Monotone nonlinear Finite Volume Scheme for Flow in Porous Media

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Overview DuMu$^X$

- **DuMu$^X$:** DUNE for Multi-{Phase, Component, Scale, Physics, ...} Flow and Transport in Porous Media
- Development started 2007
- Based on DUNE

  ![Dune](image)

  Distributed and Unified Numerics Environment

- Current release: 2.9 (March 2016, git repository)
- Recently started to use opm-grid (corner-point grids), “straight forward” because of the dune grid interface
- Interesting for us: using other opm modules like upscaling …
Why nonlinear Finite Volume Methods?

Desirable features:

- **accuracy**
  - locally mass conservative

- **efficiency**
  - sparse matrices

- **flexibility**
  - unstructured grids
  - anisotropic, heterogeneous tensors

- **discretization**
  - MPFA
  - Mixed Finite Element
  - Mimetic Finite Difference

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Why nonlinear Finite Volume Methods?

Desirable features:

- **accuracy**
  - locally mass conservative
  - monotone
  - extremum principles

- **efficiency**
  - sparse matrices

- **flexibility**
  - unstructured grids
  - anisotropic, heterogeneous tensors

- **discretization**
  - MPFA
  - Mixed Finite Element
  - Mimetic Finite Difference
  - Nonlinear Schemes
Idea of flux calculation

Flux Approximation: (elliptic equation)

\[- \nabla \cdot (K \nabla p) = q \quad \rightarrow \quad -\int_{\partial V_i} (K \nabla p) \cdot n \, dS = \int_{V_i} q \, dV\]

\[K = K^T, \quad d := K \cdot n \quad \rightarrow \quad -\sum_{\sigma} \int_{\sigma} \nabla p \cdot d \, dS = \int_{V_i} q \, dV\]

For each cell face \(\sigma \subset \partial V_i\) approximate the fluxes

\[f_\sigma = -|\sigma| \nabla p \cdot d, \quad d := K \cdot n\]
Idea of flux calculation for homogeneous permeability tensor

\[ f_1 = -|\sigma| \nabla p \cdot d, \quad d := K \cdot n \]

Conormal decomposition:
Idea of flux calculation for homogeneous permeability tensor

\[ f_1 = -|\sigma| \left( \alpha_1 (p_j - p_i) + \right) \]

conormal decomposition:
Idea of flux calculation for homogeneous permeability tensor

\[ f_1 = -|\sigma| (\alpha_1 (p_j - p_i) + \alpha_2 (p_k - p_i)) \]

conormal decomposition:
Idea of flux calculation for homogeneous permeability tensor

\[ f_1 = -|\sigma| (\alpha_1 (p_j - p_i) + \alpha_2 (p_k - p_i)) \quad f_2 = -|\sigma| (\beta_1 (p_i - p_j) + \beta_2 (p_l - p_j)) \]

conormal decomposition: \(\alpha, \beta \geq 0\)  

averaging
Averaged Flux Approximation

\[ f_\sigma := \mu_1 f_1 - \mu_2 f_2, \quad \mu_1 + \mu_2 = 1, \quad 0 \leq \mu_1, \mu_2 \leq 1 \]

\[ = |\sigma| (\mu_1 (\alpha_1 + \alpha_2) + \mu_2 \beta_1) p_i \]
\[ - |\sigma| (\mu_2 (\beta_1 + \beta_2) + \mu_1 \alpha_1) p_j \]
\[ - |\sigma| (\mu_1 \alpha_2 p_k - \mu_2 \beta_2 p_l) \]

Possible choice: \( \mu_1 = \mu_2 = 0.5 \)

Averaged Multi-Point Flux Approximation: AvgMPFA
Averaged Flux Approximation

\[ f_\sigma := \mu_1 f_1 - \mu_2 f_2, \quad \mu_1 + \mu_2 = 1, \quad 0 \leq \mu_1, \mu_2 \leq 1 \]

\[ = |\sigma| (\mu_1 (\alpha_1 + \alpha_2) + \mu_2 \beta_1) p_i \]
\[ - |\sigma| (\mu_2 (\beta_1 + \beta_2) + \mu_1 \alpha_1) p_j \]
\[ - |\sigma| (\mu_1 \alpha_2 p_k - \mu_2 \beta_2 p_l) \]
\[ \overset{1}{=} 0 \]

\[ \rightarrow f_\sigma = t_1(p_k, p_l)p_i - t_2(p_k, p_l)p_j \]

