Physics-Preserving Discretizations for Subsurface Flows

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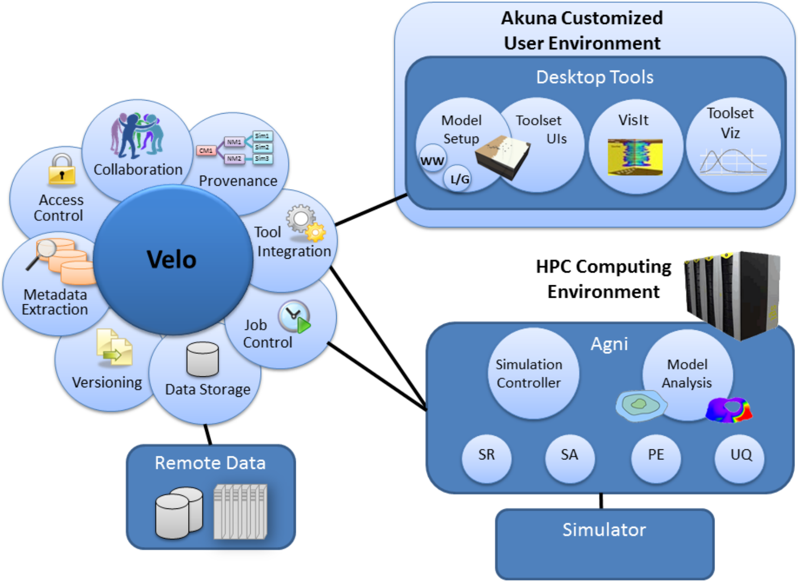
Outline

1. **ASCEM Program and open source code Amanzi**
2. **Mathematical and physical requirements for discrete schemes**
3. **Mimetic finite difference (MFD) method**
4. **Nonlinear finite volume (NFV) method**
5. **Application to nonlinear solvers**

ASCEM Program

Advanced Simulation Capability for Environmental Management



Open source simulator Amanzi (github.com/amanzi)

Amanzi is the Multi-Process HPC Simulator for coupled flow and reactive transport

- modular C++ design, uses 22 external libraries
- polytopal (MSTK), structured AMR (BoxLib) meshes
- automatic update of state fields via a dependency graph
- state-of-the-art solvers (Hypre, Trilinos, Amanzi)
- parallel IO (ParMETIS, Exodus, HDF5)
- chemistry packages (PFloTran, CrunchFlow, Amanzi)
- standard and advanced discretization methods
- quality control (400+ unit and 100+ regression tests)

Simplified PDE model (1/2)

$$\frac{\partial(\phi\,\rho\,s)}{\partial t} + \mathrm{div}(\rho\,\mathbf{q}) = Q, \qquad \mathbf{q} = -\frac{k_r}{\mu}\mathbb{K}\,(\nabla p - \rho\mathbf{g})$$

$$\frac{\partial(\phi\,s\,C_i)}{\partial t} + \mathrm{div}(\mathbf{q}\,C_i) - \mathrm{div}(\phi_e\,s\,\mathbb{D}_i\nabla C_i) = R(C_1,\ldots,C_n)$$

where ϕ, ϕ_e - **porosities**

ρ, μ - **density and viscosity of water**

s - **saturation**

$\mathbb{K}$, k_r - **absolute and relative permeabilities**

C_i - **molar concentration of chemical species**

Various extensions include the dual porosity model, energy equation, water vapor model, coupled surface and subsurface flow and transport, and multiphase flows.

Simplified PDE model (2/2)

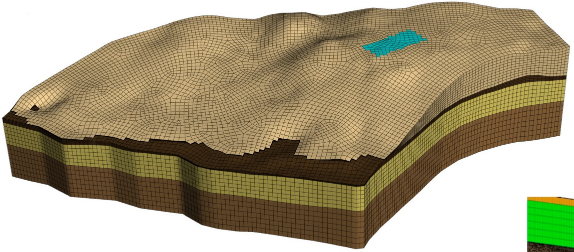
$$\frac{\partial(\phi\, s)}{\partial t} + \mathrm{div}(\mathbf{q}) = 0, \qquad \mathbf{q} = -\mathbb{K}\, k_r\, (\nabla p - \rho \mathbf{g})$$

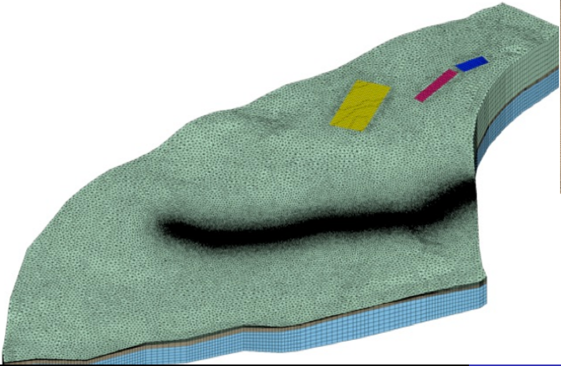
$$\frac{\partial(\phi\, s\, C_i)}{\partial t} + \mathrm{div}(\mathbf{q}\, C_i) - \mathrm{div}(\phi\, s\, \mathbb{D}_i \nabla C_i) = 0$$

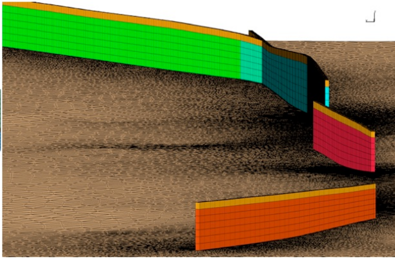
Mathematical and physical properties

- **conservation laws (water, species)**
- **positivity of concentration**
- **maximum principles (hydraulic head, pressure)**
- **symmetry and positive definiteness of operators**

