Numerical Simulations of CO_2 Geo-Sequestration using PETSc

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APPLIED GEOPHYSICS AND GEOTHERMAL ENERGY

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Overview

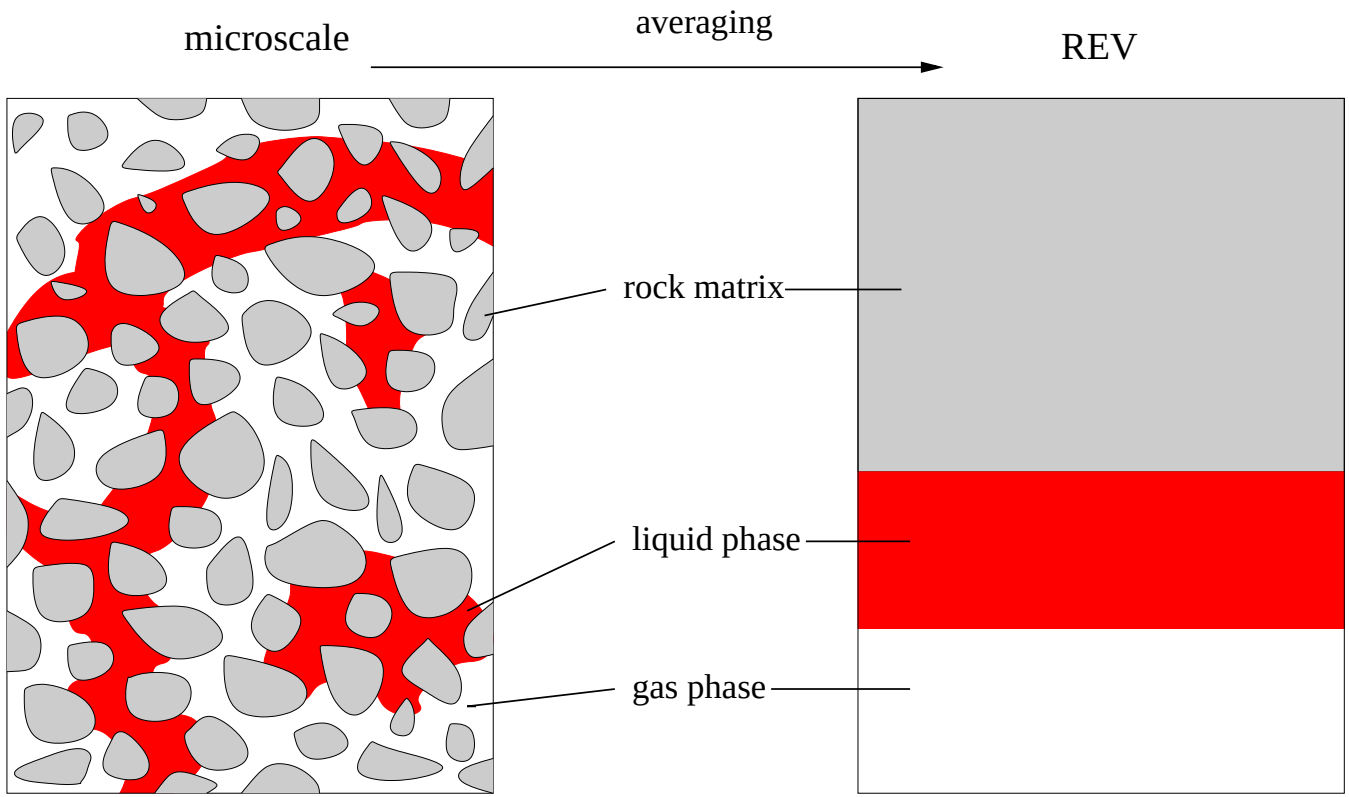
Two-phase flow in porous media

Numerical method and test example

Two-phase two-component flow

Properties of CO_2 and brine

Representative elementary volume (REV)



Porosity: $\phi = \frac{V_{\text{pores}}}{V_{\text{total}}}$, Saturation of phase α: $S_\alpha = \frac{V_\alpha}{V_{\text{pores}}}$,
Absolute permeability: $\mathbb{K} = k_f \frac{\mu}{\rho g}$.

Initial-Boundary-Value problem

p_w-S_n-formulation

$$\frac{\partial(\phi\rho_w(1-S_n))}{\partial t} + \operatorname{div}\left(\rho_w \frac{k_{rw}(S_n)}{\mu_w}\mathbb{K}(\nabla p_w - \rho_w \boldsymbol{g})\right) = \rho_w q_w$$

$$\frac{\partial(\phi\rho_n S_n)}{\partial t} + \operatorname{div}\left(\rho_n \frac{k_{rn}(S_n)}{\mu_n}\mathbb{K}(\nabla p_w + \nabla p_c(S_n) - \rho_n \boldsymbol{g})\right) = \rho_n q_n$$

Initial conditions

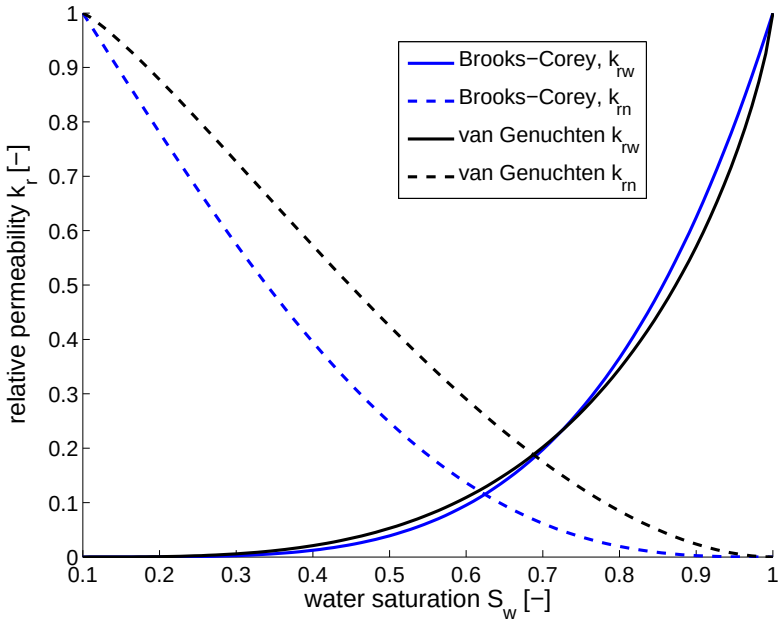
$$S_n(\boldsymbol{x},0) = S_{n0}(\boldsymbol{x}), \qquad p_w(\boldsymbol{x},0) = p_{w0}(\boldsymbol{x}) \quad \boldsymbol{x} \in \Omega$$

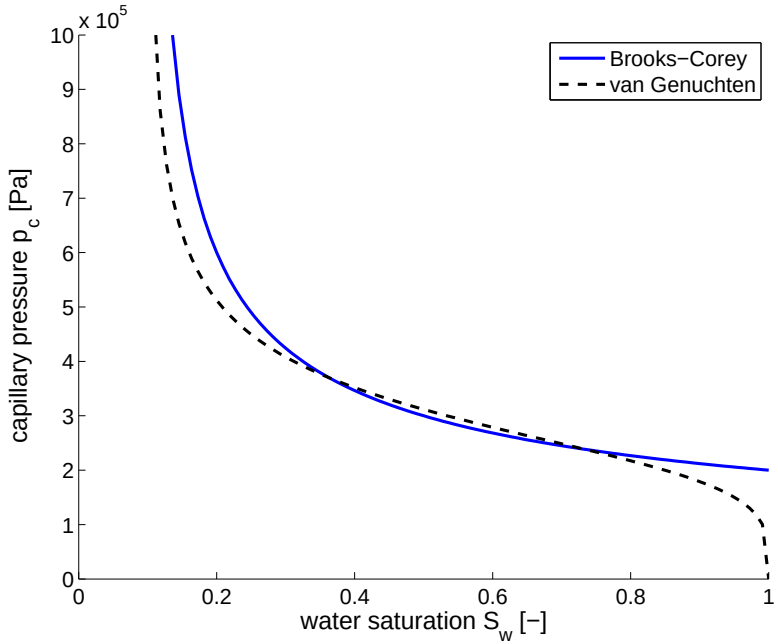
Boundary conditions

$$p_w(\boldsymbol{x},t) = g_{Dw}(\boldsymbol{x},t) \text{ on } \Gamma_{Dw} \qquad \rho_w \boldsymbol{v}_w \cdot \boldsymbol{n} = g_{Nw}(\boldsymbol{x},t) \text{ on } \Gamma_{Nw}$$

$$S_n(\boldsymbol{x},t) = g_{Dn}(\boldsymbol{x},t) \text{ on } \Gamma_{Dn} \qquad \rho_n \boldsymbol{v}_n \cdot \boldsymbol{n} = g_{Nn}(\boldsymbol{x},t) \text{ on } \Gamma_{Nn}$$