Nonlinear Flux Approximation: NLTPFA


Heterogeneous permeability tensor

Harmonic Averaging Point: \[ \overline{p}_\sigma = \frac{c_i p_i + c_j p_j}{c_i + c_j} \]

\[ \overline{x}_\sigma = \frac{c_i x_i + c_j x_j + (K_i - K_j) n_{ij}}{c_i + c_j} \]

\[ c_i = \frac{n_{ij} \cdot K_i \cdot n_{ij}}{\text{dist}(x_i, \sigma)} \]

\[ c_j = \frac{n_{ij} \cdot K_j \cdot n_{ij}}{\text{dist}(x_j, \sigma)} \]

Agélás et al., "A nine-point finite volume scheme for the simulation of diffusion in heterogeneous media."
Generalization of conormal decomposition
Generalization of conormal decomposition

\[
\min_{\alpha \in \mathbb{R}^{NF}} F(\alpha)
\]

subject to

\[
d_\sigma = A\alpha
\]

\[
\sum \alpha_i \geq c, \quad \alpha_i \geq 0
\]

\[
A = (x_{\sigma_1} - x_c, \ldots, x_{\sigma_{NF}} - x_c)
\]

example:

\[
F(\alpha) = \sum \alpha_i
\]
Generalization of conormal decomposition

\[
\min_{\gamma \geq 0, \alpha \in \mathbb{R}^{NF}} \kappa \gamma + F(\alpha)
\]

subject to \( d_\sigma = A\alpha \)

\[
\sum \alpha_i \geq c, \quad \alpha_i \geq -\gamma
\]

\[
A = (x_{\sigma_1} - x_c, \ldots, x_{\sigma_{NF}} - x_c)
\]

example:

\[
F(\alpha) = \sum \alpha_i
\]

\[
\kappa \gg F(\alpha)
\]

If \( \gamma > 0 \) then there exists no conormal decomposition with only positive coefficients.

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Modification of nonlinear TPFA

\[ f_{\sigma} = t_1(\mu_1, \mu_2)p_i - t_2(\mu_1, \mu_2)p_j \]

\[ \underbrace{-\mu_1 \lambda_1 + \mu_2 \lambda_2} \]

\[ : R_{\sigma} = 0 \]

\[ \lambda_1 := \sum \alpha_{k,j} p_j, \quad \lambda_2 := \sum \alpha_{l,j} p_j. \]

\[ \rightarrow R_{\sigma} = 0, \quad \text{if } \lambda_1 \lambda_2 > 0 \]

\[ \text{if } \lambda_1 \lambda_2 < 0 : \quad f_{\sigma} = \left( t_1(\mu_1, \mu_2) + \frac{|R_{\sigma}| + R_{\sigma}}{2(p_i + \varepsilon)} \right) p_i \]

\[ - \left( t_2(\mu_1, \mu_2) + \frac{|R_{\sigma}| - R_{\sigma}}{2(p_j + \varepsilon)} \right) p_j \]
Literature overview NLTPFA

Existing results in literature:

- proof of monotonicity
- convergence behavior for elliptic equation (numerically)
  (second order for pressure, first order for flux)

Focus of this talk:

- comparison with commonly used linear schemes
- influence of additional nonlinearity due to nonlinear flux approximation
- challenging grids
- complex physics
Monotonicity

\[-\nabla \cdot (K \nabla p) = 0, \quad \Omega = [0, 1] \times [0, 1],\]

Setting:

\[p = 0\]

\[p = 10^5\]

\[K\]

\[K = R\left(\frac{\pi}{6}\right) \begin{pmatrix} 1000 & 0 \\ 0 & 1 \end{pmatrix} R\left(\frac{\pi}{6}\right)^{-1}\]
Monotonicity

NLTPFA (nnz 192544)

AvgMPFA (nnz 192544)

TPFA (nnz 132800)

MPFA-L (nnz 185883)

MPFA-O (nnz 238372)