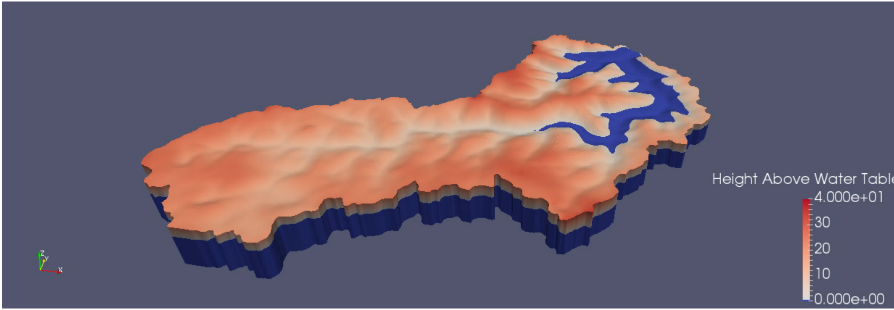
Additional challenge: polytopal meshes







Additional challenge



Development of physics-preserving schemes becomes more challenging on polytopal meshes

Requirement for the ideal scheme

- **be conservative**
- **be convergent on polytopal meshes**
- **handle degenerate and strongly varying coefficients**
- **lead to an SPD matrix (e.g. for elliptic operators)**
- **have discrete maximim principles**

Discretization methods implemented in Amanzi

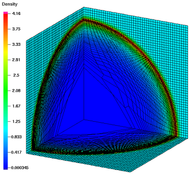
- **Finite volume scheme**
- **Mimetic finite differences (MFD) with optimization**
- **Nonlinear finite volume (NFV) scheme**

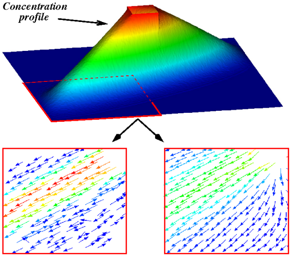
Mimetic finite differences

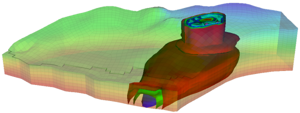
Mimetic finite different method

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

Mimetic schemes preserve or mimic critical mathematical and physical properties of systems of PDEs such as conservation laws, exact identities, and symmetries.





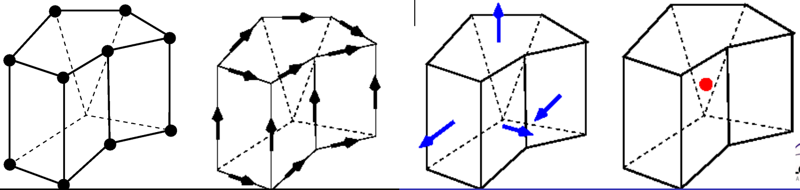


Coordinate invariant definition of primary mimetic operators using the Stokes theorem in one, two and three dimensions.

$$\int_e \frac{\partial p}{\partial \boldsymbol{\tau}_e}\,\mathrm{d}x = p(\mathbf{x}_{n_2}) - p(\mathbf{x}_{n_1}) \qquad \left(\mathrm{GRAD}\, p_h\right)_e = \frac{p_{n_2} - p_{n_1}}{|e|}$$

$$\int_f (\mathbf{curl}\,\mathbf{u})\cdot\mathbf{n}_f\,\mathrm{d}x = \oint_{\partial f} \mathbf{u}\cdot\boldsymbol{\tau}\,\mathrm{d}x \qquad \left(\mathcal{CURL}\,\mathbf{u}_h\right)_f = \frac{1}{|f|}\sum_{e\in\partial f} \alpha_{f,e}\,|e|\,u_e$$

$$\int_c \mathrm{div}\,\mathbf{u}\,\mathrm{d}x = \oint_{\partial c} \mathbf{u}\cdot\mathbf{n}\,\mathrm{d}x \qquad \left(\mathrm{DIV}\,\mathbf{u}_h\right)_c = \frac{1}{|c|}\sum_{f\in\partial c} \alpha_{c,f}\,|f|\,u_f$$



Duality between primary and derived mimetic operators.

$$\int_\Omega (\operatorname{div}\mathbf{u})\, p \,\mathrm{d}x = -\int_\Omega \mathbf{u}\cdot\nabla p \,\mathrm{d}x \quad \forall \mathbf{u}\in H_{div}(\Omega),\ p\in H_0^1(\Omega)$$

We define $\widetilde{\mathrm{GRAD}} = -\mathrm{DIV}^*$ **with respect to inner products**

$$\big[\mathrm{DIV}\mathbf{u}_h,\, p_h\big]_{\mathcal{C}_h} = -\big[\mathbf{u}_h,\, \widetilde{\mathrm{GRAD}} p_h\big]_{\mathcal{F}_h} \quad \forall \mathbf{u}_h\in\mathcal{F}_h,\ p_h\in\mathcal{C}_h$$

An inner product is defined by an SPD matrix, e.g.

$$[\mathbf{u}_h,\, \mathbf{v}_h]_{\mathcal{F}_h} = (\mathbf{u}_h)^T\, \mathbb{M}_{\mathcal{F}_h}\, \mathbf{v}_h$$

Consequence of design principles

- **Exact identities, e.g.**

$$\mathrm{DIV}\,\mathcal{CURL} = 0, \qquad \widetilde{\mathcal{CURL}}\,\widetilde{\mathrm{GRAD}} = 0$$