Nonlinearities





Brooks-Corey

$$k_{rw} = S_e^{\frac{2+3\lambda}{\lambda}}$$

$$k_{rn} = (1 - S_e)^2 \left(1 - S_e^{\frac{2+\lambda}{\lambda}}\right)$$

$$p_c = p_d S_e^{-1/\lambda}$$

van Genuchten

$$k_{rw} = \sqrt{S_e}\left(1 - (1 - S_e^{1/m})^m\right)^2$$

$$k_{rn} = (1 - S_e)^{\frac{1}{3}} \left(1 - S_e^{\frac{1}{m}}\right)^{2m}$$

$$p_c = \frac{1}{\alpha}(S_e^{-1/m} - 1)^{1/n}$$

Effective saturation: $S_e = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{nr}}, \quad 0 \leq S_e \leq 1$

Numerical method

$$\frac{\partial(\phi\rho_\alpha S_\alpha)}{\partial t} + \operatorname{div}\left(\rho_\alpha \frac{k_{r\alpha}}{\mu_\alpha}\mathbb{K}(\nabla p_\alpha - \rho_\alpha \boldsymbol{g})\right) = \rho_\alpha q_\alpha \qquad \alpha \in \{\mathrm{w}, \mathrm{n}\}$$

- First step: Semidiscretization in space with two-point flux approximation. Leads to a system of ordinary differential equations.
- Second step: Time-Integration with implicit Euler method.

Leads to a system of nonlinear algebraic equations (remember relative permeabilities and capillary pressure).

$$F(\boldsymbol{u}) = \mathbf{0} \quad \text{with } \boldsymbol{u} = \begin{pmatrix} \boldsymbol{p}_w \\ \boldsymbol{S}_n \end{pmatrix} \text{ and } F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}$$

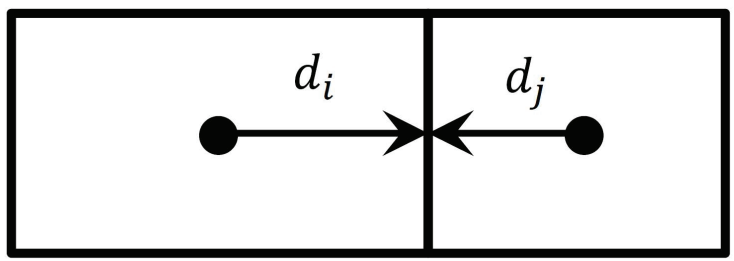
Linearize this nonlinear system of equations with Newton's method.

Numerical method

$$\sum_{\alpha} \phi \frac{(\rho_\alpha S_\alpha)_i^{n+1} - (\rho_\alpha S_\alpha)_i^n}{\Delta t} V_i$$

$$+ \sum_{\alpha} \sum_{j} \left(\rho_\alpha \frac{k_{r\alpha}}{\mu_\alpha} \boldsymbol{K} \right)_{ij}^{n+1} \left(\frac{p_{w,j} - p_{w,i}}{d_i + d_j} - \rho_{ij} g_{ij} \right)^{n+1} A_{ij}$$

$$- \sum_{\alpha} q_{\alpha,i}^{n+1} V_i = 0$$



Two-point flux approximation for two neighbouring grid cells i and j with distances d_i and d_j to the interface separating the two control volumes with area A_{ij}.

Newton's method

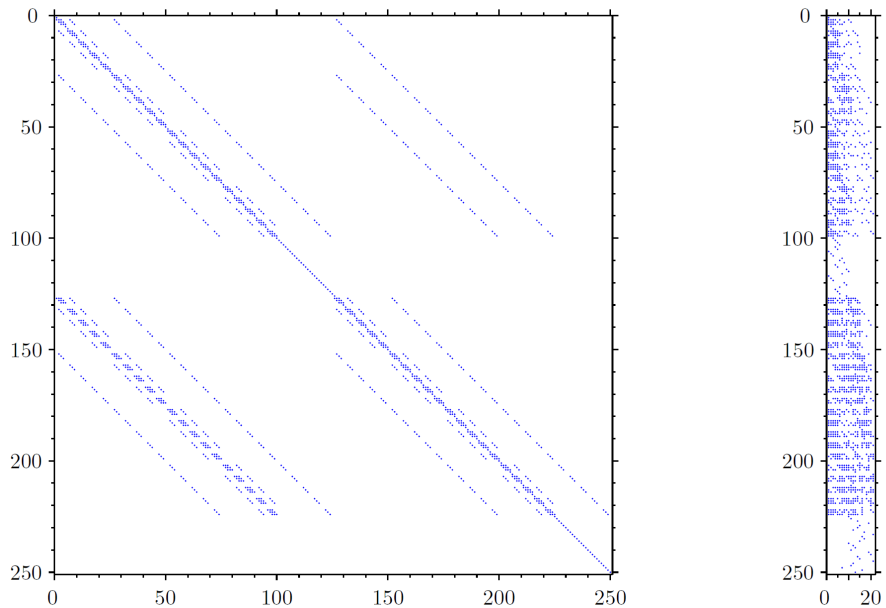
Transformation into linear system

$$\frac{\partial F(\boldsymbol{u})}{\partial \boldsymbol{u}} \Delta \boldsymbol{u} = -F(\boldsymbol{u})$$

Jacobian $J := \frac{\partial F(\boldsymbol{u})}{\partial \boldsymbol{u}}$ and $\Delta \boldsymbol{u} := \boldsymbol{u}_{j+1} - \boldsymbol{u}_j$. Jacobian is of the form

$$J = \begin{pmatrix} \frac{\partial F_1}{\partial \boldsymbol{p}_w} & \frac{\partial F_1}{\partial \boldsymbol{S}_n} \\ \frac{\partial F_2}{\partial \boldsymbol{p}_w} & \frac{\partial F_2}{\partial \boldsymbol{S}_n} \end{pmatrix}$$

Exact Jacobian computed by *Automatic Differentiation* (AD) using **ADiMat**, **TAPENADE** or **TAF**.