Box (nnz 241152)

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Monotonicity

NLTPFA

AvgMPFA ~2.5%

TPFA

MPFA-L ~3%

MPFA-O ~7%

Box ~2.2%

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Properties of NLTPFA

• second order accuracy for pressure, first order for flux (numerical results)

• monotonicity
Challenging grids (corner-point grids)

- curved faces
- degenerated points
- degenerated faces
- non-convex cells
- centroid outside of cell
- non-matching grids

opm-grid
Example: non-matching grid

Setting:

\[ \Omega_1 \]

\[ \Omega_2 \]

generated with MRST

\[ \mathbf{K}_1 = \begin{pmatrix} 3 & 1 & 0 \\ 1 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

\[ \mathbf{K}_2 = \begin{pmatrix} 10 & 3 & 0 \\ 3 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

\[ p_1 = 6x + 1.6y + 4xy - 2y^2 + z + 1.4 \]

\[ p_2 = x + 2.8y + 2xy - 2y^2 + z + 4.4 \]
Example: non-matching grid
Example: non-matching grid

\[ e_p = 2.74 \cdot 10^{-4} \]

\[ e_p = 7.02 \cdot 10^{-5} \]

\[ |p_{ex} - p_h| \]

\[ O(h^2) \]

\[ e_p = 1.77 \cdot 10^{-5} \]

\[ |p_{ex} - p_h| \]
Example: corner-point grid

Setting:

- Cell volumes differ by five orders of magnitude
- optimization: approx. 7% of cells with negative coefficients

opm-grid
Example: corner-point grid

Setting:

\[ p = 1 \cdot 10^5 \text{ Pa} \]

\[ p = 2 \cdot 10^5 \text{ Pa} \]

- Cell volumes differ by five orders of magnitude
- Optimization: approx. 7% of cells with negative coefficients

opm-grid
Example: corner-point grid

- Grid
  - 5m
  - 62.5m
  - 125m

- Exact
  - \( p_{\text{exact}} \)
    - 2.0e+05
    - 1.7e+05
    - 1.5e+05
    - 1.3e+05
    - 1.0e+05

- Linear TPFA
- Nonlinear TPFA

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Example: corner-point grid

grid

5m

62.5m

125m

exact

$p_{exact}$

linear TPFA

$|p_{exact} - p_{tpfa}|$

nonlinear TPFA

$|p_{exact} - p_{ntpfa}|$

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Example: corner-point grid

grid

5m
62.5m
125m

exact

\( p_{\text{exact}} \)

linear TPFA

\[ |p_{\text{exact}} - p_{\text{tpfa}}| \]

nonlinear TPFA

\[ |p_{\text{exact}} - p_{\text{ntpfa}}| \]

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Example: corner-point grid

grid

125m

5m

62.5m

exact

linear TPFA

$p_{exact} - p_{tpfa}$

$|p_{exact} - p_{tpfa}|$

nonlinear TPFA

$|p_{exact} - p_{ntpfa}|$

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Example: corner-point grid

nonlinear TPFA
Example: corner-point grid

nonlinear TPFA

opm-grid
Properties of NLTPFA

• second order accuracy for pressure, first order for flux (numerical results)

• monotonicity

• handling of complex grids like corner-point grids
Comparison of different schemes

Setting:

- \( p_w = 2 \cdot 10^5 \text{ Pa} \)
- \( S_w = 1 \)
- \( S_{w,\text{init}} = 0 \)
- \( u_w = 0 \)
- \( u_n = \frac{1.5 \cdot 10^{-3}}{1460} \text{ m/s} \)

- incompressible two-phase flow
- no gravity
- no capillary pressure
Comparison of different schemes

Setting 1:

Setting 2:

Setting 3: permeability distribution

Setting 4:
Comparison of different schemes

Setting 1:

Setting 2:

Setting 3:

Setting 4:

NLTPFA solution

similar results for all schemes:

AvgMPFA
Box
TPFA
MPFA-L
MPFA-O
Comparison of different schemes

- NLTPFA
- AvgMPFA
- MPFA-L
- MPFA-O
- Box
- TPFA

Total Newton iter vs setting

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Comparison of different schemes

\[ \bar{\kappa} = \frac{\sum_i \Delta t_i \sqrt{\kappa_1(J_i)\kappa_\infty(J_i)}}{\sum_i \Delta t_i} \]