- **Symmetry, positive definiteness of discrete Laplacians**

- **Helmholtz decompositions:**

$$\mathbf{v}_h = \widetilde{\mathrm{GRAD}}\,q_h + \mathcal{CURL}\,\mathbf{u}_h$$

where $\mathbf{v}_h \in \mathcal{F}_h$**,** $q_h \in \mathcal{C}_h$**, and** $\mathbf{u}_h \in \mathcal{E}_h$ **with** $\widetilde{\mathrm{DIV}}\,\mathbf{u}_h = 0$**,**

$$\mathbf{v}_h = \mathrm{GRAD}\,q_h + \widetilde{\mathcal{CURL}}\,\mathbf{u}_h$$

where $\mathbf{v}_h \in \mathcal{E}_h$**,** $q_h \in \mathcal{N}_h$**, and** $\mathbf{u}_h \in \mathcal{F}_h$ **with** $\mathrm{DIV}\,\mathbf{u}_h = 0$

- **Treatment of polyhedral meshes with curved faces**[1]

[1] F.Brezzi, K.L., M.Shashkov, V.Simoncini, CMAME, 2007

Flexibility the mimetic framework

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

leads to primary DIV **that approximates** $\mathrm{div}(\cdot)$ **and derived** $\widetilde{\mathrm{GRAD}}$ **that approximates** $\mathbb{K}\,\nabla(\cdot)$**.**

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

leads to primary DIV **that approximates** $\mathrm{div}(k\,\cdot)$ **and derived** $\widetilde{\mathrm{GRAD}}$ **that approximates** $\nabla(\cdot)$**. Symmetry is preserved even when** k **is upwinded on each mesh face.**[2]

[2] K.L., G.Manzini, D.Moulton, M.Shashkov, JCP, 2016

Related methods and frameworks

- **Cell method**
- **Compatible discrete operators**
- **Co-volume method**
- **Summation by parts**
- **Hybrid FV, mixed FV, discrete duality FV**
- **Mixed FE, weak Galerkin, VEM, Kuznetsov-Repin FE**
- **Enhanced mixed FE**
- **Exterior calculus**

Local inner products

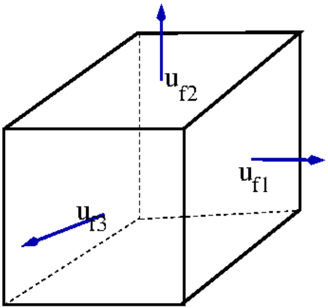
Inner products are built cell-by-cell:

$$\left[\mathbf{v}_h,\ \mathbf{u}_h\right]_{\mathcal{F}_h} = \sum_{c\in\Omega_h} \left[\mathbf{v}_{c,h},\ \mathbf{u}_{c,h}\right]_{c,\mathcal{F}_h}$$

The cell-based inner product is defined by SPD matrix:

$$\left[\mathbf{v}_{c,h},\ \mathbf{u}_{c,h}\right]_{c,\mathcal{F}_h} = (\mathbf{v}_{c,h})^T \mathbb{M}_{c,\mathcal{F}_h}\, \mathbf{u}_{c,h} \approx \int_c \mathbf{v}\cdot\mathbf{u}\,\mathrm{d}x$$

Degrees of freedom



$$u_{f_i} = \frac{1}{|f_i|} \int_{f_i} \mathbf{u} \cdot \mathbf{n} \, \mathrm{d}x$$

Decomposition of matrix $\mathbb{M}_{c,\mathcal{F}_h}$

Derivation of an accurate inner product is based on the consistency and stability conditions:

$$\mathbb{M}_{c,\mathcal{F}_h} = \underbrace{\mathbb{M}^{(0)}_{c,\mathcal{F}_h}}_{consistency} + \underbrace{\mathbb{M}^{(1)}_{c,\mathcal{F}_h}}_{stability}$$

Admissible inner product matrix is not unique

Consistency condition

Let $\mathcal{V}_c$ be specially designed Hilbert space, and $\mathbf{u}_{c,h} = \Pi_c(\mathbf{u})$:

$$\left[\Pi_c(\mathbf{u}^0),\, \Pi_c(\mathbf{v})\right]_{c,\mathcal{F}_h} = \int_c \mathbf{u}^0 \cdot \mathbf{v}\, \mathrm{d}x \quad \forall \mathbf{u}^0 \in \mathcal{P}_0(c), \quad \mathbf{v} \in \mathcal{V}_c$$

The space $\mathcal{V}_c$ is typically infinite dimensional (see VEM framework[3] where $\mathcal{V}_c$ has finite dimension):

$$\mathcal{V}_c = \left\{\mathbf{v} :\; \mathbf{v} \cdot \mathbf{n}_f \in \mathcal{P}^0(f),\; \mathrm{div}(\mathbf{v}) \in \mathcal{P}^0(c)\right\}$$

[3] L.Beiro da Veiga, F.Brezzi, A.Cangiani, G.Manzini, L.D.Marini, A.Russo, M3AS, 2013

Algebraic form of consistency condition (1/2)

Since $\mathbf{u}^0 = \nabla q^1$ **and** $\displaystyle\int_c q^1 \mathrm{d}x = 0$**, we have**

$$\left[\Pi_c(\mathbf{u}^0),\, \Pi_c(\mathbf{v})\right]_{c,\mathcal{F}_h} = (\mathbf{u}^0_{c,h})^T \mathbb{M}_{c,\mathcal{F}}\, \mathbf{v}_{c,h} = \int_c \nabla q^1 \cdot \mathbf{v}\, \mathrm{d}x$$

$$= -\int_c q^1 \mathrm{div}(\mathbf{v})\, \mathrm{d}x + \int_{\partial c} q^1\, \mathbf{v} \cdot \mathbf{n}\, \mathrm{d}x$$