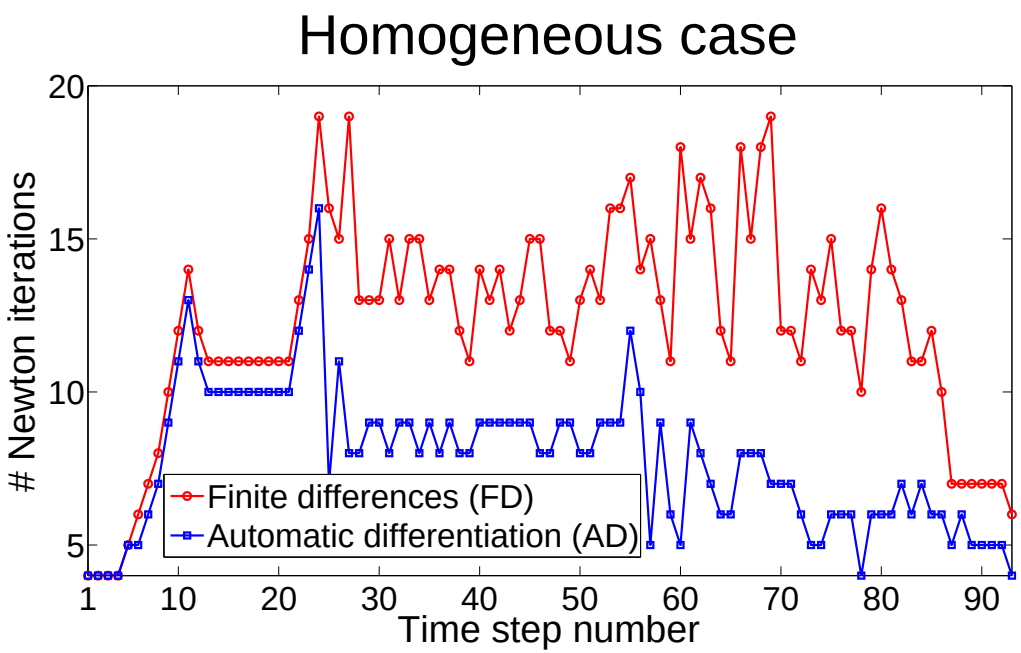


Every quadrant has non-zero entries due to coupling of equations.

Comparison of exact and approximate Jacobians

$$J_{ij} = \frac{\partial F_i(\boldsymbol{u})}{\partial u_j} \approx \frac{F_i(\ldots, u_{j-1} + \Delta u_j, u_{j+1}, \ldots) - F_i(\ldots, u_{j-1} - \Delta u_j, u_{j+1}, \ldots)}{2\Delta u_j}$$

with $\boldsymbol{u} = (\boldsymbol{p}_w, \boldsymbol{S}_n)^T = (u_1, u_2, \ldots, u_N)^T$ and $\Delta u_j = \delta \cdot u_j$.



Exact Jacobians save time: One vs. two evaluations.

Newton iterations decrease.

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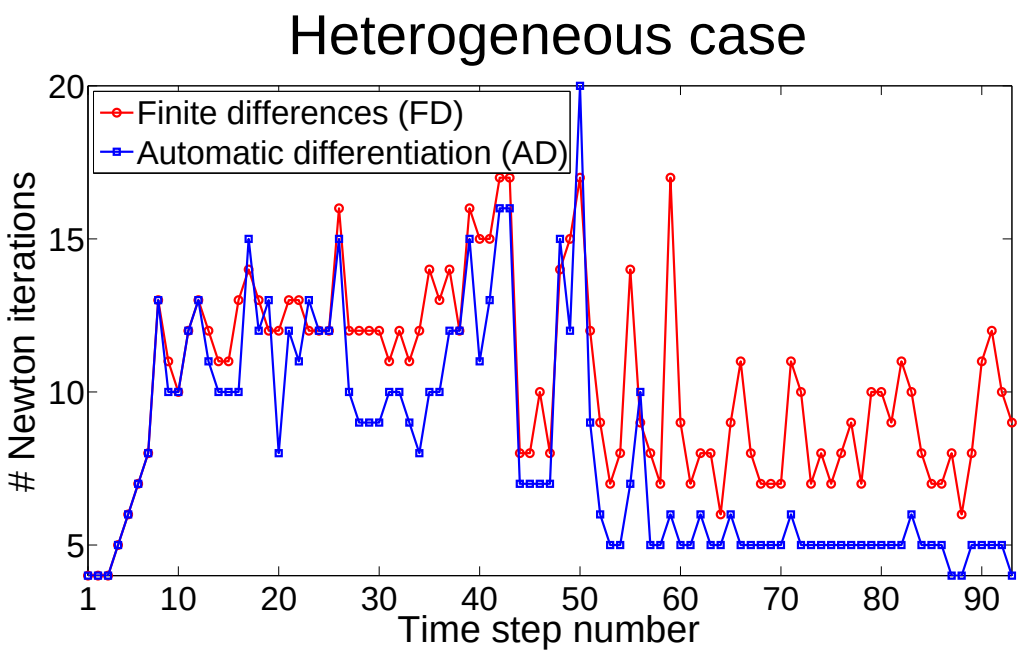

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Used preconditioners and iterative solvers Balay et al. (1997)

Algebraic multigrid

- Hypre/BoomerAMG http://acts.nersc.gov/hypre/
- Notay (2012)/AGMG http://homepages.ulb.ac.be/~ynotay/AGMG/
- PETSc/GAMG http://www.mcs.anl.gov/petsc/
- Trilinos/ML http://trilinos.sandia.gov/packages/ml/

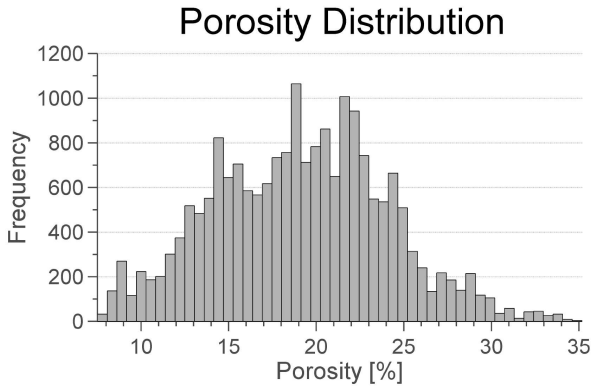
Solvers

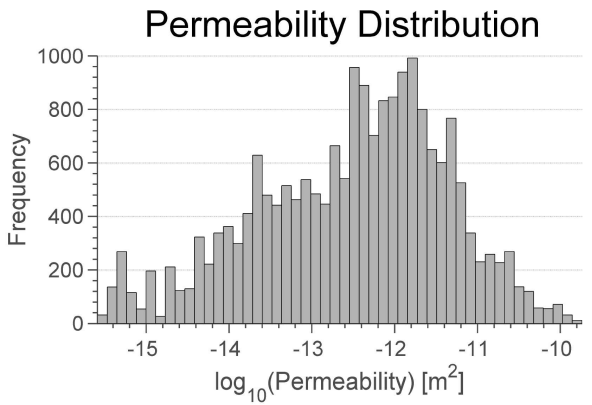
- MUMPS/LU http://graal.ens-lyon.fr/MUMPS/
- BiCGStab
- GMRES
- FGMRES
- Geometric multigrid (2 and 3 level)