Condition number influences iterative solver behavior
Comparison of different schemes

BiCGStab solver with ILUn preconditioning
Properties of NLTPFA

- second order accuracy for pressure, first order for flux (numerical results)
- monotonicity
- handling of complex grids like corner-point grids
- NLTPFA behaves better than corresponding linear scheme (AvgMPFA)
- linear and nonlinear solvers behave similar to linear schemes
More complex example

Compressible two-phase two-component nonisothermal (2p2cni) flow equations:

Mass balance:

\[
\phi \frac{\partial (\sum_{\alpha} \rho_{mol,\alpha} x_\alpha^\kappa S_\alpha)}{\partial t} - \sum_{\alpha} \text{div} \left\{ \frac{k_{r\alpha}}{\mu_\alpha} \rho_{mol,\alpha} x_\alpha^\kappa K (\nabla p_\alpha - \rho_\alpha g) \right\} - \sum_{\alpha} \text{div} \left\{ \tau \phi S_\alpha \rho_{mol,\alpha} D_\alpha^\kappa \nabla x_\alpha^\kappa \right\} - q^\kappa = 0, \quad \kappa \in \{\text{CO}_2, \text{Brine}\}.
\]

Energy balance:

\[
\phi \frac{\partial (\sum_{\alpha} \rho_\alpha u_\alpha S_\alpha)}{\partial t} + (1 - \phi) \frac{\partial \rho_s c_s T}{\partial t} - \text{div}(\lambda_{pm} \nabla T) - \sum_{\alpha} \text{div} \left\{ \frac{k_{r\alpha}}{\mu_\alpha} \rho_\alpha h_\alpha K (\nabla p_\alpha - \rho_\alpha g) \right\} - q^h = 0.
\]

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**Numerical Examples**

**Setting:**

- $k = 10^{-19}, \quad \phi = 0.001$
- $k = 10^{-15}, \quad \phi = 0.05$
- $k = 3.0 \cdot 10^{-14}, \quad \phi = 0.2$

**Simulation Time:**

~6.3 years

**CO₂ Injection**

**Unstructured Grid:**

**Cell Areas:**

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Solution of NLTPFA

After grid refinement, ~60000 cells

\( S_n \)

\( p_n \)

\( x_w^{Brine} \)

\( T \)
Adaptive Grid

TPFA:

NLTPFA:

$S_n$

0.00

0.280

0.278

0.557

0.835

0.839

0.559

0.280

0.557

0.835

0.839
Properties of NLTPFA

- second order accuracy for pressure, first order for flux (numerical results)
- monotonicity
- handling of complex grids like corner-point grids
- NLTPFA behaves better than corresponding linear scheme (AvgMPFA)
- linear and nonlinear solvers behave similar to linear schemes
- (straight forward) applicability for physically complex nonlinear equations (2p2cni)
Conclusion

• second order accuracy for pressure, first order for flux (numerical results)

• monotonicity

• handling of complex grids like corner-point grids

• NLTPFA behaves better than corresponding linear scheme (AvgMPFA)

• linear and nonlinear solvers behave similar to linear schemes

• (straight forward) applicability for physically complex nonlinear equations (2p2cni)


**Conclusion**

- second order accuracy for pressure, first order for flux (numerical results)
- monotonicity
- handling of complex grids like corner-point grids
- NLTPFA behaves better than corresponding linear scheme (AvgMPFA)
- linear and nonlinear solvers behave similar to linear schemes
- (straight forward) applicability for physically complex nonlinear equations (2p2cni)
**Implementation in DuMu\(^X\)**

**dumux-stable:**
Box and TPFA method for fully-implicit porous media flow

**current development:**
- Unification of finite volume schemes for fully-implicit models (linear and nonlinear schemes)
- Schemes differ in face stencil classes, which provide iterators for flux calculation or matrix assembly
- Generalization of *fvGeometry*, *fluxVars*, … classes, to be able to handle grids like corner-point grids (dynamic implementation)
- Models independent of discretization
Thank you very much!

References:


