Discretization methods for AD-GPRS

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SUPRI-B meeting

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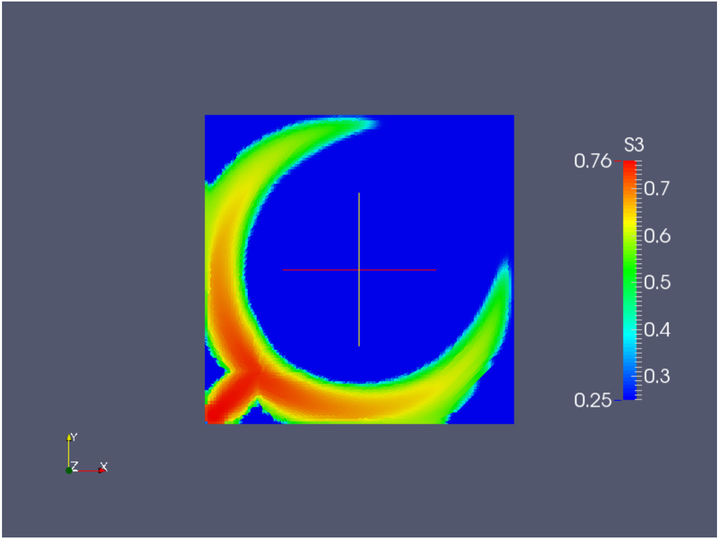
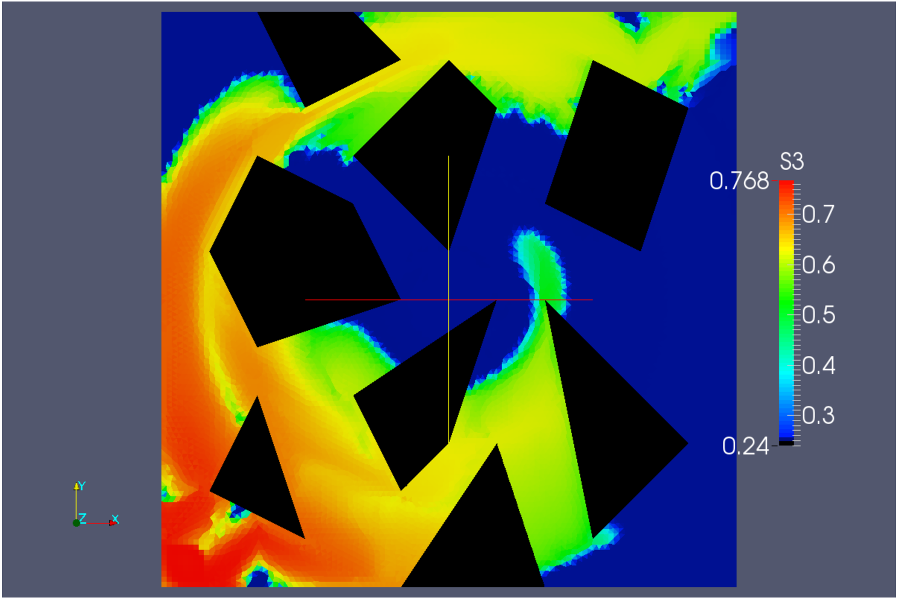
- Nonlinear Finite Volume Schemes.
- Discretization Toolkit for AD-GPRS.
- Performance improvements for AD-GPRS.

Intro video



Intro video



Nonlinear Finite Volume Schemes

Next slides

Derivation of one of the schemes.

Nonlinear Finite Volume Schemes

Why one would like to use nonlinear scheme?

- To obtain wanted properties of the schemes:
  - Positivity of the solution.
  - Satisfy discrete maximum principle.
- To improve robustness and speed of the simulator.

Is there anything wrong with them?

Yes!

- Proof of convergence requires coercivity.
- DMP schemes require specific nonlinear solvers.

In the following: derivation of one of the nonlinear schemes.