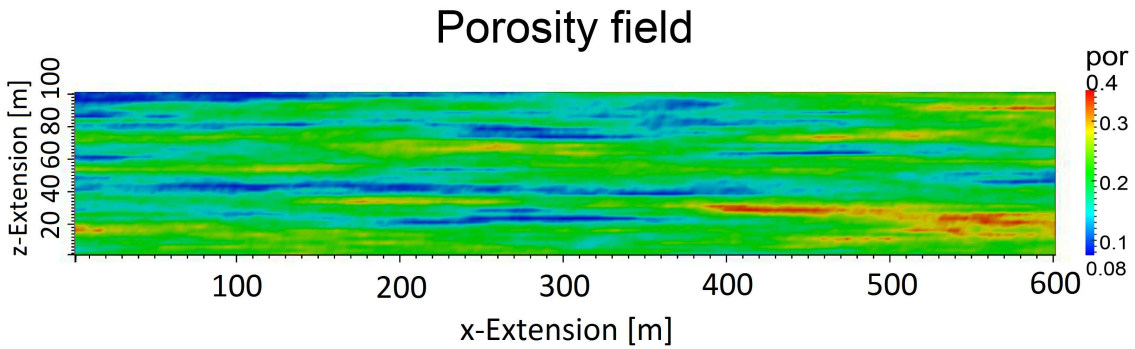
Preconditioners

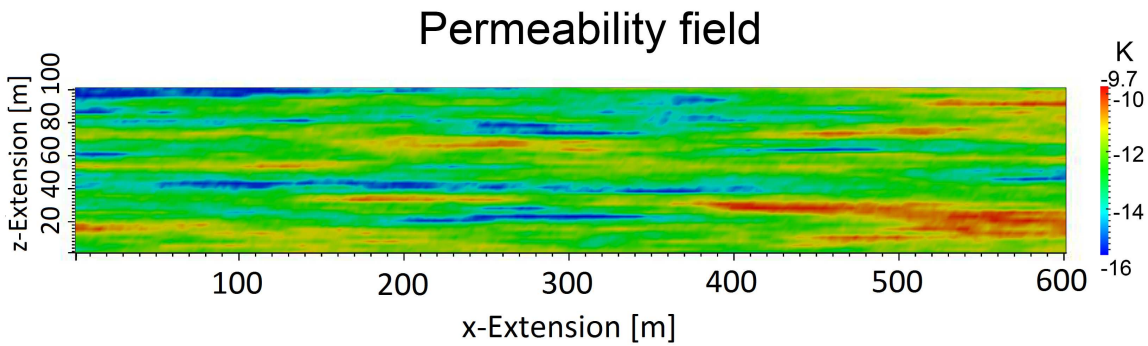
- Incomplete LU
- Hypre/Euclid
- Block-Jacobi

Heterogeneous porosity and permeability





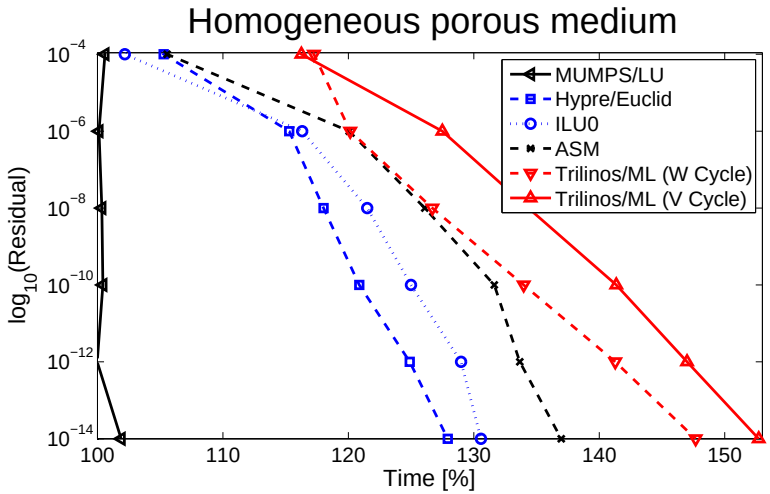


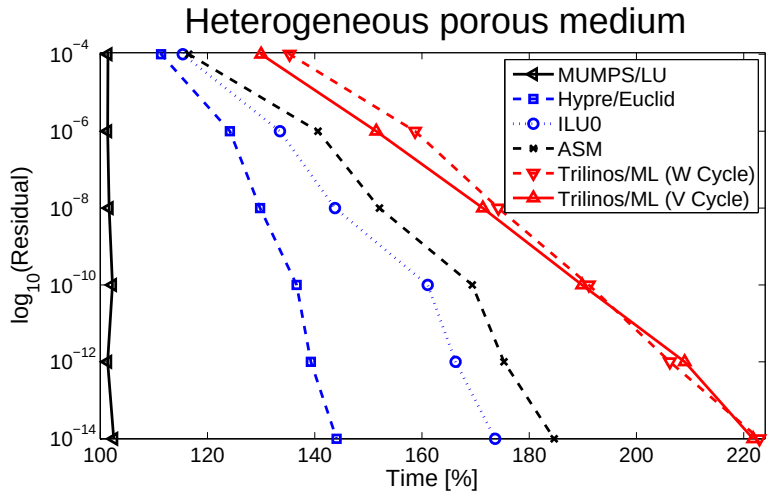


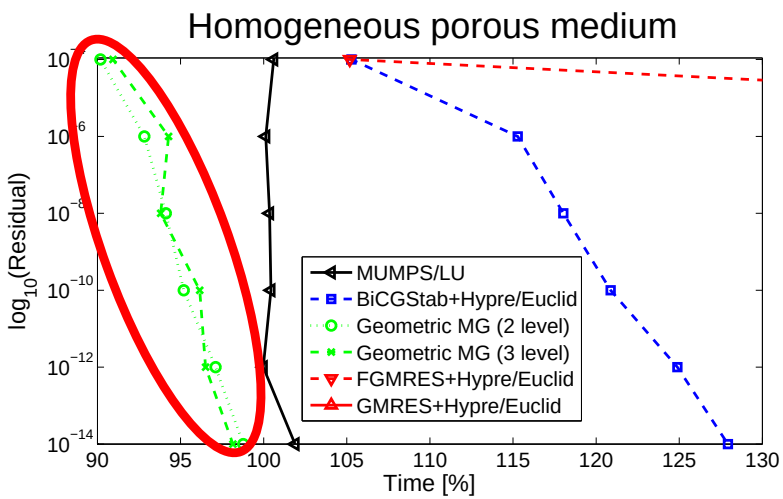
Gaussian distribution for Porosity field. Permeability after Pape et al. (1999). Fractal model valid for Rotliegend sandstone of NE-German basin:

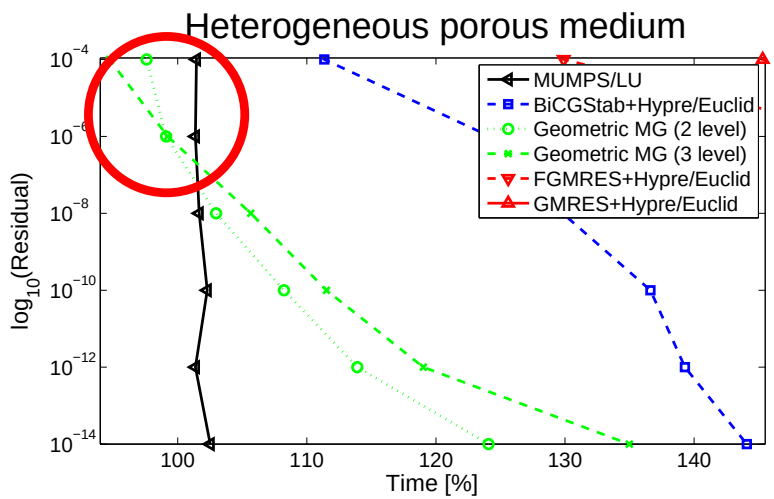
$$K = 155\,\phi + 37315\,\phi^2 + 630(10\,\phi)^{10}.$$