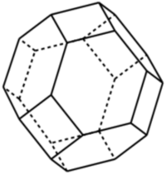
$$= \sum_{f \in \partial c} v_f \int_f q^1\, \mathrm{d}x$$

Since $\mathrm{v}_{c,h}$ **is an arbitrary vector of DOFs, we conclude with the matrix equation w.r.t. unknown** $\mathbb{M}_{c,\mathcal{F}_h}$**:**

$$\mathbb{M}_{c,\mathcal{F}_h}\, \mathbf{u}^0_{c,h} = \mathbf{r}_{c,h}$$

Algebraic form of consistency condition (2/2)

$$\mathbb{M}_{c,\mathcal{F}} \begin{pmatrix} u^0_{f_1} \\ \vdots \\ u^0_{f_m} \end{pmatrix} = \begin{pmatrix} \int_{f_1} q^1 \, \mathrm{d}x \\ \vdots \\ \int_{f_m} q^1 \, \mathrm{d}x \end{pmatrix} \qquad \forall \mathbf{u}^0 = \nabla q^1$$



It is sufficient to consider only linearly independent functions q^1. In 3D, we have $q^1_a = x - x_c$, $q^1_b = y - y_c$, and $q^1_c = z - z_c$.

$$\underbrace{\mathbb{M}_{c,\mathcal{F}_h}}_{m\times m} \underbrace{\mathbb{N}_c}_{m\times 3} = \underbrace{\mathbb{R}_c}_{m\times 3}$$

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

Solution of the mimetic matrix equation

Lemma

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

$$\mathbb{M}_{c,\mathcal{F}_h} = \underbrace{\mathbb{M}^{(0)}_{c,\mathcal{F}_h}}_{consistency} + \underbrace{\mathbb{M}^{(1)}_{c,\mathcal{F}_h}}_{stability}$$

where

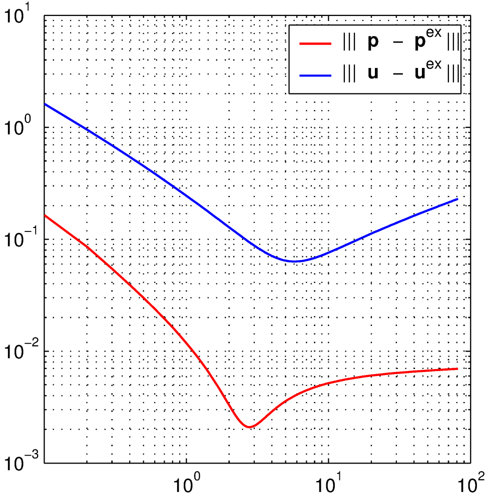
$$\mathbb{M}^{(0)}_{c,\mathcal{F}_h} = \mathbb{R}_c\,(\mathbb{R}_c^T\,\mathbb{N}_c)^{-1}\,\mathbb{R}_c^T, \qquad \mathbb{R}_c^T\,\mathbb{N}_c = |c|\,\mathbb{I}$$

and

$$\mathbb{M}^{(1)}_{c,\mathcal{F}_h} = \left(\mathbb{I} - \mathbb{N}_c\left(\mathbb{N}_c^T\mathbb{N}_c\right)^{-1}\mathbb{N}_c^T\right)\mathbb{P}_c\left(\mathbb{I} - \mathbb{N}_c\left(\mathbb{N}_c^T\mathbb{N}_c\right)^{-1}\mathbb{N}_c^T\right)$$

where $\mathbb{P}_c$ is an SPD matrix.

Consider a model elliptic problem and calculate Darcy flux and pressure errors as functions of one normalize parameter:



$$\mathbb{P}_c = a_c \mathbb{I}$$

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

Stability condition (2/2)

$\mathbb{M}_{c,\mathcal{F}_h}$ **should behave like a mass matrix:**

$$\mathbb{M}_{c,\mathcal{F}_h} \sim |c|\,\mathbb{I}$$

This imposes restrictions on the parameter matrix:

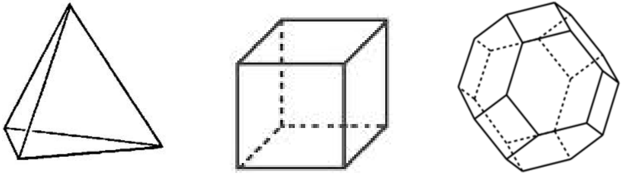
$$\sigma_\star |c|\,\|\mathbf{v}_{c,h}\|^2 \leq \mathbf{v}_{c,h}^T\,\mathbb{M}_{c,\mathcal{F}_h}^{(0)}\mathbf{v}_{c,h} + \mathbf{v}_{c,h}^T\,\mathbb{M}_{c,\mathcal{F}_h}^{(1)}\mathbf{v}_{c,h} \leq \sigma^\star |c|\,\|\mathbf{v}_{c,h}\|^2$$

In practice, a good choice is given by the scalar matrix

$$\mathbb{P}_c = \frac{1}{3}|c|\,\mathbb{I}.$$

How rich is the family of MFD scheme?

