by the DOE Office of Science Advanced Scientific Computing Research (ASCR) Program in Applied Mathematics Research.

- It would be very hard to test new discretization methods without the **MSTK library** written by Rao Garimella, T-5, LANL.

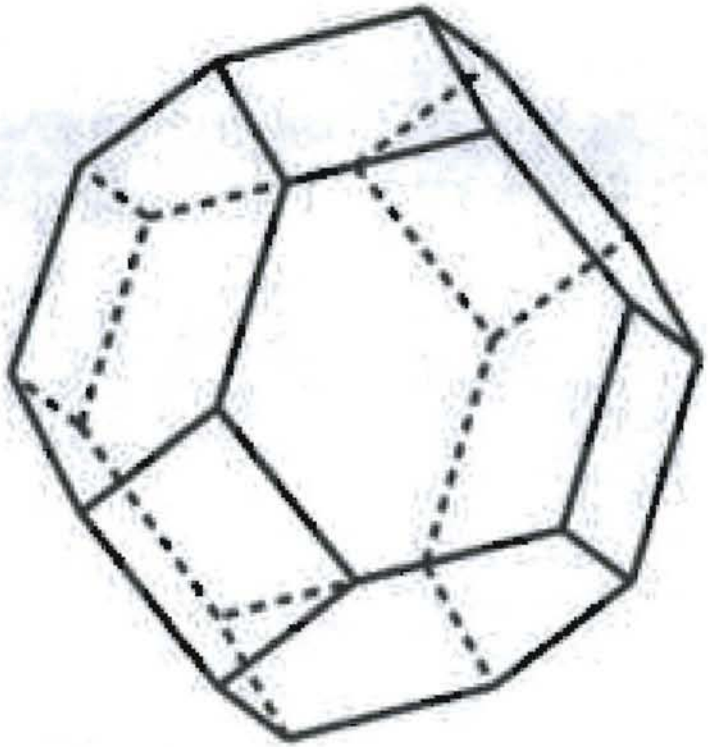
Talk flow

1. Discrete vector and tensor calculus
2. Tools for analysis of MFD methods
3. Applications: diffusion, Stokes, magnetostatics
4. Outreach
5. Alternative approach to the maximum principle
6. Applications: artificial viscosity, flows in porous media
7. Summary and future work

Nature chooses polyhedra

In 1887, Lord Kelvin formulated a conjecture about how the space should be partitioned into cells of equal volume with the least area of surface between them

Kelvin (1887)



tetrakaidecahedron

Weaire-Phelan (1994)

We often mimic the nature

The **Weaire-Phelan structure** is the inspiration for the design of the aquatic center for the 2008 Olympics in Beijing in China.

The design is ideally suited to **absorbing the energy from earthquakes**.

Discrete Vector and Tensor Calculus

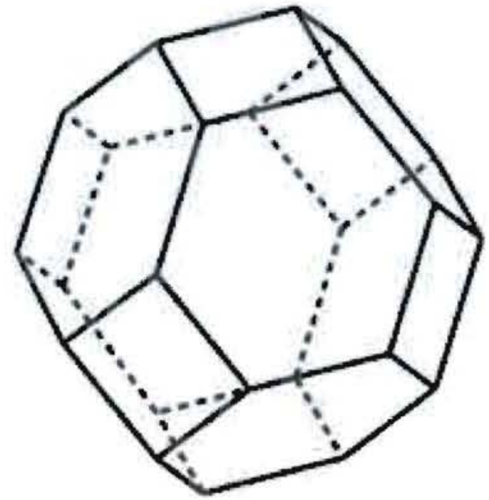
Primary and derived operators

$\mathbf{N}$ — space of node-based functions

$\mathbf{R}$ — space of edge-based functions

$\mathbf{X}$ — space of face-based functions

$\mathbf{Q}$ — space of element-based functions



Primary operators	Derived operators
$\mathcal{DIV}: \mathbf{X} \to \mathbf{Q}$	$\widetilde{\mathcal{GRAD}}: \mathbf{Q} \to \mathbf{X}$
$\mathcal{GRAD}: \mathbf{N} \to \mathbf{R}$	$\widetilde{\mathcal{DIV}}: \mathbf{R} \to \mathbf{N}$
$\mathcal{CURL}: \mathbf{R} \to \mathbf{X}$	$\widetilde{\mathcal{CURL}}: \mathbf{X} \to \mathbf{R}$

Primary operators

Using the divergence theorem, directional derivative, and Stokes's theorem, we define the primary operators:

div $\vec{u}$ $\qquad (\mathcal{DIV}\,\boldsymbol{u})_E = \frac{1}{|E|} \sum_{f \in \partial E} \boldsymbol{u}_f\,|f|$

$\nabla s \cdot \vec{\tau}$ $\qquad (\mathcal{GRAD}\,\boldsymbol{s})_\ell = \frac{\boldsymbol{s}_{v_1} - \boldsymbol{s}_{v_2}}{|\ell|}$

curl $\vec{e}$ $\qquad (\mathcal{CURL}\,\boldsymbol{e})_f = \frac{1}{|f|} \sum_{\ell \in \partial f} \boldsymbol{e}_\ell\,|\ell|$

Derived gradient operator

Let $p = 0$ on the boundary. We start with

$$\int_\Omega \vec{u} \cdot \mathbb{K}^{-1}(\mathbb{K}\nabla p)\,\mathrm{d}x = -\int_\Omega p\,\mathrm{div}\,\vec{u}\,\mathrm{d}x$$

and use approximations

$$\int_\Omega \vec{u} \cdot \mathbb{K}^{-1}\vec{v}\,\mathrm{d}x \approx \boldsymbol{v}^T\,\mathbb{M}_{\boldsymbol{X}}\,\boldsymbol{u}$$

and

$$\int_\Omega p\,q\,\mathrm{d}x \approx \boldsymbol{p}^T\,\mathbb{M}_{\boldsymbol{Q}}\boldsymbol{q}.$$

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Derived gradient operator

The discrete integration by parts formula is

$$\boldsymbol{v}^T \, \mathbb{M}_{\boldsymbol{X}} \, \widetilde{\mathcal{GRAD}} \boldsymbol{p} = -\boldsymbol{p}^T \, \mathbb{M}_{\boldsymbol{Q}} \mathcal{DIV} \boldsymbol{v}.$$

Since $\boldsymbol{p}$ and $\boldsymbol{v}$ are arbitrary, we get

$$\widetilde{\mathcal{GRAD}} = -\mathbb{M}_{\boldsymbol{X}}^{-1} \, \mathcal{DIV}^T \, \mathbb{M}_{\boldsymbol{Q}}.$$

Derived operators

$$\widetilde{\mathcal{GRAD}} = -\mathbb{M}_{\boldsymbol{X}}^{-1}\,\mathcal{DIV}^T\,\mathbb{M}_{\boldsymbol{Q}}$$

$$\widetilde{\mathcal{DIV}} = -\mathbb{M}_{\boldsymbol{N}}^{-1}\,\mathcal{GRAD}^T\,\mathbb{M}_{\boldsymbol{R}}$$

$$\widetilde{\mathcal{CURL}} = \mathbb{M}_{\boldsymbol{R}}^{-1}\,\mathcal{CURL}^T\,\mathbb{M}_{\boldsymbol{X}}$$

Derivation of accurate inner product matrices $\mathbb{M}$ is the heart of mimetic methods

Summary of properties

- $\mathcal{DIV}\boldsymbol{u} = 0$ iff $\boldsymbol{u} = \mathcal{CURL}\boldsymbol{e}$ for some $\boldsymbol{e} \in \boldsymbol{R}$
- $\mathcal{CURL}\boldsymbol{e} = 0$ iff $\boldsymbol{e} = \mathcal{GRAD}\boldsymbol{s}$ for some $\boldsymbol{s} \in \boldsymbol{N}$

- $\widetilde{\mathcal{DIV}}\boldsymbol{e} = 0$ iff $\boldsymbol{e} = \widetilde{\mathcal{CURL}}\boldsymbol{u}$ for some $\boldsymbol{u} \in \boldsymbol{X}$
- $\widetilde{\mathcal{CURL}}\boldsymbol{u} = 0$ iff $\boldsymbol{u} = \widetilde{\mathcal{GRAD}}\boldsymbol{p}$ for a $\boldsymbol{p} \in \boldsymbol{Q}$