Nonlinear Finite Volume Schemes

Toy problem

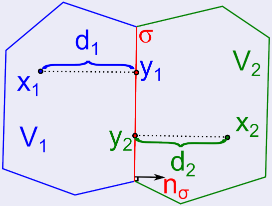
Solve for p that satisfy anisotropic diffusion equation with source f:

$$\begin{cases} -\nabla \cdot \mathbb{K} \nabla p = f & \text{in} \quad \Omega, \\ \mathbb{K} \dfrac{\partial p}{\partial \vec{n}} = f_N & \text{in} \quad \Gamma_N, \\ p = f_D & \text{in} \quad \Gamma_D. \end{cases}$$

Where domain Ω is decomposed into polyhedral mesh, $\mathbb{K}$ is a symmetric positive definitive and piecewise-constant on each polyhedron of the mesh and $\Gamma_N \cup \Gamma_D = \partial\Omega$ is a piecewise-linear boundary.

Nonlinear Finite Volume Schemes

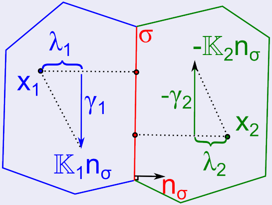
Approximation of the gradient in two materials



$$\nabla_1 p = \frac{p(\mathbf{y}_1) - p_1}{d_1}\vec{n}_\sigma + \vec{g}_\sigma,$$

$$-\nabla_2 p = \frac{p(\mathbf{y}_2) - p_2}{d_2}\vec{n}_\sigma + \vec{g}_\sigma.$$

Representation of co-normals in two materials



$$\lambda_1 = \vec{n}_\sigma \cdot \mathbb{K}_1 \vec{n}_\sigma, \qquad \vec{\gamma}_1 = (\mathbb{K}_1 - \lambda_1 \mathbb{I})\vec{n}_\sigma,$$

$$\lambda_2 = \vec{n}_\sigma \cdot \mathbb{K}_2 \vec{n}_\sigma, \qquad \vec{\gamma}_2 = (\mathbb{K}_2 - \lambda_2 \mathbb{I})\vec{n}_\sigma.$$

Nonlinear Finite Volume Schemes

Flux continuity condition on interface σ

$$\mathbb{K}_1 \nabla_1 p - \mathbb{K}_2 \nabla_2 p = 0$$

or

$$\lambda_1 \frac{p(\mathbf{y}_1) - p_1}{d_1} + \vec{\gamma}_1 \cdot \vec{g}_\sigma = \lambda_2 \frac{p_2 - p(\mathbf{y}_2)}{d_2} + \vec{\gamma}_2 \cdot \vec{g}_\sigma .$$

Interpolation on interface σ

$$p(\mathbf{y}_1) = p(\mathbf{y}) + (\mathbf{y}_1 - \mathbf{y}) \cdot \vec{g}_\sigma , \qquad p(\mathbf{y}_2) = p(\mathbf{y}) + (\mathbf{y}_2 - \mathbf{y}) \cdot \vec{g}_\sigma .$$

We want to get an expression for $p(\mathbf{y})$ on σ.

Nonlinear Finite Volume Schemes

Interpolation on interface σ

$$p(\mathbf{y}) = \frac{\lambda_1 d_2 p_1 + \lambda_2 d_1 p_2}{\lambda_1 d_2 + \lambda_2 d_1} + \frac{d_1 d_2}{\lambda_1 d_2 + \lambda_2 d_1}(\gamma_2 - \gamma_1) \cdot \vec{g}_\sigma + \left(\mathbf{y} - \frac{\lambda_1 d_2 \mathbf{y}_1 + \lambda_2 d_1 \mathbf{y}_2}{\lambda_1 d_2 + \lambda_2 d_1}\right) \cdot \vec{g}_\sigma.$$

Harmonic averaging point

$$\mathbf{y}_\sigma = \frac{\lambda_1 d_2 \mathbf{y}_1 + \lambda_2 d_1 \mathbf{y}_2 + d_1 d_2 (\gamma_1 - \gamma_2)}{\lambda_1 d_2 + \lambda_2 d_1},$$

$$p(\mathbf{y}_\sigma) = \frac{\lambda_1 d_2 p_1 + \lambda_2 d_1 p_2}{\lambda_1 d_2 + \lambda_2 d_1}.$$

Nonlinear Finite Volume Schemes

Harmonic averaging point

Léo Agelas, Robert Eymard, Raphaèle Herbin: *A nine-point finite volume scheme for the simulation of diffusion in heterogeneous media*, C. R. Acad. Sci. Paris 2009

We will proceed in derivation the decomposition of the total flux into **transverse** and **normal** parts.