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



Equivalent solution of the mimetic matrix equation

Lemma

A family of SPD solutions to $\mathbb{N}_c = \left(\mathbb{M}_{c,\mathcal{F}_h}\right)^{-1} \mathbb{R}_c$ is

$$\left(\mathbb{M}_{c,\mathcal{F}_h}\right)^{-1} = \mathbb{W}_{c,\mathcal{F}_h} = \underbrace{\mathbb{W}^{(0)}_{c,\mathcal{F}_h}}_{consistency} + \underbrace{\mathbb{W}^{(1)}_{c,\mathcal{F}_h}}_{stability}$$

where

$$\mathbb{W}^{(0)}_{c,\mathcal{F}_h} = \mathbb{N}_c \, (\mathbb{N}_c^T \, \mathbb{R}_c)^{-1} \, \mathbb{N}_c^T$$

and

$$\mathbb{W}^{(1)}_{c,\mathcal{F}_h} = \left(\mathbb{I} - \mathbb{R}_c \left(\mathbb{R}_c^T \mathbb{R}_c\right)^{-1} \mathbb{R}_c^T\right) \mathbb{P}_c \left(\mathbb{I} - \mathbb{R}_c \left(\mathbb{R}_c^T \mathbb{R}_c\right)^{-1} \mathbb{R}_c^T\right)$$

where $\mathbb{P}_c$ is an SPD matrix.

Maximum principle (1/2)

The cell-based stiffness matrix for an elliptic equation appearing in the mixed-hydrid formulations looks like:

$$\mathbb{A}_c = \begin{bmatrix} \mathbb{C}_c^T\, \mathbb{W}_{c,\mathcal{F}_h}\, \mathbb{C}_c & -\mathbb{C}_c^T\, \mathbb{W}_{c,\mathcal{F}_h}\, \mathbb{B}_c \\ -\mathbb{B}_c^T\, \mathbb{W}_{c,\mathcal{F}_h}\, \mathbb{C}_c & \mathbb{B}_c^T\, \mathbb{W}_{c,\mathcal{F}_h}\, \mathbb{B}_c \end{bmatrix}, \quad \mathbb{B}_c = \mathbb{C}_c \mathbf{1}$$

Direct control of M-matrix property is not practical. We use stronger criteria:

Lemma

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

Maximum principle (2/2)

Cell-based matrix of parameters:

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

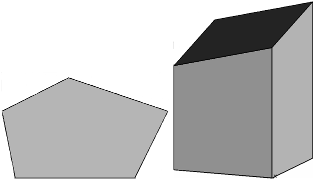
- **Z-matrix property** $(\mathbb{W}_{c,\mathcal{F}_h})_{ij} \le 0$ **for** $i \ne j$ **leads to linear inequality constraints**
- $(\mathbb{W}_{c,\mathcal{F}_h}\, \mathbb{B}_c)_i \ge \epsilon > 0$ **are also linear inequality constraints**

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

$$\Phi(a_1, \ldots, a_3) = \sum_{i,j=1}^{m} (\mathbb{W}_{c,\mathcal{F}_h})_{ij}.$$

Cost of the simplex method

cell	Random perturbation		Rotation of anisotropic $\mathbb{K}$	
	optimized	default	optimized	default
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

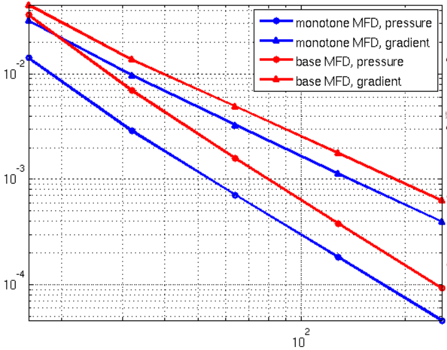


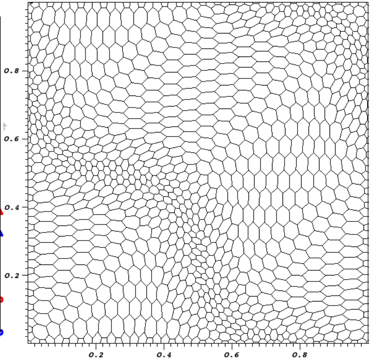
- The optimized MFD method is 3-6 times more expensive than the default method with $\mathbb{P}_c = \alpha_c \mathbb{I}$
- The simplex method returns diagonal matrix $\mathbb{W}_{c,\mathcal{F}_h}$ on Voronoi meshes and for scalar $\mathbb{K}$

Model diffusion problem

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

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



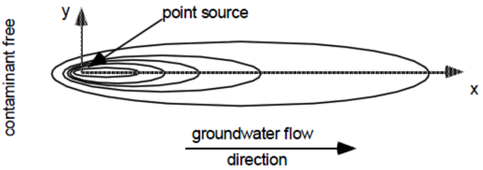


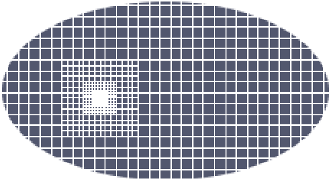
We observed that optimization typically improves errors on polygonal meshes.

PORFLOW Test 5.2.1

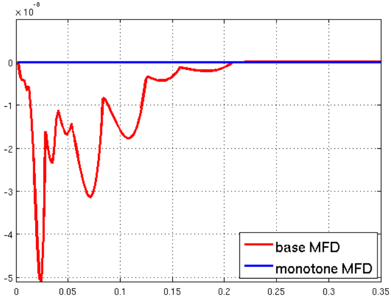
$$\frac{\partial C}{\partial t} + \mathrm{div}(\mathbf{q}C) - \mathrm{div}(\mathbb{D}\nabla C) = Q, \qquad \mathbb{D} = \alpha_L \frac{\mathbf{q}\mathbf{q}}{\|\mathbf{q}\|^2} + \alpha_T \left(\mathbb{I} - \frac{\mathbf{q}\mathbf{q}}{\|\mathbf{q}\|^2}\right)$$

Velocity makes angle 30° with the x-axis.