Performance of iterative solvers and preconditioners



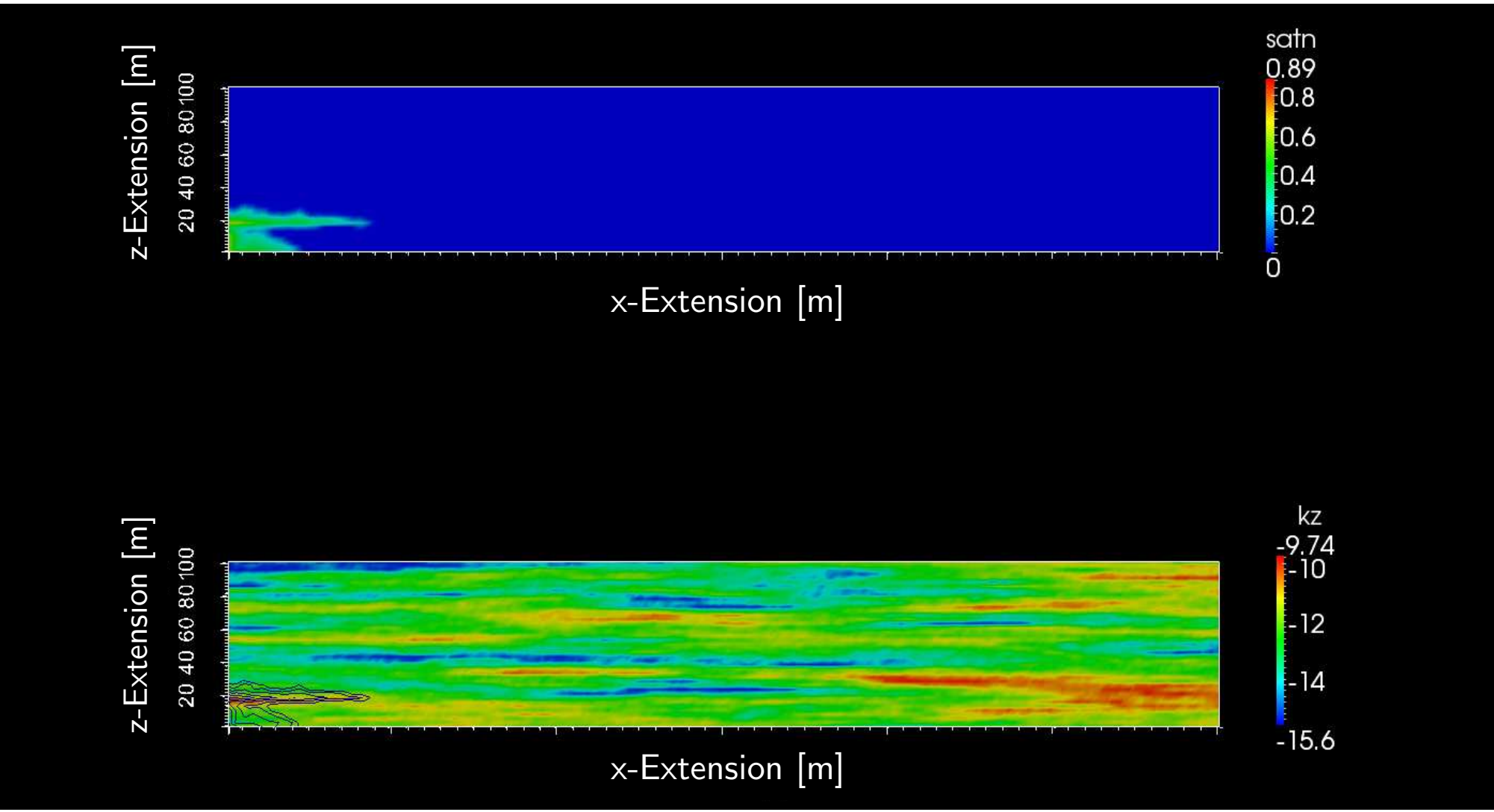






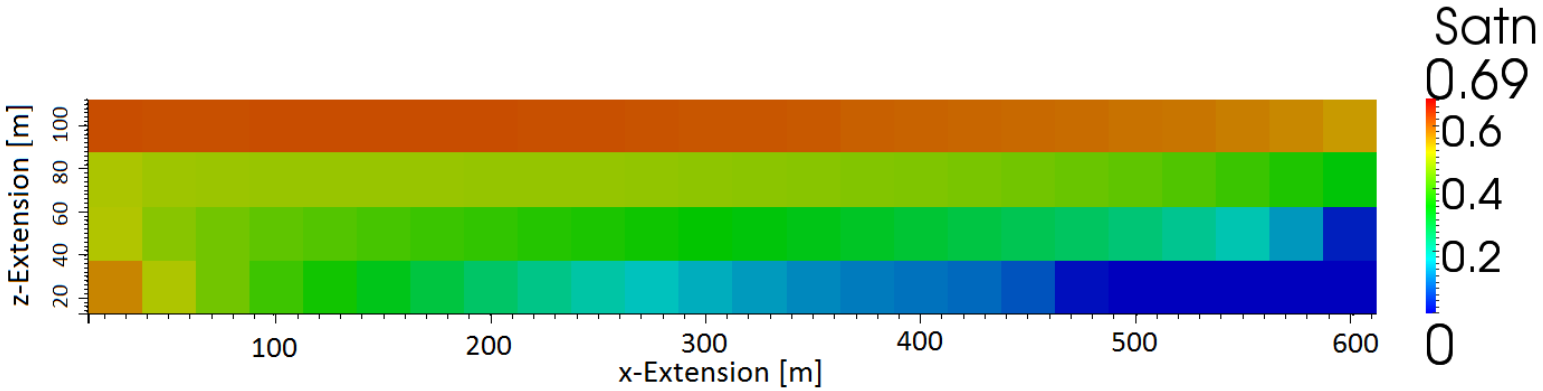
Geometric multigrid best. Necessity for large-scale problems.

CO_2 injection into heterogeneous porous media.



Convergence study

Grid size: $I0 \cdot J0 \cdot K0 = (2^x \cdot 6+1) \cdot 2 \cdot (2^x+1)$ $\quad \mathrm{EOC}_{i+1} = \log(2)^{-1} \left| \log\left(\frac{e_i}{e_{i+1}} \right) \right|$



x	Nodes	MUMPS/LU [s]	ILU0 [s]	GeoMG3 [s]	EOC(p_w)
2	250	114	75	106	1.32

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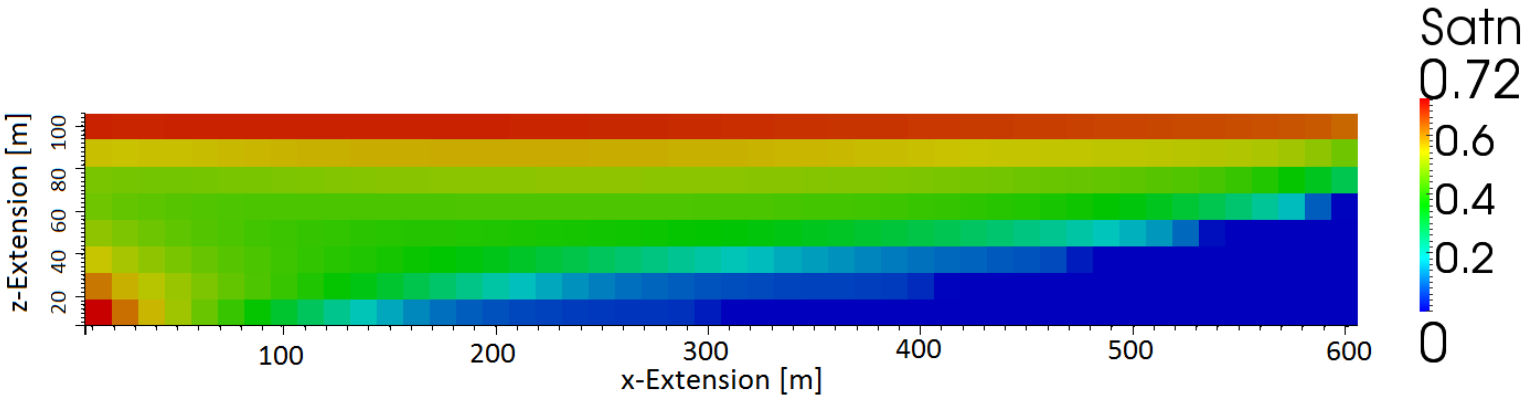

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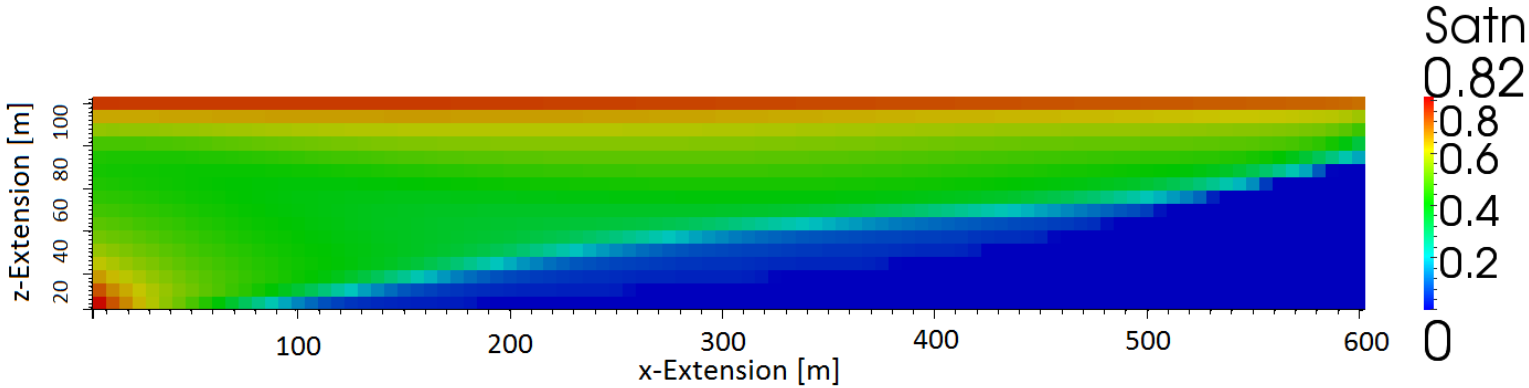

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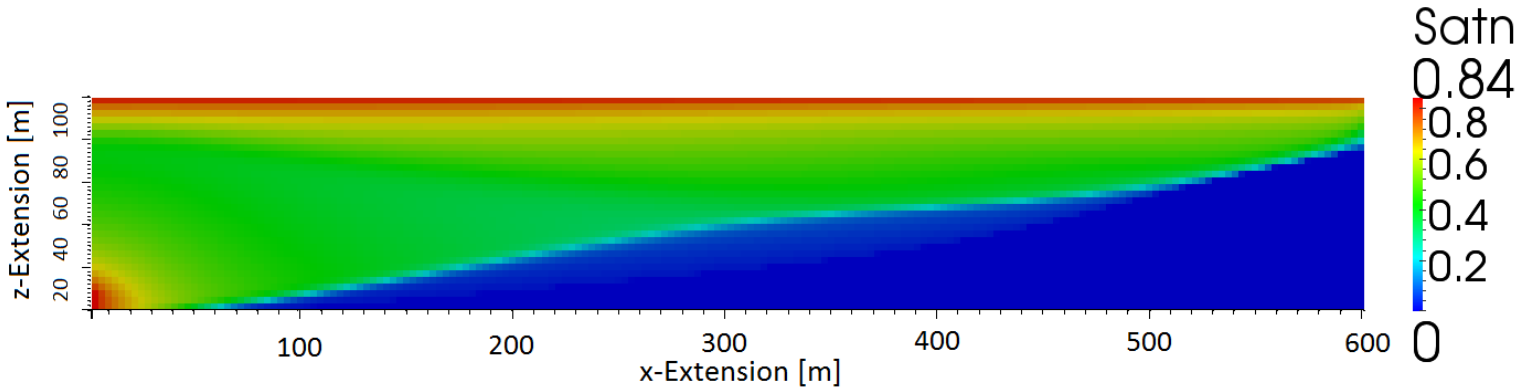

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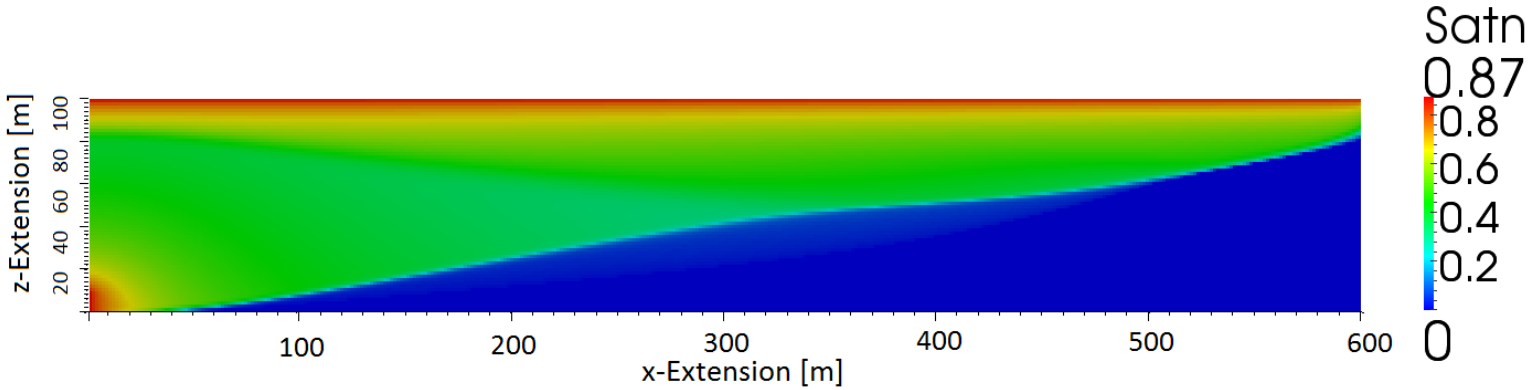

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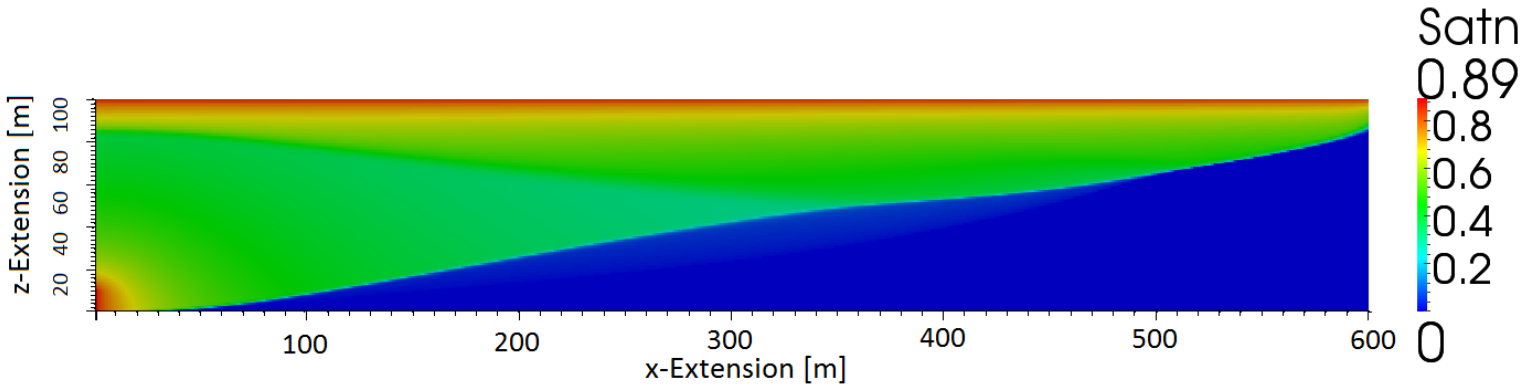

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6	50050	28350	45476	22336	1.00
7	198402	152108	189875	187140	

Two-phase two-component flow

$$\sum_{\alpha\in\{w,n\}} \frac{\partial(\phi\rho_\alpha x_\alpha^\kappa S_\alpha)}{\partial t} - \sum_{\alpha\in\{w,n\}} \mathrm{div}(\rho_\alpha\lambda_\alpha x_\alpha^\kappa \mathbb{K}(\nabla p_\alpha - \rho_\alpha \boldsymbol{g})$$
$$- \sum_{\alpha\in\{w,n\}} \mathrm{div}(\rho_\alpha D_{\mathrm{pm},\alpha}^\kappa \nabla x_\alpha^\kappa) - q^\kappa = 0, \qquad \kappa \in \{H_2O, CO_2\} \tag{2p2c}$$

Special case: Two-phase flow

$$x_n^{CO_2} = 1, \qquad x_n^{H_2O} = 0$$
$$x_w^{CO_2} = 0, \qquad x_w^{H_2O} = 1$$

$$\frac{\partial\phi\rho_w S_w}{\partial t} - \mathrm{div}(\rho_w\lambda_w\mathbb{K}(\nabla p_w - \rho_w\boldsymbol{g})) = q_w$$
$$\frac{\partial\phi\rho_n S_n}{\partial t} - \mathrm{div}(\rho_n\lambda_n\mathbb{K}(\nabla p_n - \rho_n\boldsymbol{g})) = q_n \tag{2p}$$

Closure relations and primary variables

Algebraic closure relations:

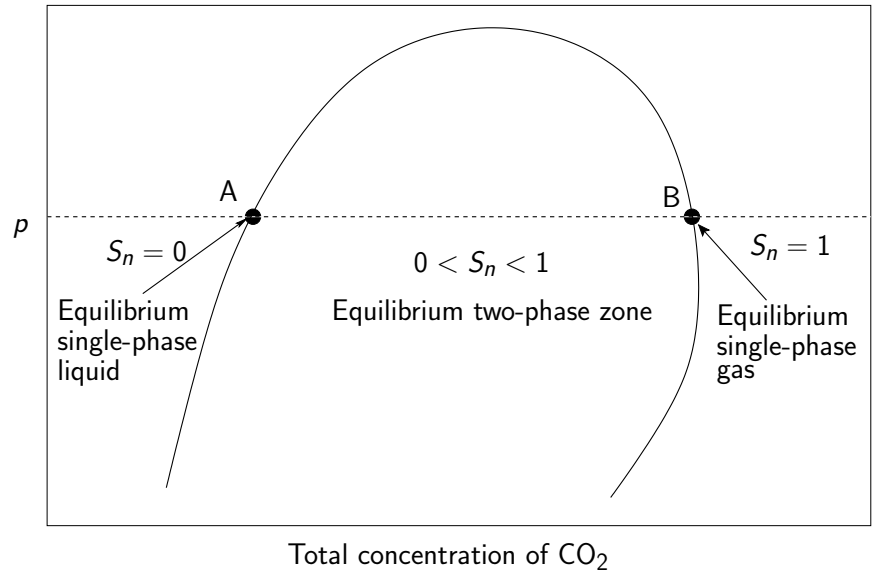
$$\sum_{\alpha \in \{w,n\}} S_\alpha = 1, \qquad p_c = p_n - p_w$$

$$\sum_{c \in \{H_2O, CO_2\}} x_\alpha^c = 1, \qquad \alpha \in \{w, n\}$$

Choose primary variables: p_w, S_n. Dependent variables:
$x_\alpha^c = x_\alpha^c(p_n, T, \text{sal})$, $\rho_\alpha = \rho_\alpha(p_\alpha, T, \text{sal}, x_\alpha^c)$, $\mu_\alpha = \mu_\alpha(p_\alpha, T, \text{sal})$.

Phase diagram

Phase diagram for two-component system



x_α^c gives mole of component c per total mole in phase α when the two phases are in equilibrium.
Problem: Equations only hold for two-phase regions. Not in single-phase regions.
Limit of equations for $S_n \to 0$:

$$\frac{\partial(\phi \rho_w x_w^c)}{\partial t} - \operatorname{div}\left(\frac{\rho_w}{\mu_w} x_w^c \mathbb{K}(\nabla p_w - \rho_w \boldsymbol{g})\right) - \operatorname{div}(\rho_w D_w^c \nabla x_w^c) + q^c = 0, \qquad c \in \{H_2O, CO_2\} \quad (2c)$$

Extended Saturations

Solution:

- Introduce residual saturations and avoid single-phase regions $\rightarrow$ unrealistic.
- Switch primary variables, choose e.g. $x_w^{CO_2}$ and p_w.
- Extend concept of saturation and use two-phase flow equations everywhere.

Method of extended saturations after Abadpour & Panfilov (2008).

Idea: Introduce imaginary gas phase in zone of undersaturated liquid and imaginary liquid phase for zone of oversaturated gas.

$$\begin{aligned} \tilde{S} &< 0 && \text{undersaturated liquid} \\ 0 \leq \tilde{S} &\leq 1 && \text{in the two-phase region} \\ \tilde{S} &> 1 && \text{oversaturated gas} \end{aligned} \qquad S_n = \begin{cases} 0 & \text{if } \tilde{S} < 0 \\ \tilde{S} & \text{if } 0 \leq \tilde{S} \leq 1 \\ 1 & \text{if } \tilde{S} > 1. \end{cases}$$

Consistence conditions

Consistence conditions for imaginary gas: $\tilde{S} < 0$ (undersaturated liquid).

$$\rho_n = \rho_w, \quad \mu_n = \mu_w$$
$$k_{rw}(\tilde{S}) = 1 - \tilde{S}, \quad k_{rn}(\tilde{S}) = \tilde{S}$$
$$p_c(\tilde{S}) = 0$$
$$D_n = D_w \left(1 + \frac{x_n^{CO_2} - x_w^{CO_2}}{\tilde{S}} \nabla \tilde{S} \, \nabla^{-1} x_n^{CO_2}\right)$$
$$x_n^{CO_2} = x_n^{CO_2}(p_n, T), \quad x_w^{CO_2} = x_w^{CO_2}(p_n, T)$$

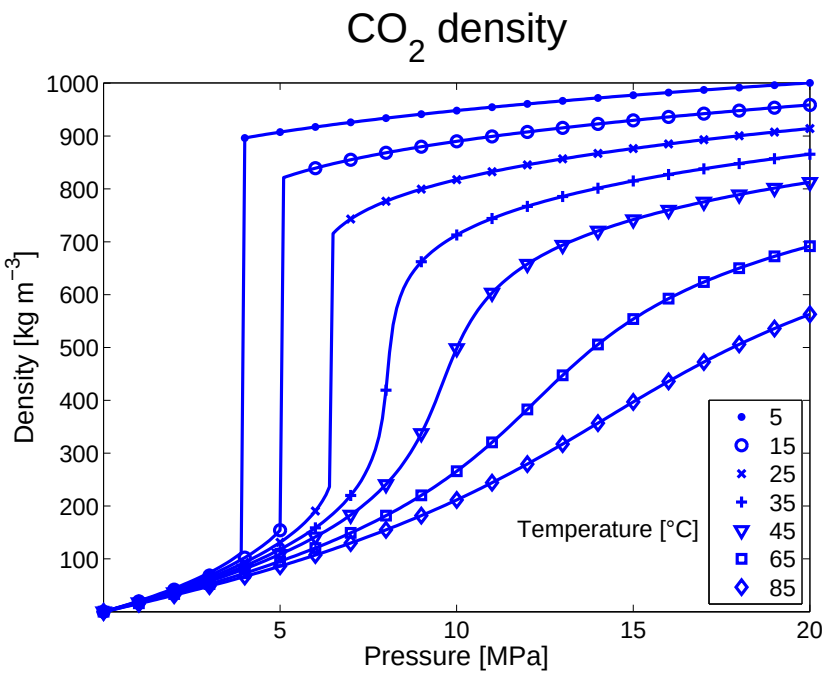
Plugging consistence equations into (2p2c) leads to correct single-phase equations (2c).