Nonlinear Finite Volume Schemes

Normal component of the flux

$$\frac{\lambda_1}{d_1}(p(\mathbf{y}_\sigma)-p_1) = \frac{\lambda_2}{d_2}(p_2-p(\mathbf{y}_\sigma)) = \frac{\lambda_1\lambda_2}{\lambda_1 d_2+\lambda_2 d_1}(p_2-p_1).$$

Which is exectly definition of the Two-Point Flux Approximation or TPFA.

Transverse direction of the flux

$$\vec{\gamma} = \mathbb{K}_1\vec{n}_\sigma - \frac{\lambda_1}{d_1}(\mathbf{y}_\sigma - \mathbf{x}_1) = \mathbb{K}_2\vec{n}_\sigma - \frac{\lambda_2}{d_2}(\mathbf{x}_2 - \mathbf{y}_\sigma)$$
$$= \frac{\lambda_1\lambda_2(\mathbf{y}_1 - \mathbf{y}_2) + \lambda_2 d_1\vec{\gamma}_1 + \lambda_1 d_2\vec{\gamma}_2}{\lambda_1 d_2 + \lambda_2 d_1}.$$

Nonlinear Finite Volume Schemes

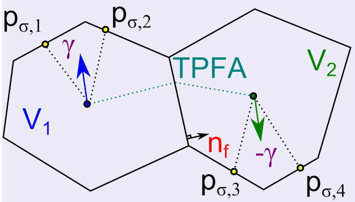
Transverse direction of the flux

Lina Chang, Guangwei Yuan: *An efficient and accurate reconstruction algorithm for the formulation of cell-centered diffusion schemes*, J. Comp. Phys., 2012

How do we approximate the **transverse** part of the flux? In each polyhedron V_1 and V_2 adjacent to the interface σ we search a positive-definite basis.

Nonlinear Finite Volume Schemes

Transverse flux approximation



$$\vec{\gamma} \cdot \nabla_1 p = \sum_{i_1=1}^{dim} \alpha_{i_1}(p_{\sigma,i_1} - p_1),$$

$$-\vec{\gamma} \cdot \nabla_2 p = \sum_{i_2=1}^{dim} \beta_{i_2}(p_{\sigma,i_2} - p_2),$$

$$\forall i_1, i_2 \in [1, dim] : \alpha_{i_1}, \beta_{i_2} \geq 0.$$

We define transverse flux $\gamma = \vec{\gamma} \cdot \nabla p$ as a convex combination of two parts $\gamma_1 = \vec{\gamma} \cdot \nabla_1 p$ and $\gamma_2 = \vec{\gamma} \cdot \nabla_2 p$.

Nonlinear Finite Volume Schemes

Transverse flux approximation

$$\begin{cases} \gamma = \mu_1 \gamma_1 + \mu_2 \gamma_2, \\ \mu_1 + \mu_2 = 1. \end{cases}$$

Choice of $\mu_1 = \mu_2 = \frac{1}{2}$ is not very stable. We can follow two approaches of the definition of weights μ_1 and μ_2.

Nonlinear Two-Point Flux Approximation

Christophe Le Potier *Schéma volumes finis monotone pour des opérateurs de diffusion fortement anisotropes sur des maillages de triangles non structurés* C. R. Acad. Sci. Paris, 2005

Nonlinear Finite Volume Schemes

Nonlinear Two-Point Flux Approximation

Expanded expressions for one-sided fluxes:

$$\gamma_1 = \alpha_1(p_{\sigma,1} - p_1) + \alpha_2(p_{\sigma,2} - p_1),$$
$$\gamma_2 = \beta_3(p_2 - p_{\sigma,3}) + \beta_4(p_2 - p_{\sigma,4}).$$

Linear combination:

$$\gamma = \mu_2(\beta_3 + \beta_4)p_2 - \mu_1(\alpha_1 + \alpha_2)p_1 + \mu_1(\alpha_1 p_{\sigma,1} + \alpha_2 p_{\sigma,2}) - \mu_2(\beta_3 p_{\sigma,3} + \beta_4 p_{\sigma,4}).$$

We define μ_1 and μ_2 so that expression in red is zero and convexity $\mu_1 + \mu_2 = 1$ is satisfied. If we freeze μ_1 and μ_2 on each iteration then the matrix obtained is an M-matrix with nonnegative column-sum.