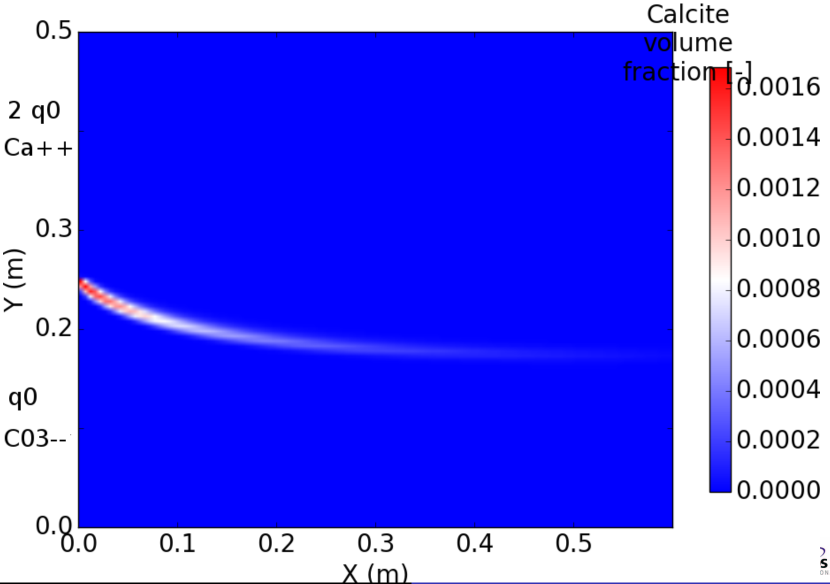


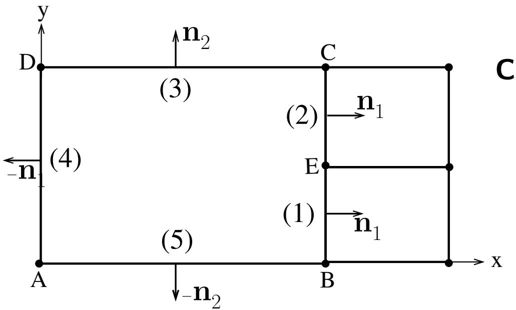
Small undershoots were observed in the base MFD method. They go to zero as the contamination front moves away from the source.



Precipitation of calcite along mixing interfaces

$$Ca^{2+} + CO_3^{2-} \leftrightarrow CaCO_3$$





Cell aspect ratio:

$$r = \frac{|AD|}{|AB|}$$

Let $\mathbb{K}$ be diagonal. Then, the optimized MFD scheme has the discrete maximum principle if

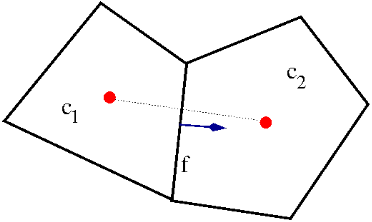
$$r^2 < 4\frac{\mathbb{K}_{yy}}{\mathbb{K}_{xx}}$$

Nonlinear finite volumes

Brief history of nonlinear schemes

- 1998 **Nonlinear scheme with the DMP for simplicial meshes and scalar k (Bertolazzi)**
- 2005 **Its theoretical analysis (Bertolazzi,Manzini)**
- 2005 **TPFA scheme for triangular meshes (Le Potier)**
- 2009 **Interpolation-free scheme (L,Svyatsky,Vassilevski)**
- 2010 **1st-order FV scheme with DMP (Le Potier)**
- 2011 **2nd-order FV scheme with DMP (Sheng,Yuan)**
- 2011 **Convergence analysis (Le Potier, Droniou)**
- 2012 **Interpolation-free scheme with DMP (L,Svyatsky,Vassilevski)**
- 2014 **Multiphase flows (Nikitin,Terekhov,Vassilevski)**
- 2016 **Non-isothermal two-phase flow (Schneider,Flemisch,Helmig)**
- 2017 **Richards' equation (L,Svyatsky)**

Two-point flux approximation

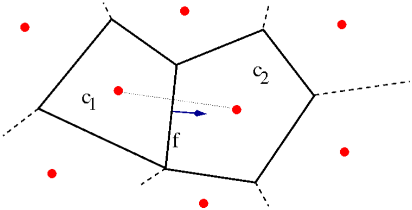


The classical 2-point flux approximation is

$$\mathbf{q}_f = T_f \frac{p_{c_1} - p_{c_2}}{d_{12}}$$

The formula becomes inaccurate for arbitrarily-shaped cells and/or tensorial material properties.