- For any $\boldsymbol{u} \in \boldsymbol{X}$ with given values on $\partial\Omega$, we have

$$\boldsymbol{u} = \widetilde{\mathcal{GRAD}}\boldsymbol{p} + \mathcal{CURL}\boldsymbol{e}, \qquad \boldsymbol{p} \in \boldsymbol{Q},\ \boldsymbol{e} \in \boldsymbol{R}$$

- For any $\boldsymbol{e} \in \boldsymbol{R}$ with given values on $\partial\Omega$, we have

$$\boldsymbol{e} = \mathcal{GRAD}\boldsymbol{s} + \widetilde{\mathcal{CURL}}\boldsymbol{u}, \qquad \boldsymbol{s} \in \boldsymbol{N},\ \boldsymbol{u} \in \boldsymbol{X}$$

Tools for Analysis, I

Algebraic consistency conditions

Matrix $\mathbb{M}$ is assembled from elemental matrices $\mathbb{M}_E$. Consider matrix $\mathbb{M}_{\boldsymbol{X},E}$. Let $\boldsymbol{X}_E$ be restriction of $\boldsymbol{X}$ to element E and $\vec{u} = \mathbb{K}_E \nabla p$ correspond to $\boldsymbol{u}_E \in \boldsymbol{X}_E$:

$$\int_E \mathbb{K}_E^{-1}(\mathbb{K}_E \nabla p)\vec{v}\,\mathrm{d}x = -\int_E p\,\mathrm{div}\vec{v}\,\mathrm{d}x + \int_{\partial E} p\,\vec{v}\cdot\boldsymbol{n}\,\mathrm{d}x$$

Its discrete analog is

$$\boldsymbol{u}_E^T \mathbb{M}_{\boldsymbol{X},E}\,\boldsymbol{v}_E = -(\mathcal{DIV}\boldsymbol{v}_E)\int_E p\,\mathrm{d}x + \sum_{f\in\partial E} \boldsymbol{v}_f \int_f p\,\mathrm{d}x$$

Algebraic consistency conditions

$$\boldsymbol{u}_E^T \mathbb{M}_{\boldsymbol{X},E}\, \boldsymbol{v}_E = -(\mathcal{DIV}\boldsymbol{v}_E) \int_E p \,\mathrm{d}x + \sum_{f\in\partial E} \boldsymbol{v}_f \int_f p \,\mathrm{d}x$$

Since $\boldsymbol{v}_E$ is arbitrary, we get

$$\mathbb{M}_{\boldsymbol{X},E}\, \boldsymbol{u}_E = \begin{pmatrix} \displaystyle\int_{f_1} p \,\mathrm{d}x - \frac{|f_1|}{|E|} \int_E p \,\mathrm{d}x \\ \vdots \\ \displaystyle\int_{f_n} p \,\mathrm{d}x - \frac{|f_n|}{|E|} \int_E p \,\mathrm{d}x \end{pmatrix}$$

Algebraic consistency conditions

We search for an SPD matrix $\mathbb{M}_{\boldsymbol{X},E}$ such that the above condition is exact for linear p and corresponding constant $\vec{u} = \mathbb{K}_E \nabla p$. Taking $p = x, y, z$, we get three equations:

$$\mathbb{M}_{\boldsymbol{X},E} \mathbb{N}_\alpha = \mathbb{R}_\alpha, \qquad \alpha = x, y, z.$$

The algebraic consistency condition is

$$\mathbb{M}_{\boldsymbol{X},E} \mathbb{N} = \mathbb{R},$$

where $\mathbb{N} = [\mathbb{N}_x, \mathbb{N}_y, \mathbb{N}_z]$ and $\mathbb{R} = [\mathbb{R}_x, \mathbb{R}_y, \mathbb{R}_z]$. By construction

$$\mathbb{N}^T \mathbb{R} = |E| \, \mathbb{K}_E = \mathbb{R}^T \mathbb{N}.$$

Algebraic consistency conditions

$$\mathbb{M}_{\boldsymbol{X},E}\,\mathbb{N} = \mathbb{R}$$

Solution of this matrix equation requires to calculate the null space of $\mathbb{N}^T$. Let $\mathbb{N}^T\mathbb{D} = 0$. Then

$$\mathbb{M}_{\boldsymbol{X},E} = \mathbb{R}\,(\mathbb{R}^T\mathbb{N})^{-1}\,\mathbb{R}^T + \mathbb{D}\,\mathbb{U}\,\mathbb{D}^T,$$

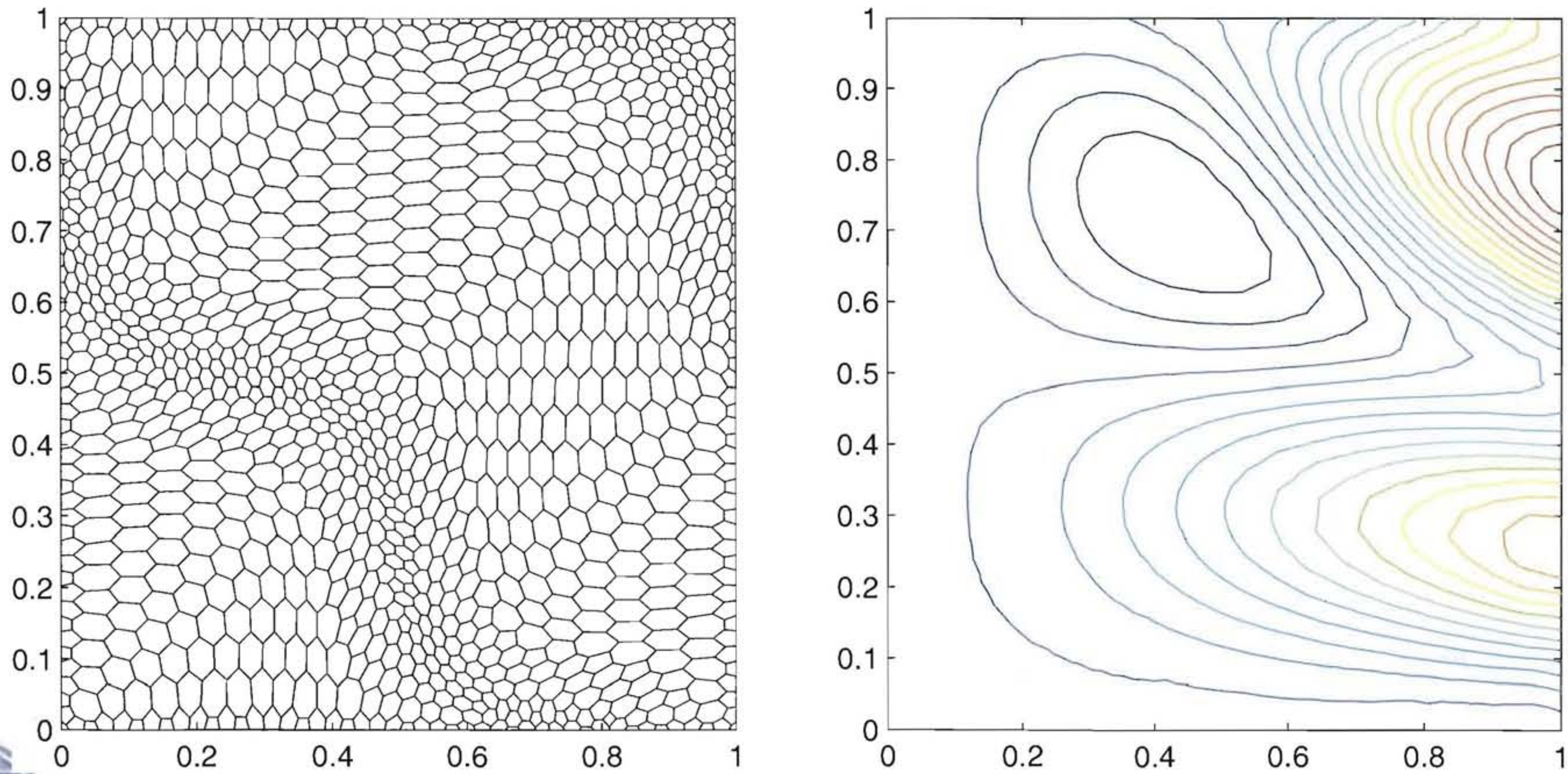
where $\mathbb{U}$ is an arbitrary matrix such that

$$\mathbb{U} = \mathbb{U}^T > 0.$$

The construction works for **non-convex, degenerate** and **generalized** polyhedra.