Nonlinear Finite Volume Schemes

Nonlinear Multi-Point Approximation

Enrico Bertolazzi, Gianmarco Manzini: *A second-order maximum principle preserving finite volume method for steady convection-diffusion problems*, SIAM J. Numer. Anal., 2005

The weights are defined as:

Nonlinear Multi-Point Approximation

$$\mu_1 = \frac{|\gamma_2|}{|\gamma_1| + |\gamma_2|}, \qquad \mu_2 = \frac{|\gamma_1|}{|\gamma_1| + |\gamma_2|}.$$

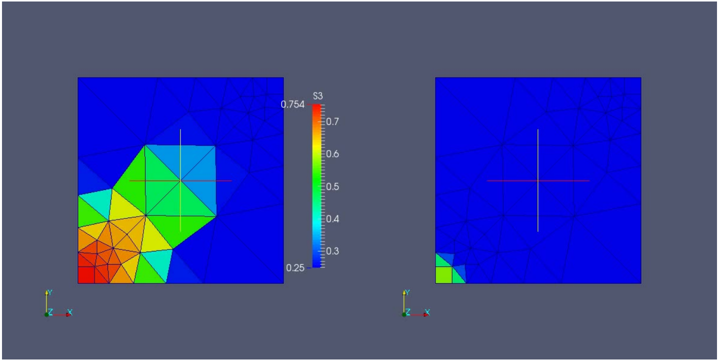
Nonlinear Finite Volume Schemes

Nonlinear Multi-Point Approximation

$$\gamma = \begin{cases} \gamma_1\mu_1 = \gamma_2\mu_2, & \gamma_1\gamma_2 > 0, \\ 0, & \gamma_1\gamma_2 < 0. \end{cases}$$
$$= \frac{|\gamma_1||\gamma_2|}{|\gamma_1| + |\gamma_2|}(\mathrm{sign}(\gamma_1) + \mathrm{sign}(\gamma_2)).$$

If we freeze μ_1 and μ_2 and will use $\gamma = \gamma_1\mu_1$ to define flux on V_1 and $\gamma = \gamma_2\mu_2$ on V_2 then on each iteration the matrix obtained will be an M-matrix with nonnegative row-sum.

Nonlinear Finite Volume Schemes



Why a new formulation for the scheme was derived?

Nonlinear Finite Volume Schemes

Convergence

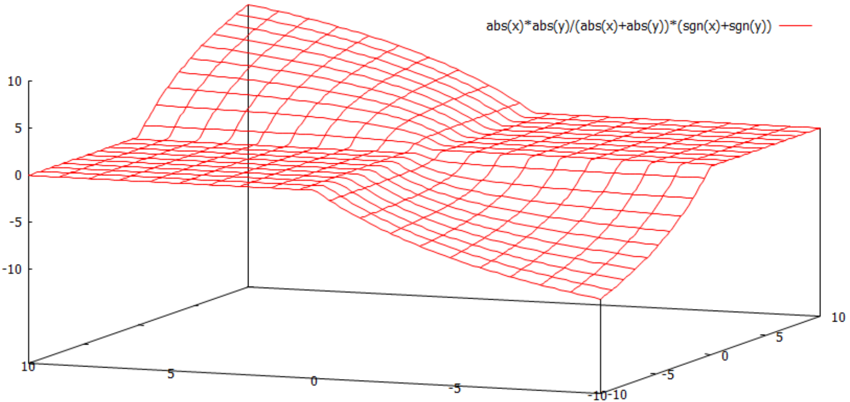
Jérôme Droniou, Christophe Le Potier:
Construction and convergence study of schemes preserving the elliptic local maximum principle, SIAM J. Numer. Anal, 2011

Nonlinear solver

Since methods are convergent under coercivity assumption we will use the Newton method with the full Jacobian.