Nonlinear FV scheme with the discrete MP (1/2)



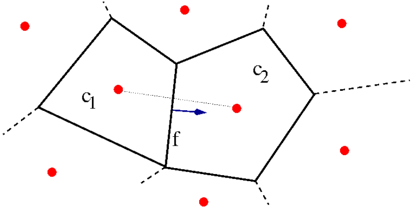
Multi-point one-sides fluxes use positive decomposition of co-normal:

$$\mathbf{q}_f^{(i)} = \alpha_{ik} \frac{p_{c_i} - p_{c_k}}{d_{ik}} + \alpha_{il} \frac{p_{c_i} - p_{c_l}}{d_{il}}, \qquad \alpha_{ik}, \alpha_{il} \geq 0$$

Unique flux:

$$\mathbf{q}_f = \frac{|\mathbf{q}_f^{(2)}|}{|\mathbf{q}_f^{(1)}| + |\mathbf{q}_f^{(2)}|} \mathbf{q}_f^{(1)} + \frac{|\mathbf{q}_f^{(1)}|}{|\mathbf{q}_f^{(1)}| + |\mathbf{q}_f^{(2)}|} (-\mathbf{q}_f^{(2)})$$

Nonlinear FV scheme with the discrete MP (2/2)

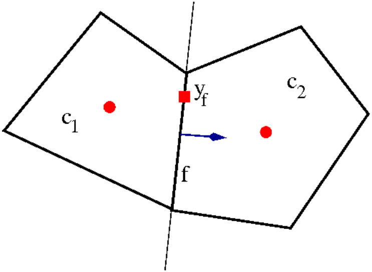


Unique flux has two equivalent representations

$$\mathbf{q}_f = \frac{2\,|\mathbf{q}_f^{(2)}|\,\mathbf{q}_f^{(1)}}{|\mathbf{q}_f^{(1)}| + |\mathbf{q}_f^{(2)}|} = -\frac{2\,|\mathbf{q}_f^{(1)}|\,\mathbf{q}_f^{(2)}}{|\mathbf{q}_f^{(1)}| + |\mathbf{q}_f^{(2)}|}$$

This leads to a cell-centered FV scheme with an M-matrix.

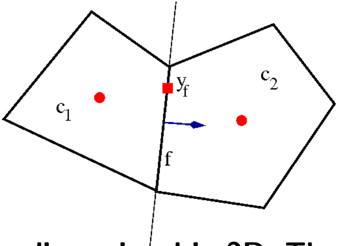
Harmonic averaging point (1/2)



Consider the affine space $\mathcal{S}$ of functions $q(\mathbf{x})$:

- $q(\mathbf{x})$ **is linear in both** c_1 **and** c_2**,** $q(\mathbf{x}_{c_i}) = p_{c_i}$
- $q(\mathbf{x})$ **is continuous of interface** f
- $q(\mathbf{x})$ **has continuous flux across the interface** f

Harmonic averaging point (2/2)



The space $\mathcal{S}$ is one-dimensional in 2D. There exists a function $q^\star \in \mathcal{S}$ and a point $\mathbf{y}_f \in f$ such that[4]

$$q^\star(\mathbf{y}_f) = \gamma_f p_{c_1} + (1-\gamma_f) p_{c_2}, \qquad 0 < \gamma_f < 1.$$

We use this value to modify the one-sided flux formula:

$$\begin{aligned} \mathbf{q}_f^{(1)} &= \alpha_{11} \frac{p_{c_1} - q^\star(\mathbf{y}_f)}{d_{1f}} + \alpha_{12} \frac{p_{c_1} - p_{c_3}}{d_{13}} \\ &= \alpha_{11}(1-\gamma_f) \frac{p_{c_1} - p_{c_2}}{d_{1f}} + \alpha_{12} \frac{p_{c_1} - p_{c_3}}{d_{13}}. \end{aligned}$$

[4] L.Agelas, R.Eymard, R.Herbin, C. R. Acad. Sci. Paris, Ser.I, 2009

Nonlinear FV scheme for Richards' equation

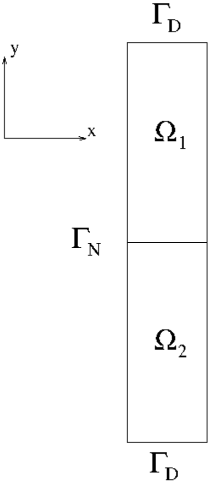
$$\frac{\partial(\phi\, s)}{\partial t} + \mathrm{div}(\mathbf{q}) = 0, \qquad \mathbf{q} = -\mathbb{K}\, k_r(\nabla p - \rho \mathbf{g})$$

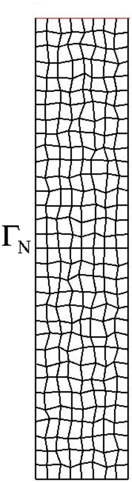
To build a second-order NFV scheme with the discrete MP, we need[5]

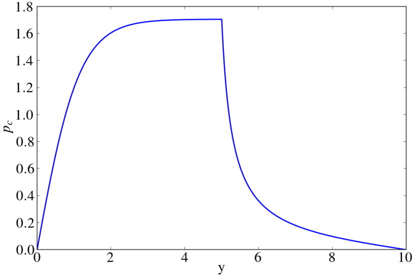
- **second-order upwind approximation of the relative permeability** k_r
- **limiter based on neighboring pressure values**

[5] D.Svyatsky, K.L., AWR, 2017

Convergence analysis



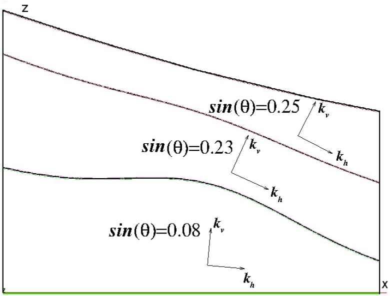


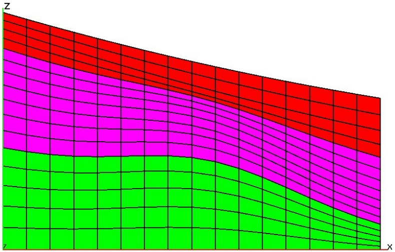


# cells	pressure error	
	1st	2nd
16x4	1.19e-01	3.34e-02
32x8	6.74e-02	1.25e-02
64x16	3.71e-02	4.34e-03
128x32	2.00e-02	1.44e-03
256x64	1.05e-02	4.35e-04