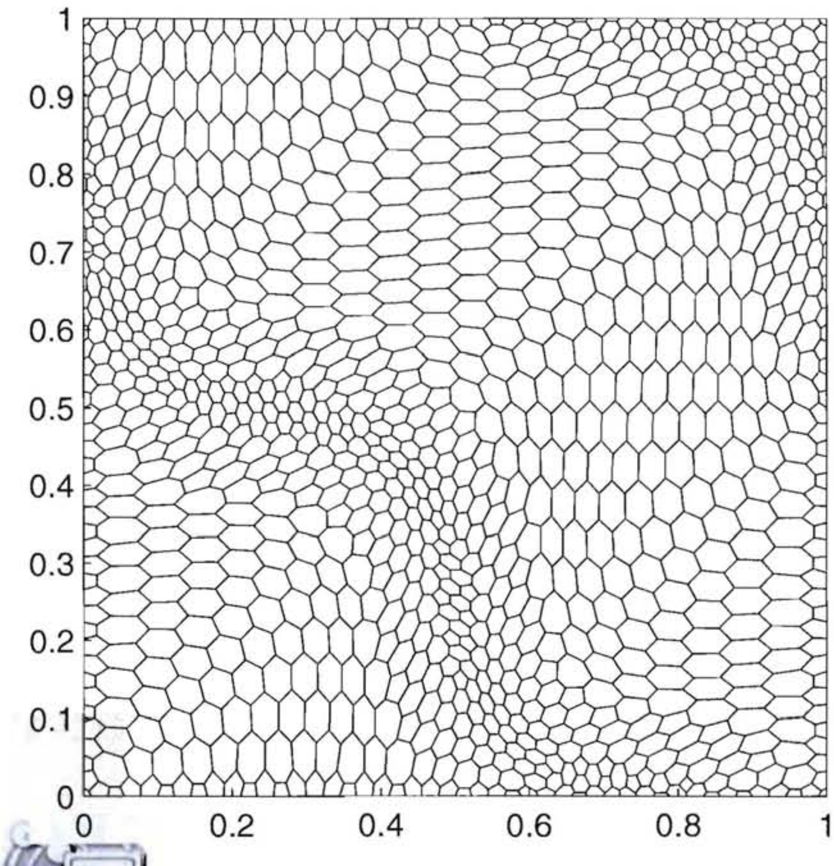
Diffusion: polygonal meshes

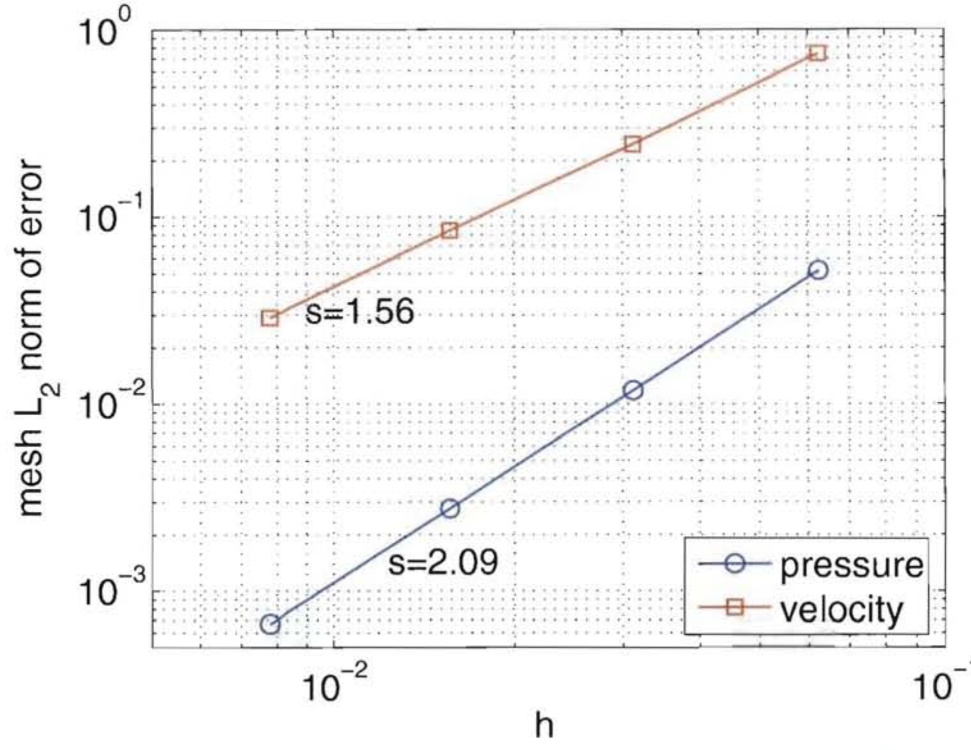
$$p(x,\,y) = x^3y^2 + x\sin(2\pi xy)\sin(2\pi y), \qquad \mathbb{K} = \begin{pmatrix} (x+1)^2 + y^2 & -xy \\ -xy & (x+1)^2 \end{pmatrix}$$



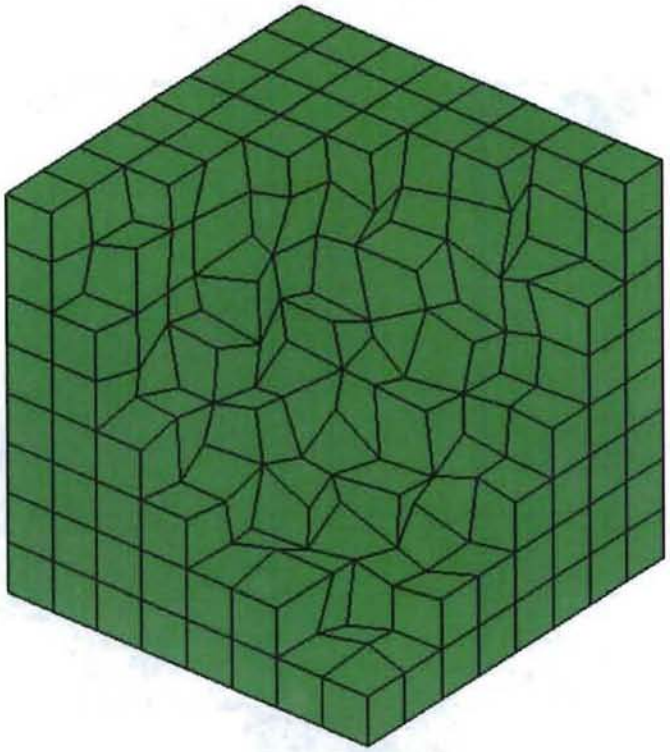
Diffusion: polygonal meshes

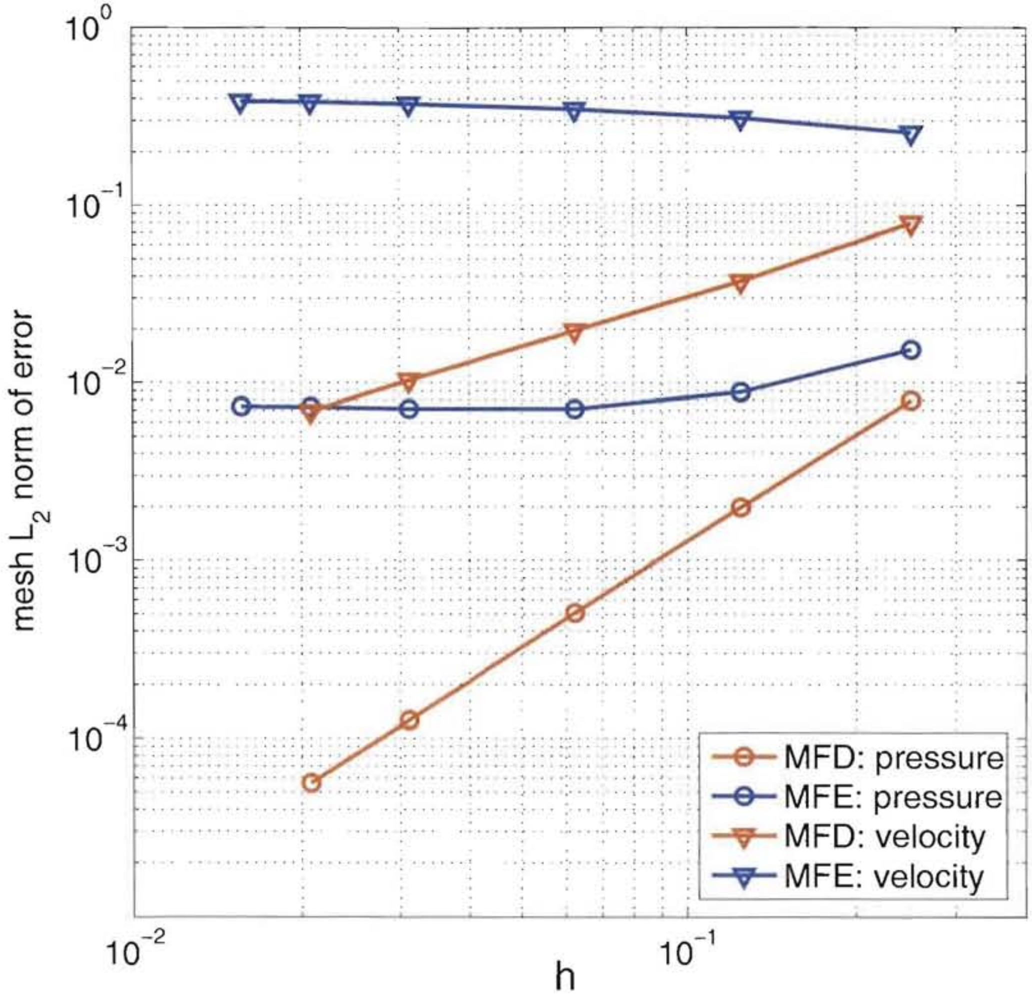
$$p(x,\,y) = x^3y^2 + x\sin(2\pi xy)\sin(2\pi y), \qquad \mathbb{K} = \begin{pmatrix} (x+1)^2 + y^2 & -xy \\ -xy & (x+1)^2 \end{pmatrix}$$





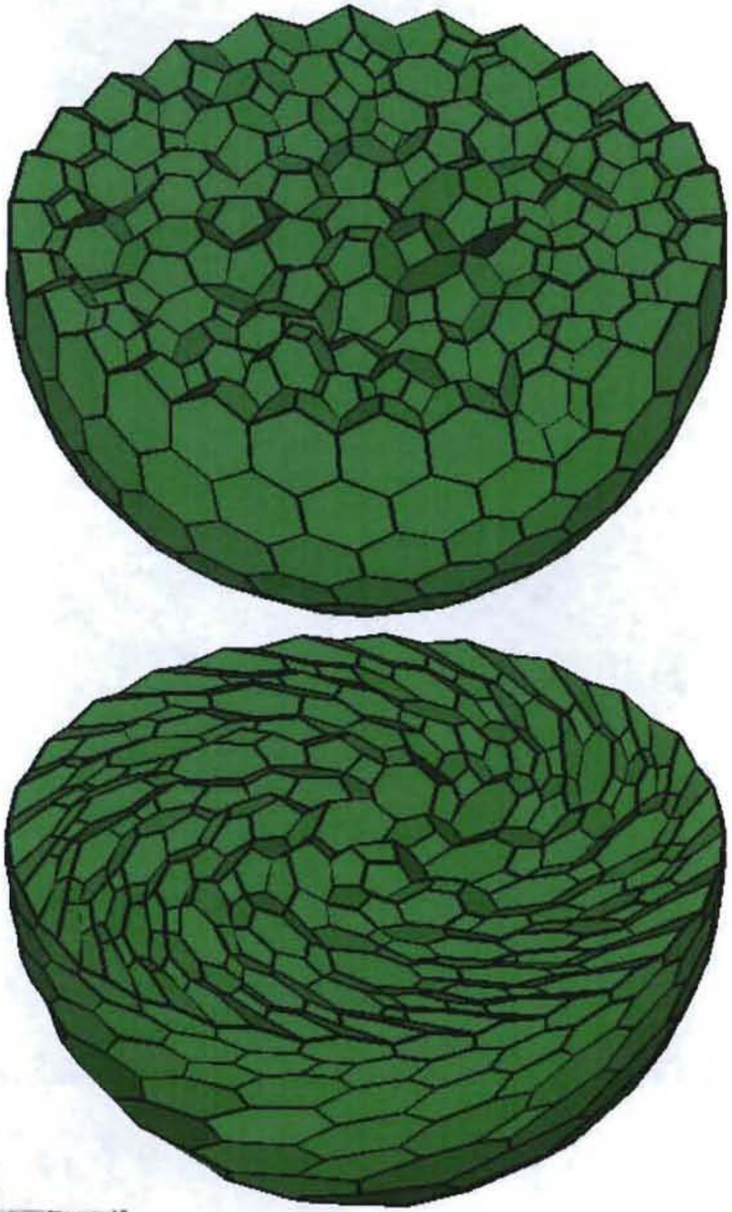
Diffusion: hexahedral meshes





Methods with one velocity unknown per strongly curved mesh face **do NOT converge**

Diffusion: polyhedral meshes



- 663 polyhedrons with up to 23 faces
- numerical results:

feature	top	bottom
CN (min)	1.002	1.009
CN (max)	2.500	115.0
CN (avg)	1.316	2.194
$\|\|\|\boldsymbol{p} - \boldsymbol{p}^h\|\|\|_Q$	8.39e-3	1.76e-2
$\|\|\|\boldsymbol{u} - \boldsymbol{u}^h\|\|\|_X$	9.20e-2	2.20e-1
$\|\|\|\boldsymbol{p} - \boldsymbol{p}^h\|\|\|_\infty$	1.68e-2	2.95e-2
$\|\|\|\boldsymbol{u} - \boldsymbol{u}^h\|\|\|_\infty$	2.43e-1	5.70e-1

Diffusion: error estimates

Assume that

- Ω has a Lipschitz continuous boundary
- Every element E is uniformly strictly star-shaped.
- Every face f is uniformly strictly star-shaped.
- The number of faces in E is uniformly bounded.

Then,

$$|||\boldsymbol{p} - \boldsymbol{p}^h|||_{\boldsymbol{Q}} + |||\boldsymbol{u} - \boldsymbol{u}^h|||_{\boldsymbol{X}} \leq Ch$$

If Ω is convex, then

$$|||\boldsymbol{p} - \boldsymbol{p}^h|||_{\boldsymbol{Q}} \leq Ch^2.$$

Stokes: consistency condition

To include elasticity, we assume that $\mathbb{C}$ is the full tensor. Taking $\vec{u}$ as a linear function, we obtain:

$$\int_E \mathbb{C}\, D(\vec{u}) : D(\vec{v})\, \mathrm{d}x = \int_{\partial E} (\mathbb{C}\, D(\vec{u}) \cdot \boldsymbol{n}) \cdot \vec{v}\, \mathrm{d}x.$$

The algebraic consistency condition is

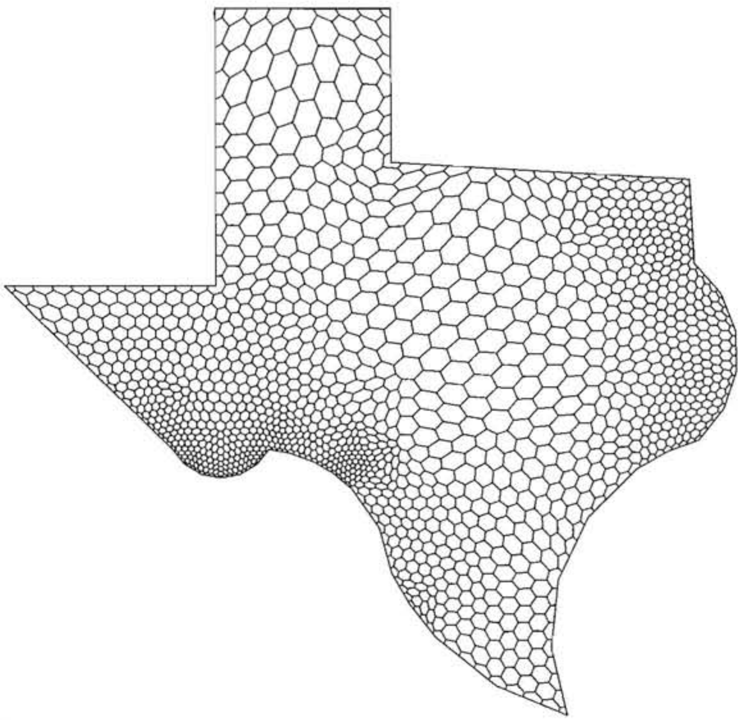
$$\mathbb{S}_{\boldsymbol{N},E}\, \mathbb{N} = \mathbb{R}.$$

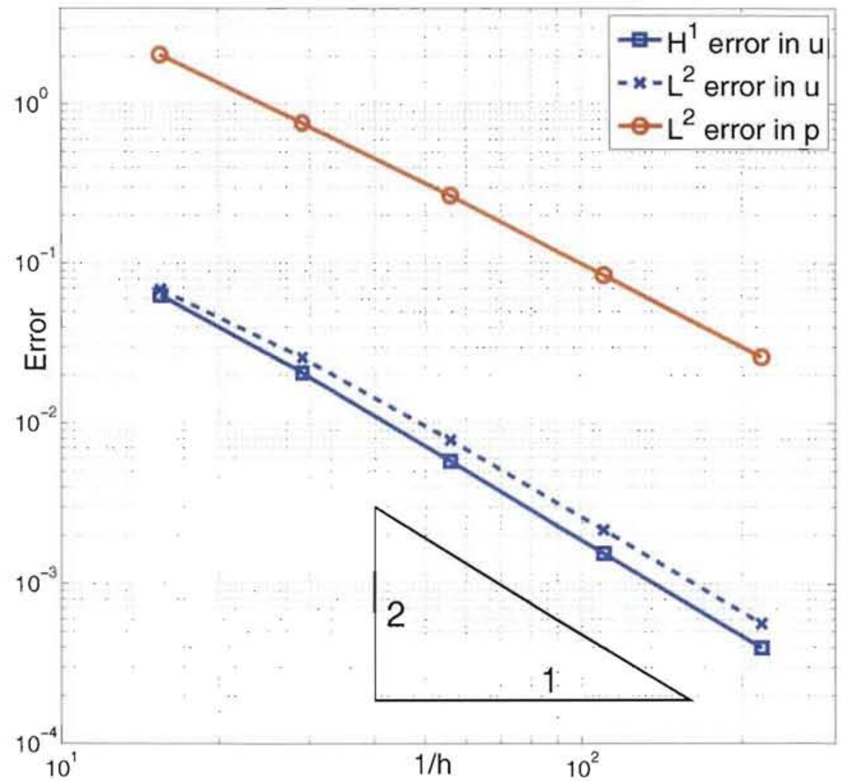
The family of symmetric solutions is

$$\mathbb{S}_{\boldsymbol{N},E} = \mathbb{R}\, (\mathbb{R}^T \mathbb{N})^{-1}\, \mathbb{R}^T + \mathbb{D}\, \mathbb{U}\, \mathbb{D}^T, \qquad \mathbb{U} = \mathbb{U}^T > 0$$

Stokes: polygonal meshes

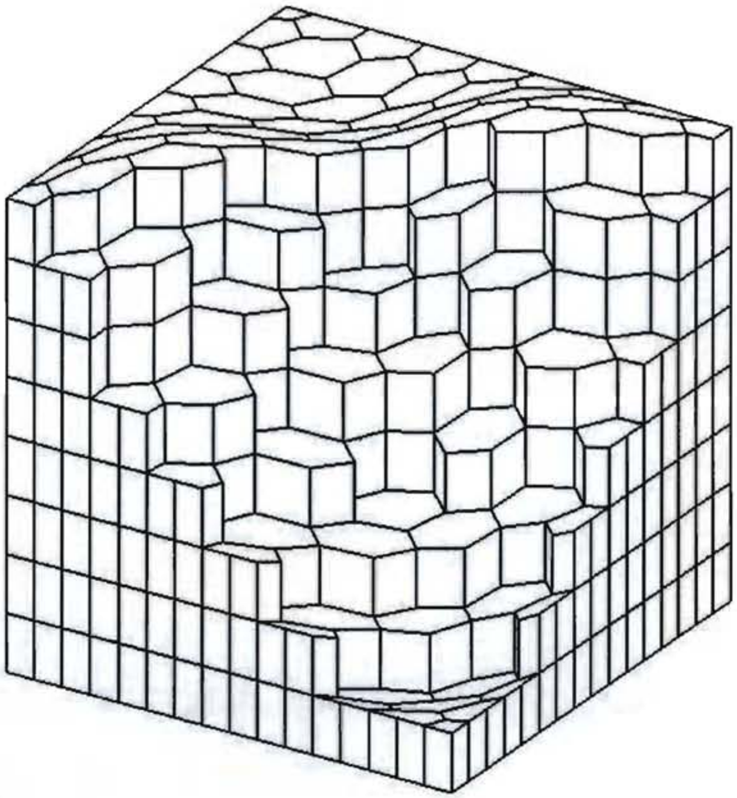
$$\vec{u}(x,y) = \begin{bmatrix} r(x)\sin(2\pi x) \\ r(x)\sin(2\pi y) \end{bmatrix}, \qquad p(x,y) = xy^2, \qquad r(x) = (1-x)\sin(2\pi x)$$

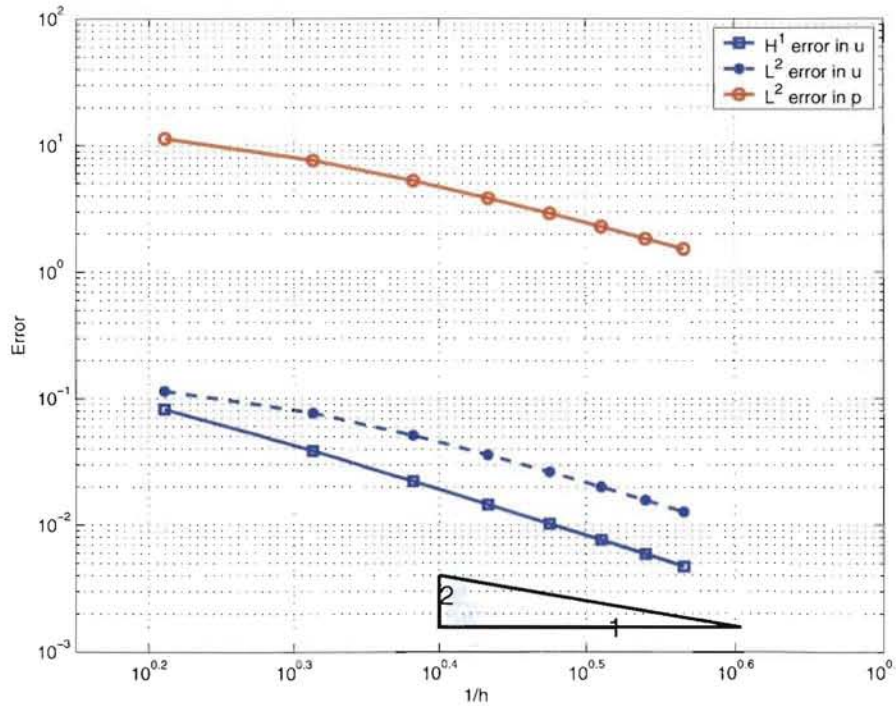




Stokes: polyhedral meshes

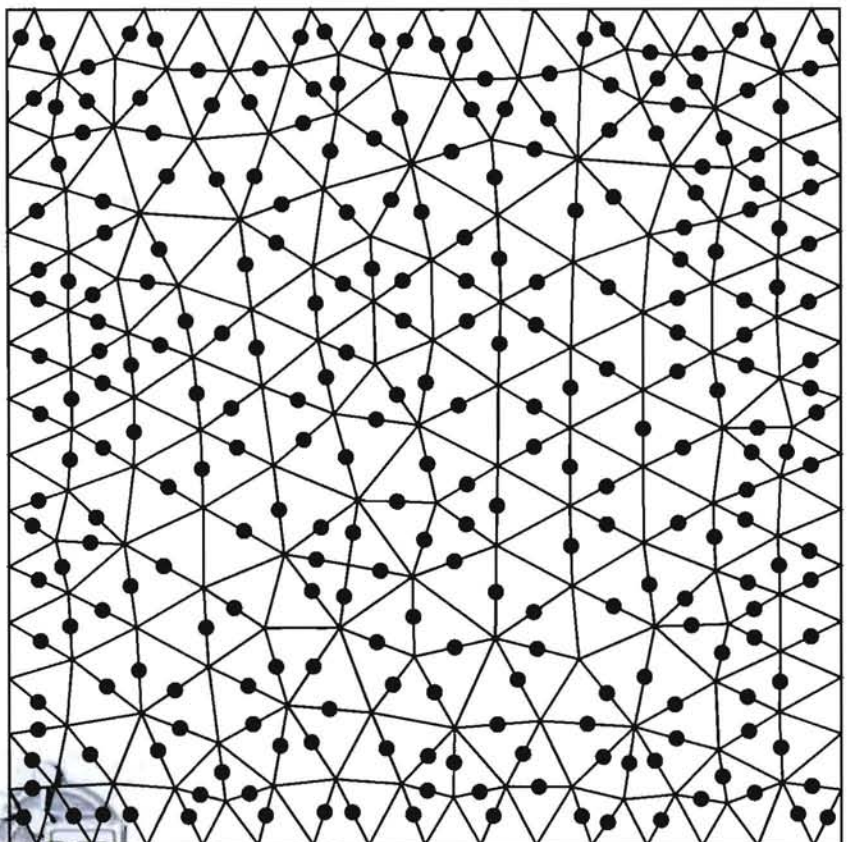
$$\vec{u} = \begin{bmatrix} 2\pi r\ \sin(2\pi y)\cos(2\pi z) \\ -r'\ \cos(2\pi y)\cos(2\pi z) \\ -2r'\ \sin(2\pi y)\sin(2\pi z) \end{bmatrix}, \quad p = \sin(2\pi x)\sin(2\pi y)\sin(2\pi z), \quad r = x^4$$

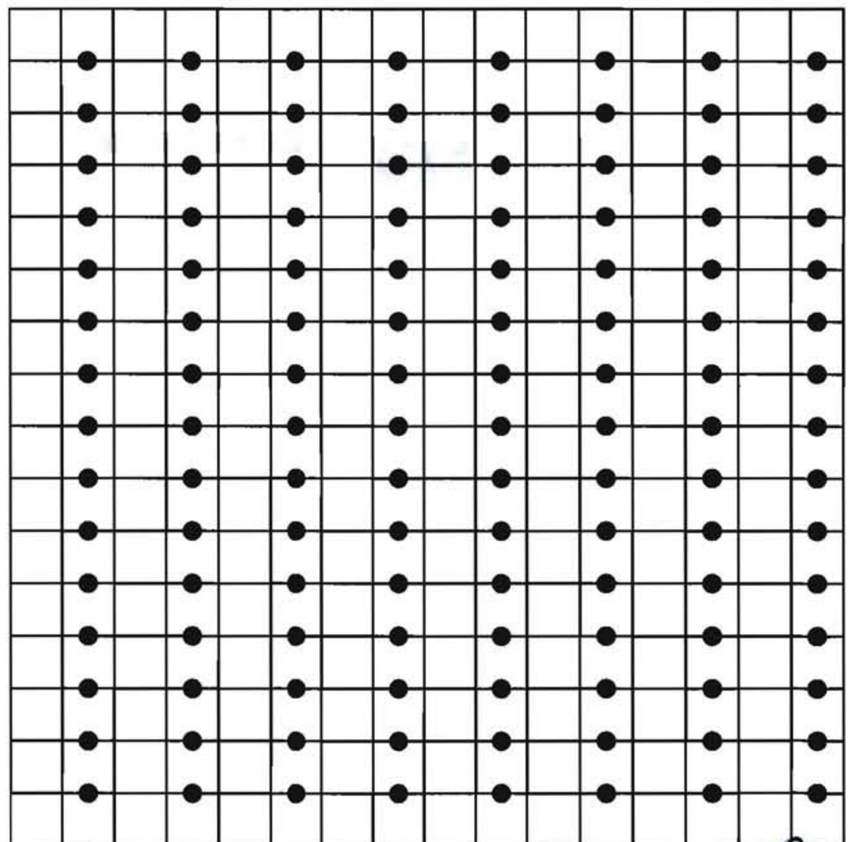




Stokes: stability analysis

We use the stabilized $P_1 - P_0$ discretization. The MFD method allows us to add the stabilizing bubbles **only** to selected edges; thus reducing the problem size.





Stokes: error estimates

Assume that

- Ω has a Lipschitz continuous boundary
- Every element E can be decomposed into the uniformly bounded number of simplexes
- Each simplex is shape-regular in a sense of Ciarlet

Then,

$$|||\boldsymbol{p} - \boldsymbol{p}^h|||_{\boldsymbol{Q}} + |||\mathbf{u} - \mathbf{u}^h|||_{1,\boldsymbol{N}} \leq Ch$$

Magnetostatics: consistency condition

Taking $\vec{u}$ as a divergence-free linear vector-function, we obtain:

$$\int_E \mathrm{curl}\vec{u} \cdot \vec{v} \, \mathrm{d}x = \int_{\partial E} \vec{v} \cdot (\boldsymbol{n} \times \vec{u}) \, \mathrm{d}x.$$

The algebraic consistency condition is

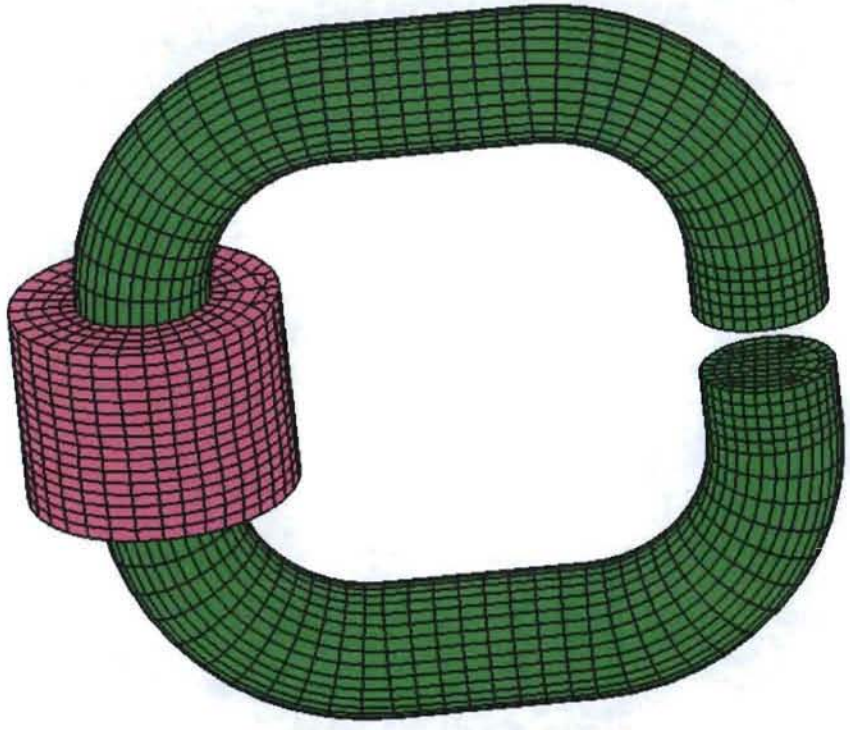
$$\mathbb{M}_{\boldsymbol{R},E} \, \mathbb{N} = \mathbb{R}.$$