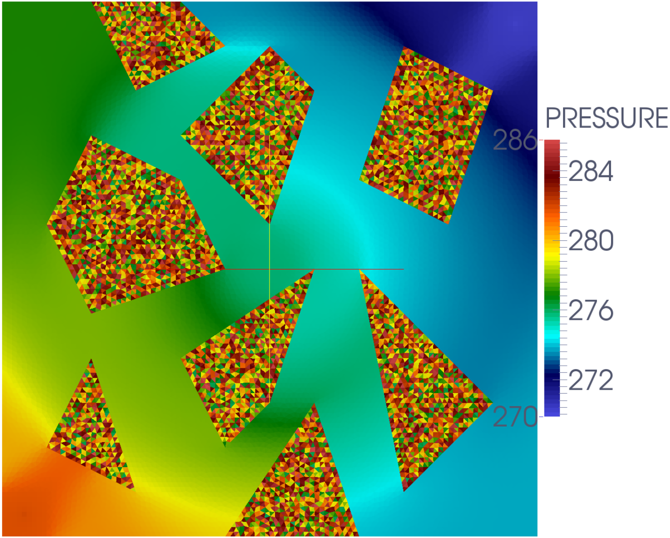
- NTPFA has a convex flux function in positive region.
- NMPFA has an upwind-style plateau in the flux and may not converge with pure newton method.

Nonlinear Finite Volume Schemes



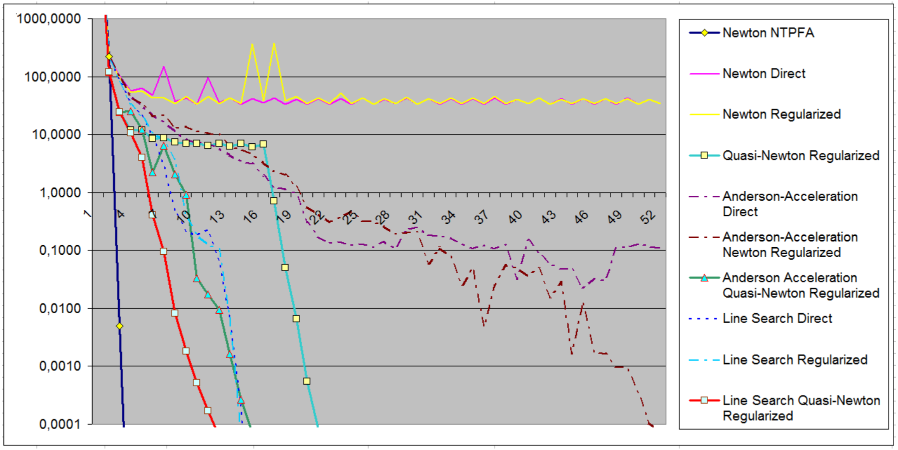
Shape of the **transverse** flux function. Presence of two plateau regions result in unconstraned behavior of transverse half-fluxes in these regions.

Nonlinear Finite Volume Schemes



Convergence of the NMPFA method on a simple problem.

Nonlinear Finite Volume Schemes



NTPFA: 3 iterations of Newton method
NMPFA: 11 iterations of Quasi-Newton + Line Search or 14 iterations of Quasi-Newton + Anderson Acceleration.

Discretization Toolkit

Next slides

Discretization toolkit for AD-GPRS.

Discretization Toolkit

Purposes

- Produce an input for AD-GPRS:
  - produce discretization for a general polyhedral mesh;
  - discretize a fracture network;
  - intersect wells with mesh geometry, compute well indices;
  - prepare geometry, initial and boundary condition for geomechanics (under work).
- Works for me as a sandbox for various methods.

Discretization Toolkit

Includes

- A dialog-style console application that produces input for AD-GPRS.
- Converter of ASCII output of AD-GPRS to grid data.
- Several models for testing purposes:
  - Anisotropic diffusion problem.
  - Black oil problem.
- Compute error norms on different grids.
- Sample grid generators and converters.