Water infiltration into dry soil (1/3)

- mass influx on the top boundary
- atmospheric pressure on the bottom boundary
- no flow otherwise
- discontinuous anisotropic permeability tensor $\mathbb{K}$

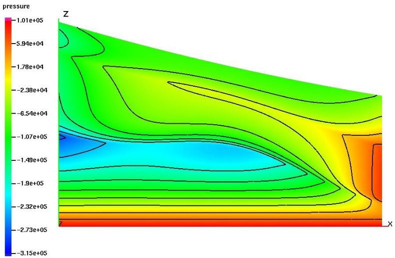




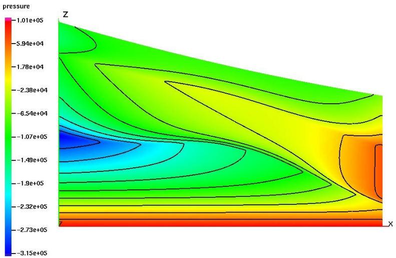
Water infiltration into dry soil (2/3)

van Genuchten parameters $n = 1.43$, $\alpha = 2.0674 \cdot 10^{-4}$ **[Pa^{-1}]**

Pressure profile at steady state satisfies maximum principles in each soil



TPFA

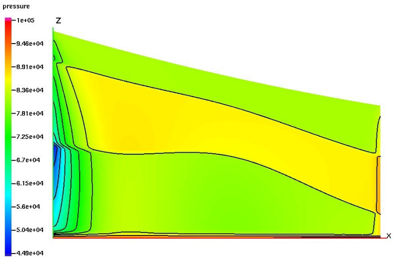


NFV

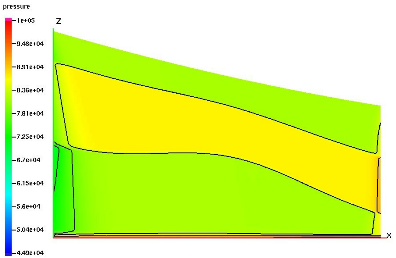
Water infiltration into dry soil (3/3)

van Genuchten parameters $n = 3.18$**,** $\alpha = 3.5959 \cdot 10^{-4}$ **[Pa^{-1}]**

Pressure profile at steady state satisfies maximum principles in each soil



TPFA



NFV

Consistent nonlinear solver

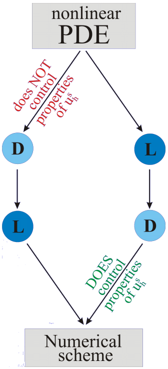
$$\frac{\partial(\phi\, s)}{\partial t} + \mathrm{div}(\mathbf{q}) = 0, \qquad \mathbf{q} = -\mathbb{K}\, k_r (\nabla p - \rho \mathbf{g})$$

Calculation of the exact Jacobian is not practical for advanced discretizations. But such schemes can be applied to continuum Jacobian[6]:

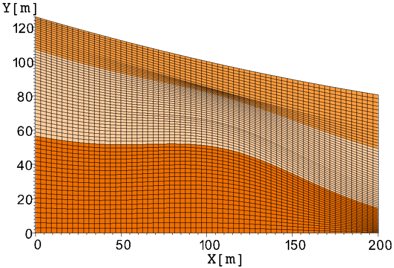
$$\mathcal{J}\,\delta p = \frac{\partial(\phi\, s)}{\partial p}\,\frac{\partial\, \delta p}{\partial t} - \mathrm{div}\big(\mathbb{K}\, k_r\, \nabla \delta p\big) + \mathrm{div}\big(\mathbf{V}\,\delta p\big)$$

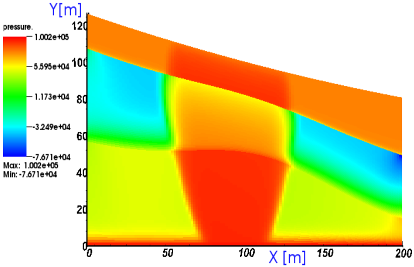
where

$$\mathbf{V} = -\mathbb{K}\frac{\partial k_r}{\partial p}(\nabla p - \rho \mathbf{g}) = \mathbf{q}\,\frac{\partial k_r}{\partial p}\,\frac{1}{k_r}$$

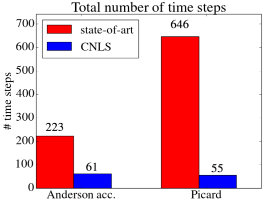


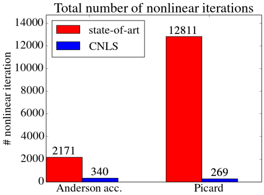
[6] J.Yue, G.Yuan, CCP 2011

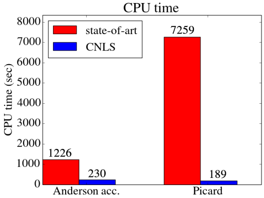




CNLS outperforms Picard and accelerated Picard:







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Conclusion

- **Physics-preserving discretizations mimic critical properties of underlying PDEs (conservation laws, symmetries, positivity, MPs).**
- **Mimetic finite difference method addresses many requirements for the ideal scheme; however, the discrete maximum principle (DMP) is only conditional.**
- **Nonlinear FV scheme is nonsymmetric but gives unconditional DMP. It is well suited for solving nonlinear Richards' equation.**
- **Consistent nonlinear solver is the promising framework for building Jacobian-free iterative methods.**