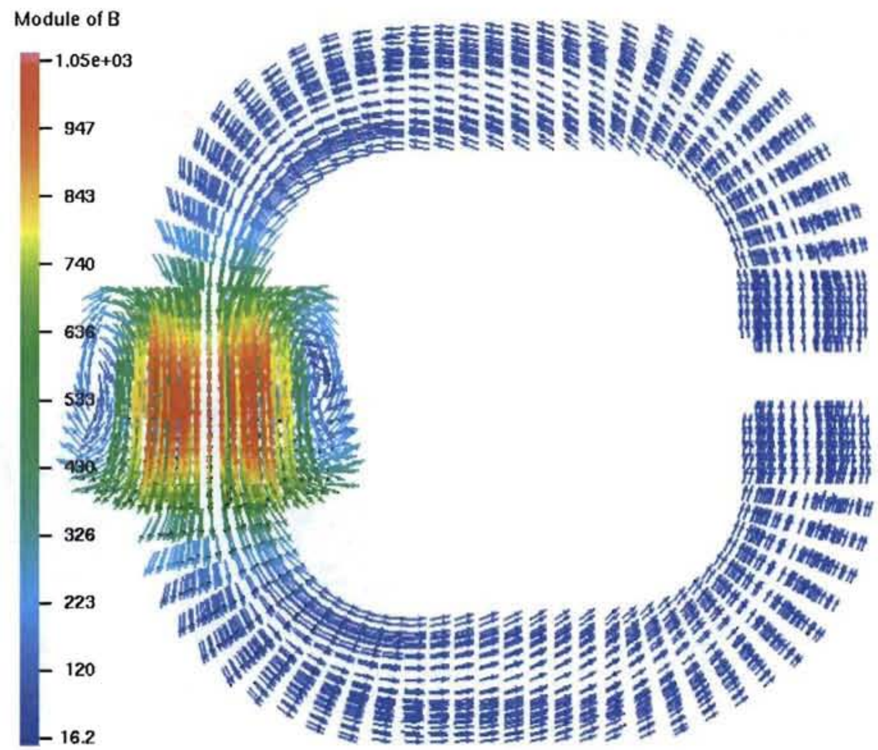
The family of symmetric solutions is

$$\mathbb{M}_{\boldsymbol{R},E} = \mathbb{R} \, (\mathbb{R}^T \mathbb{N})^{-1} \, \mathbb{R}^T + \mathbb{D} \, \mathbb{U} \, \mathbb{D}^T, \qquad \mathbb{U} = \mathbb{U}^T > 0$$

Magnetostatics: C-magnet

All-hex mesh calculation of the magnetic induction $\boldsymbol{B}$ in a C-shape magnet:





For model problems, numerical results show:

$$|||\boldsymbol{B} - \boldsymbol{B}^h|||_{\boldsymbol{X}} \le Ch$$

Tools for Analysis, II

Lifting operators

Lifting operator allows us to connect the algebraic construction of matrix $\mathbb{M}$ with basis functions. Explicit construction of the basis functions is expensive.

Example: For almost any matrix $\mathbb{M}_{\boldsymbol{X},E}$ there exist a lifting operator $\mathcal{L}_E$ from the space $\boldsymbol{X}_E$ to $H(\mathrm{div}, E)$ s.t.

- $\mathcal{L}_E(\boldsymbol{v})$ preserves constant vector functions
- $\mathcal{L}_E(\boldsymbol{v})$ has constant normal components on faces f
- $\mathcal{L}_E(\boldsymbol{v})$ has constant divergence in E
- $\boldsymbol{u}^T \mathbb{M}_{\boldsymbol{X},E} \boldsymbol{v} = \int_E \mathbb{K}_E^{-1} \mathcal{L}_E(\boldsymbol{u}) \cdot \mathcal{L}_E(\boldsymbol{v}) \,\mathrm{d}x$

Outreach

Interaction with applications:

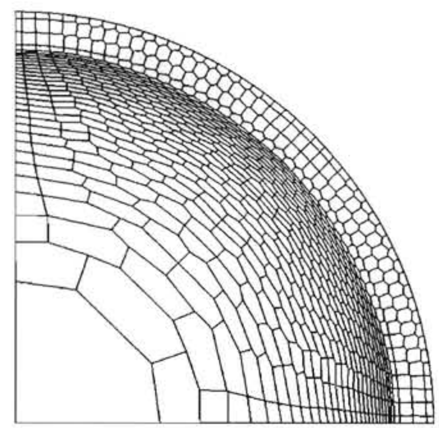
- Programmatic: MFD is used to improve accuracy of Lagrangian simulations on polyhedral meshes (more accurate diffusion discretizations; new artificial viscosity methods).

- ASCEM, SciDAC: family of MFD methods is analyzed to extract monotone methods. Nonlinear nonlinear MFD methods are developed to enforce the discrete maximum principle.

Outreach: artificial viscosity

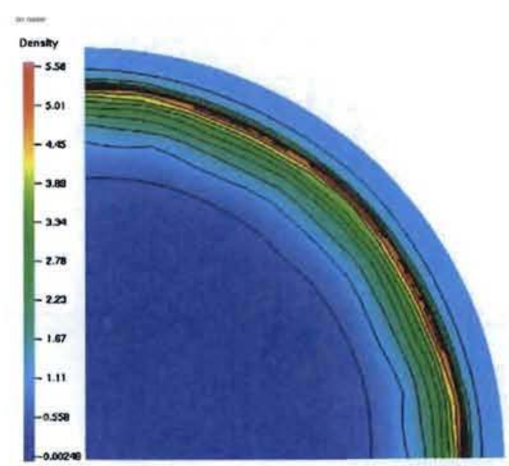
The artificial tensor viscosity can be interpreted as the mimetic approximation of the elliptic term in the modified momentum equation

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\nabla p + \operatorname{div}(\mu \nabla \boldsymbol{u})$$



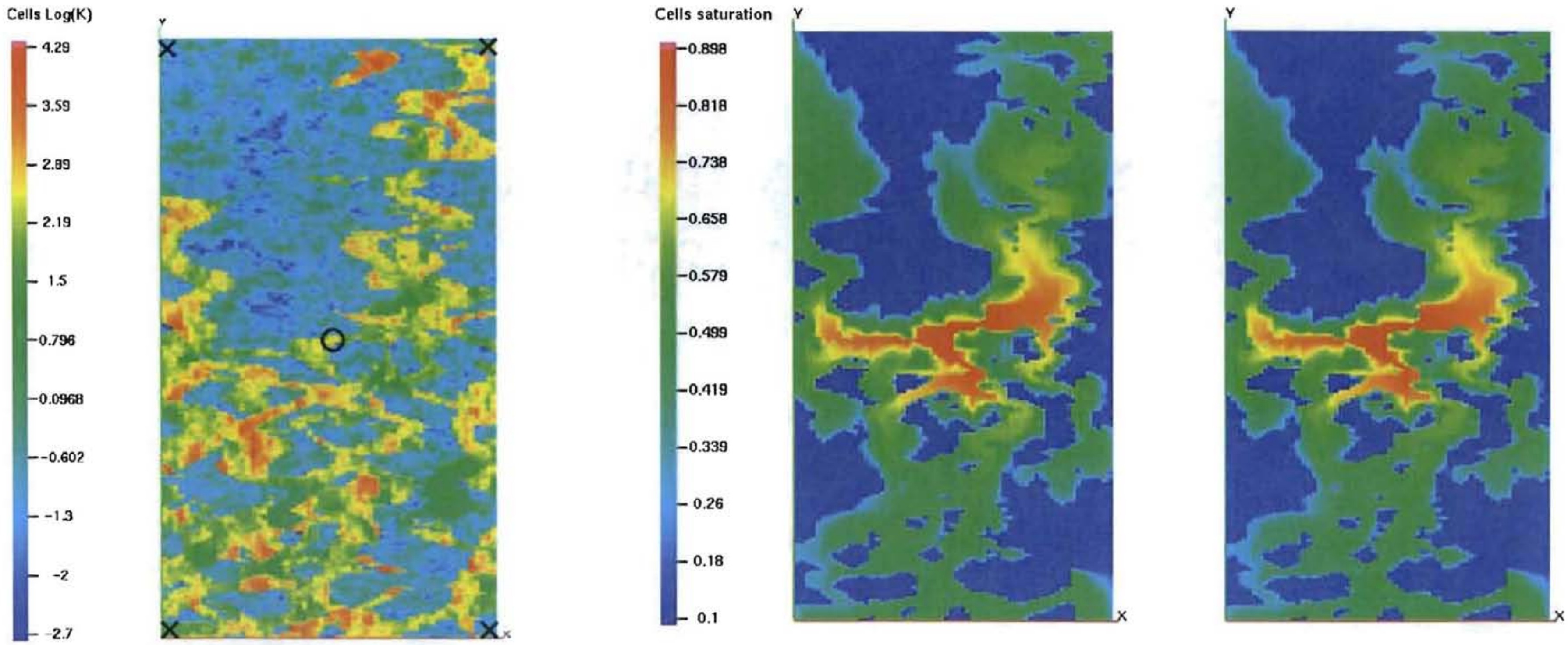
Viscosity requirements:

- zero for uniform expansion implies that the approximation must be exact for linear $\boldsymbol{u}$
- no viscosity along the shock front implies that μ must be a tensor



Outreach: flows in porous media

We developed a two-phase flow simulator for testing new algorithms for simplified but relevant problems for ASCEM and SciDAC applications.



permeability field | fine-scale solution | multiscale solution

The maximum principle

The focus is on the diffusion problem in a mixed form.

$$\mathbb{M}_{\boldsymbol{X},E} = \mathbb{R}\,(\mathbb{R}^T\mathbb{N})^{-1}\,\mathbb{R}^T + \mathbb{D}\,\mathbb{U}\,\mathbb{D}^T, \qquad \mathbb{U} = \mathbb{U}^T > 0.$$

M-matrix analysis provides a set of inequalities for the entries of the arbitrary matrix $\mathbb{U}$. Analytical solution of these inequalities is possible for

- simplicial meshes: well-know bounds are reproduced;
- parallelepiped meshes and full tensor coefficients;
- 2D orthogonal AMR meshes and full tensor coefficients

The maximum principle

Another approach to the DMP is development of nonlinear mimetic methods that generalize the work of Le Potier. The nonlinear two-point flux

$$\boldsymbol{u}_f = A(\boldsymbol{p})\boldsymbol{p}_{E_1} - B(\boldsymbol{p})\boldsymbol{p}_{E_2}$$

uses coefficients dependent on the solution. The method

- is locally conservative;
- preserves solution positivity;
- works on unstructured meshes and full tensors;
- results in a compact stencil;
- is second-order accurate.

The maximum principle

Consider the advection-dispersion-reaction equations:

$$\frac{\partial(\phi\, C^n)}{\partial t} = \mathrm{div}(\phi\, \mathbb{K} \nabla C^n) - \mathrm{div}(\vec{v} C^n) + R(C^1, \ldots, C^n).$$

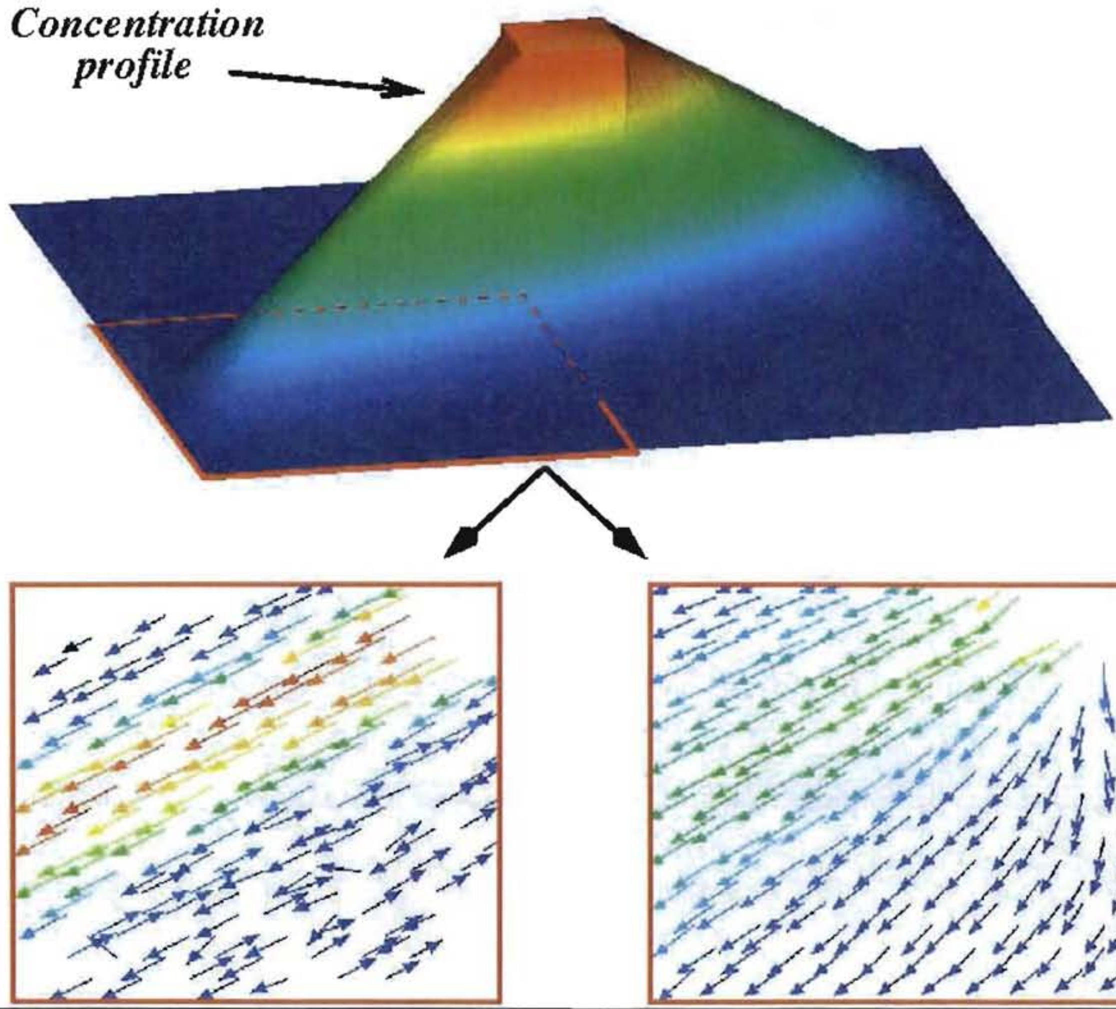
The second-order discretization of the advective flux $\vec{v}C^n$ is already nonlinear. Thus, nonlinear mimetic discretization of the dispersive flux $\phi \mathbb{K} \nabla C^n$,

$$\boldsymbol{u}_f = A(\boldsymbol{C})\boldsymbol{C}_{E_1} - B(\boldsymbol{C})\boldsymbol{C}_{E_2},$$

will not bring new numerical complications.

The maximum principle

Linear methods (left) produce oscillations and non-physical solute fluxes. Nonlinear mimetic method (right) gives a non-oscillatory solution.



Summary and future work

- Mimetic Methods (MMs) aim at a better representation of fundamental physical laws.
- Mimetic operators satisfy discrete vector and tensor identities and therefore are less sensitive to mesh non-smoothness.
- MMs are inexpensive and easy to implement on arbitrary (not totally crazy!) polyhedral meshes.
- The number of theoretical results grows.
- Future work: Continue analysis of monotone MFD methods and development of theory of high-order MFD methods.