Discretization Toolkit

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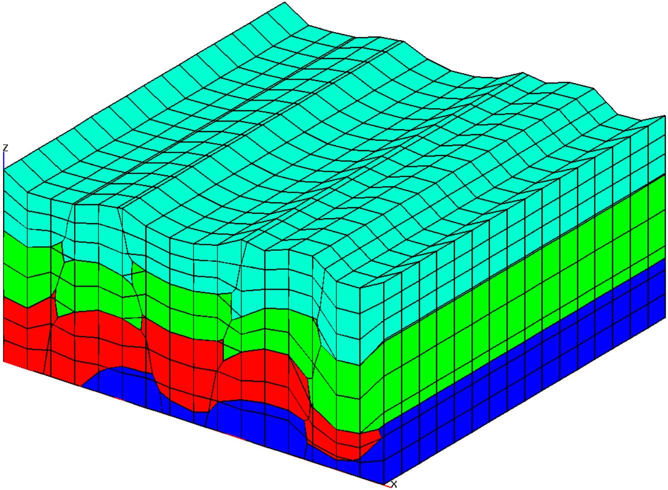
Discretization Toolkit

Workflow for AD-GPRS input

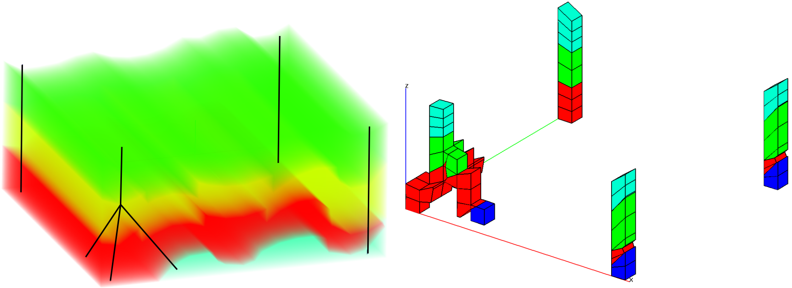
- Define properties such as porosity or permeability.
- Define apertures on the fracture faces.
- Select one of the availible schemes:
  - TPFA, MPFA-O, MPFA-L, MPFA-G, MPFA-A, MPFA-B
  - NTPFA-A, NTPFA-B, NTPFA-C
  - NMPFA-A, NMPFA-B
  - fracture treatment: full scheme, reduce to two-point inside fracture, reduce to two-point between matrix and fracture.
- Provide inclinometry of the well.
- Input initial and boundary conditions of geomechanics, not well tested yet. :(

Discretization Toolkit



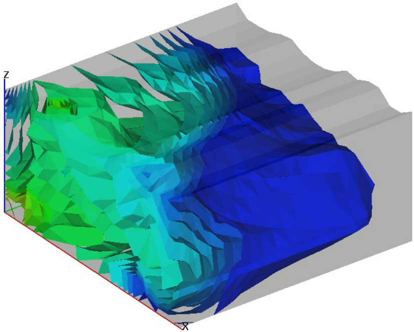
Imagine we were given a mesh like this and were asked to calculate something.

Discretization Toolkit



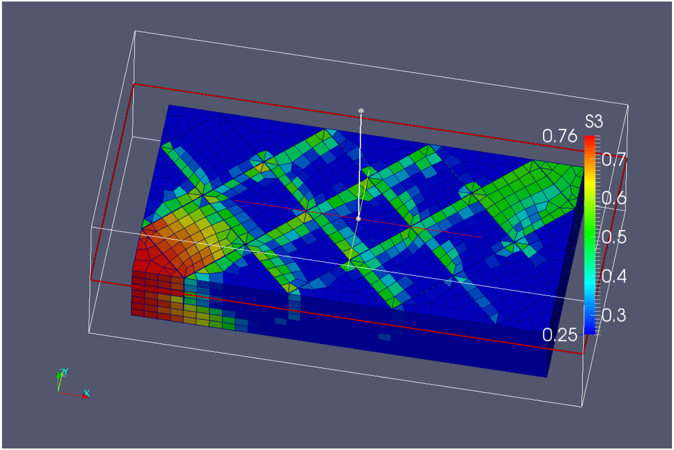
Wells definition and their intersection with mesh.

Discretization Toolkit



We feed input to AD-GPRS and run the black oil model. Convert ASCII-formated results into gmv format and make the video with GMV and ffmpeg.

Discretization Toolkit



The variant with fractures thanks to Timur Garipov.
Convert ASCII-formated results into vtk format and make the video in paraview.

Performance

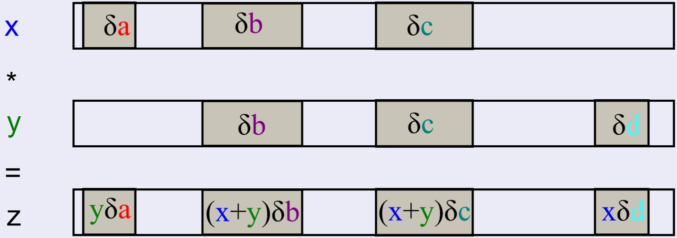
Next slides

Performance improvements and comparison of the performance of the schemes in AD-GPRS.

Performance

Operations with AD-variables

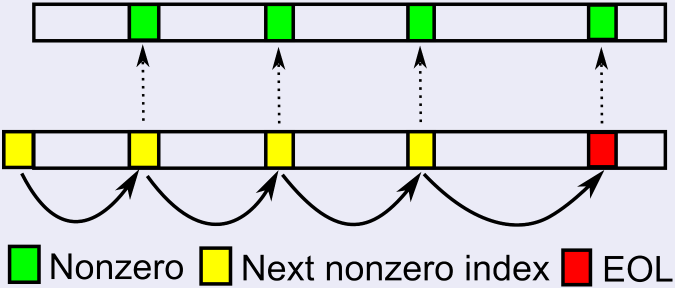
Results in the problem of calculation of linear combination of sparse vectors:



AD-GPRS analyses sparsity of sparse vectors to be combined and then uses either implicit binary tree representation or dense representation. (by Rami Younis)

Performance

Dense linked list as in ILU(τ) preconditioners

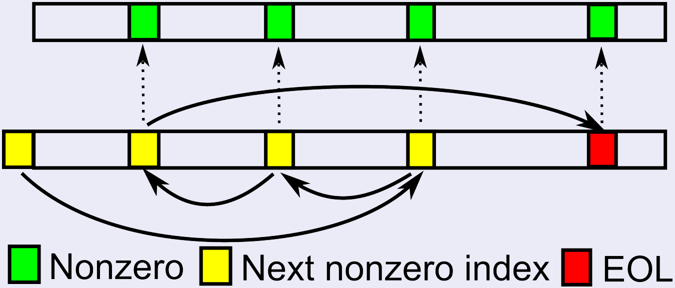


Pros and cons

- Pros: No need to test for sparsity.
- Cons: Have to rewind and search correct position to keep list sorted.

Performance

Dense linked list as for Schur complement



Pros and cons

- Pros: Insertion order is arbitrary.
- Cons: Produces unsorted result, not a big problem.

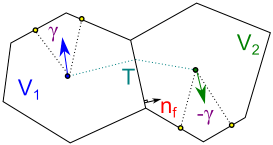
Performance

Unadressed issues

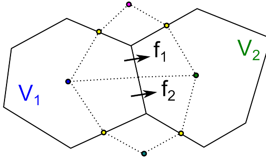
- AD-expression $\frac{x}{\sqrt{x*x+\varepsilon}}$ will result in an internal temporary representation of linear combination: $\frac{1}{\sqrt{x^2+\varepsilon}}\delta x + \frac{x^2}{2(x^2+\varepsilon)^{\frac{3}{2}}}\delta x + \frac{x^2}{2(x^2+\varepsilon)^{\frac{3}{2}}}\delta x$.
- Moreover if we multiply an expression by a constant each entry in an internal representation have to be multiplied.

Both issues greatly impact performance of nonlinear schemes.

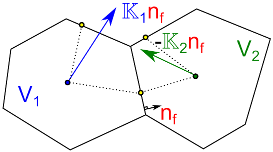
Performance



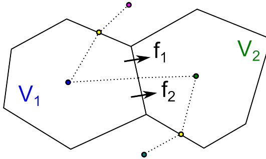
NTPFA-A



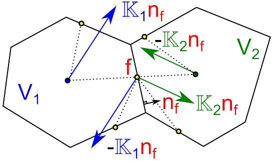
MPFA-O



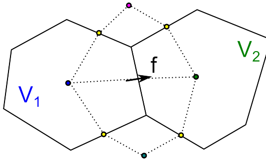
NTPFA-B



MPFA-L

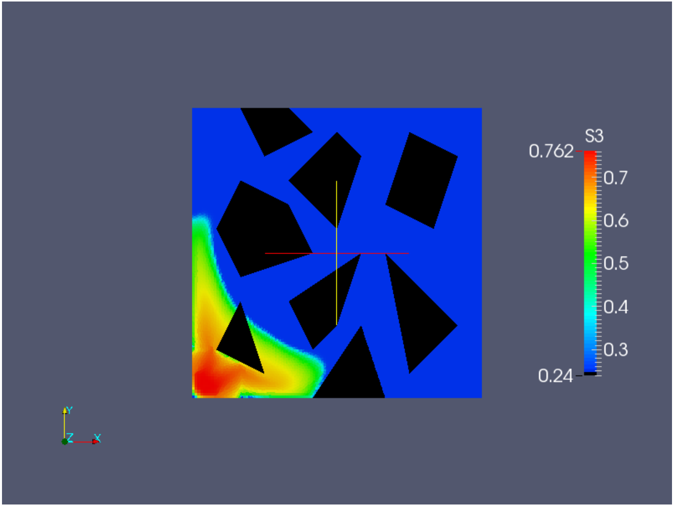


NTPFA-C



MPFA-G

Performance



Several steps of the problem for comparison with anisotropy ratio $\frac{10}{100}$.

Performance

Total time, seconds:

Method Approach	Nonlinear iterations	Linear iterations
TPFA	180	4941
MPFA-O	157	2790
MFPA-G	188+20	9475+7021
MPFA-L	180+20	12764+4053
NTPFA-A	159	4743
NTPFA-B	158	5170
NTPFA-C	170	3449

Performance

Total time, seconds:

Method Approach	SAXPY+IBTREE	Ordered LL	Unordered LL
TPFA	109.35	95.73	102.46
MPFA-O	158.90	134.07	133.01
MFPA-G	525.78	355.22	341.62
MPFA-L	435.36	306.96	273.46
NTPFA-A	160.12	123.98	129.64
NTPFA-B	162.44	133.00	136.92
NTPFA-C	162.04	126.73	127.24

Performance

Discretization, seconds:

Method Approach	SAXPY+IBTREE	Ordered LL	Unordered LL
TPFA	15.33	15.26	15.6
MPFA-O	32.66	26.35	26.51
MFPA-G	31.90	20.78	21.28
MPFA-L	22.77	16.8	17.08
NTPFA-A	24.30	17.46	18.00
NTPFA-B	22.58	17.1	17.40
NTPFA-C	41.75	26.53	26.33

Performance

Linear solver GMRES_CPR0 with tolerance 10^{-6}, seconds:

Method Approach	SAXPY+IBTREE	Ordered LL	Unordered LL
TPFA	68.42	56.8	61.85
MPFA-O	99.63	83.36	80.39
MFPA-G	440.06	242.36	228.71
MPFA-L	383.56	267.64	232.51
NTPFA-A	111.60	84.26	87.92
NTPFA-B	115.7	93.3	96.18
NTPFA-C	93.53	75.62	74.73

Future considerations

- Nonlinear schemes
  - Is it possible to make DMP scheme as fast as others?
  - How to achieve unconditional coercivity and keep method as finite-volume cell-centered?
- Discretization toolkit
  - Mimic star-delta transofrmation on fracture joints for all the schemes.
  - Improve input methods with an interpreter.
  - Finish geomechanics input.
  - In case of demand provide interactive graphical user interface.

Thank you for attention!