Density

Density of CO_2:

$\rho_n = \rho_n(p_n, T)$

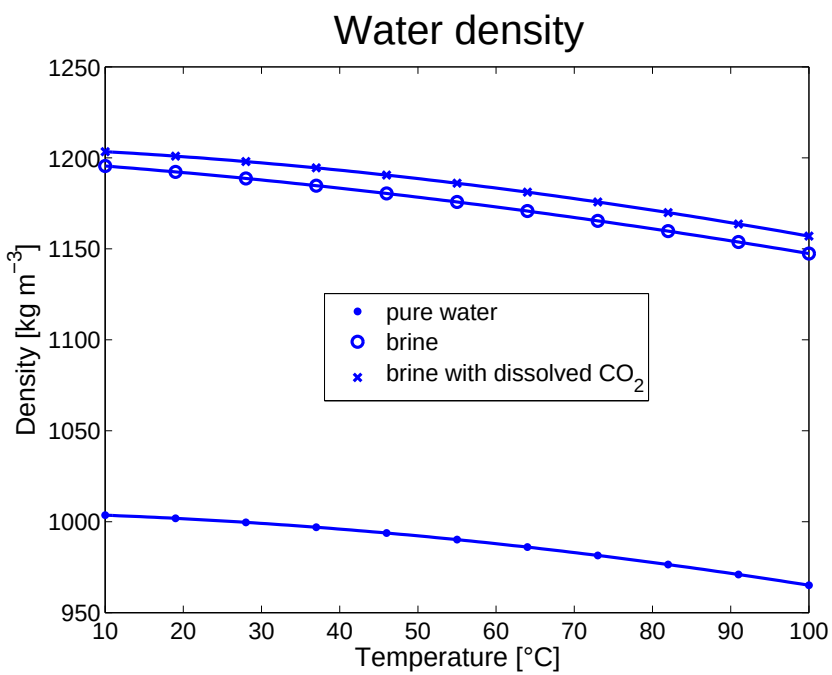
(Span & Wagner, 1996)



Density of brine:

$\rho_w = \rho_w(p_w, T, \mathrm{sal}, x_w^{CO_2})$

(Batzle & Wang, 1992; Garcia, 2001)



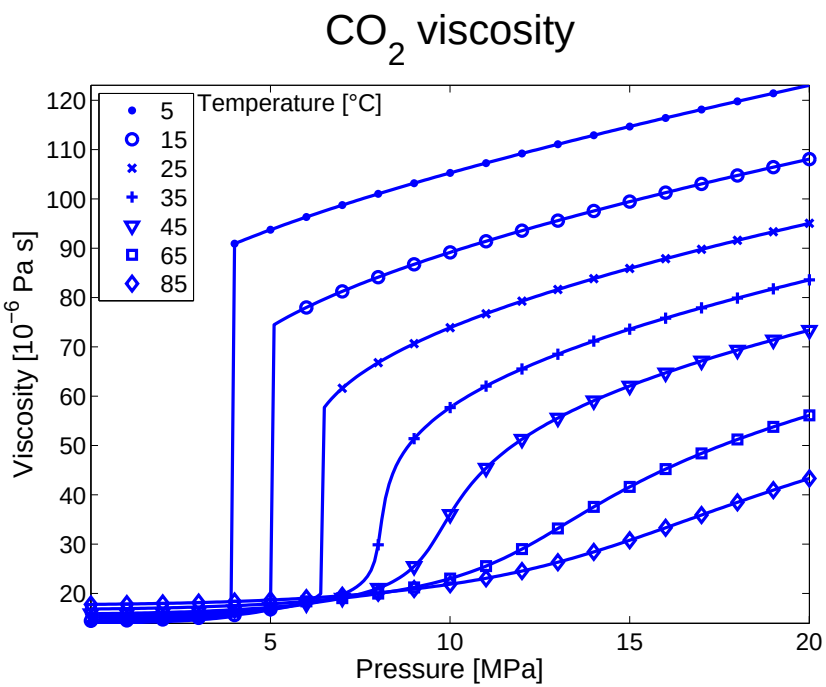
Pressure: $p_w = 10$ MPa

Salinity: $\mathrm{sal} = 0.25\ \mathrm{mol\,mol}^{-1}$

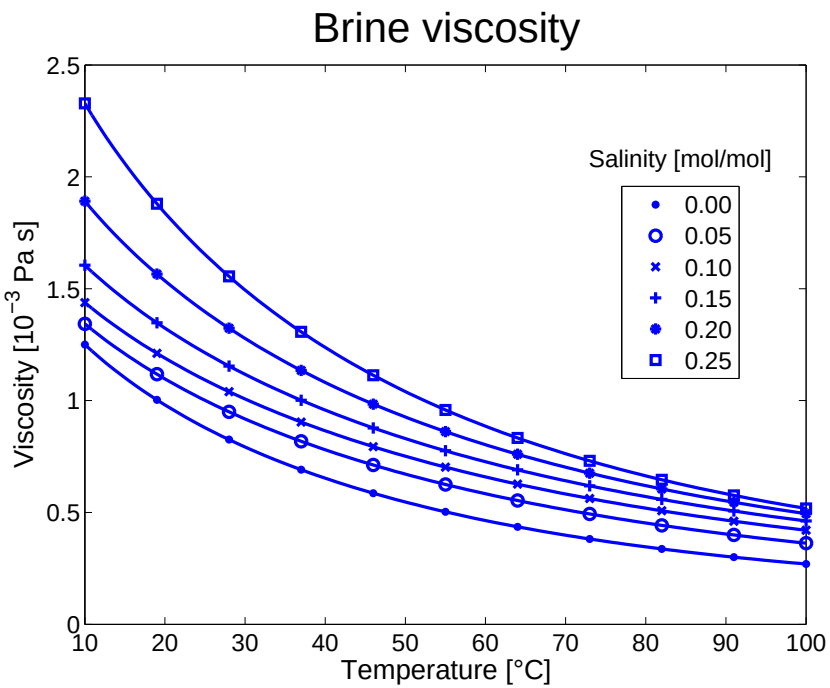
Dissolved CO_2: $x_w^{CO_2} = 0.02\ \mathrm{mol\,mol}^{-1}$

Viscosity

Viscosity of CO_2:
$\mu_n = \mu_n(p_n, T)$
(Fenghour et al., 1998)



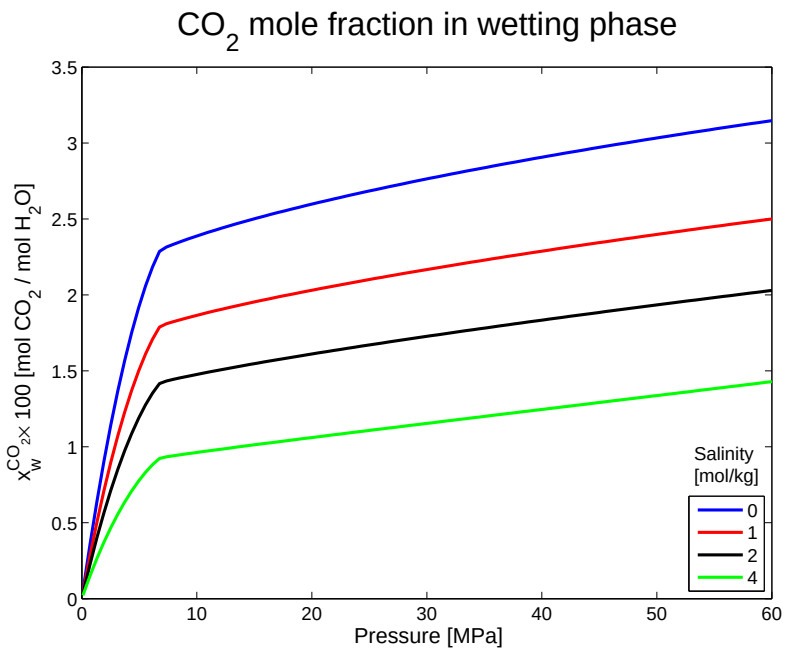
Viscosity of brine:
$\mu_w = \mu_w(T, \text{sal})$
(Batzle & Wang, 1992)

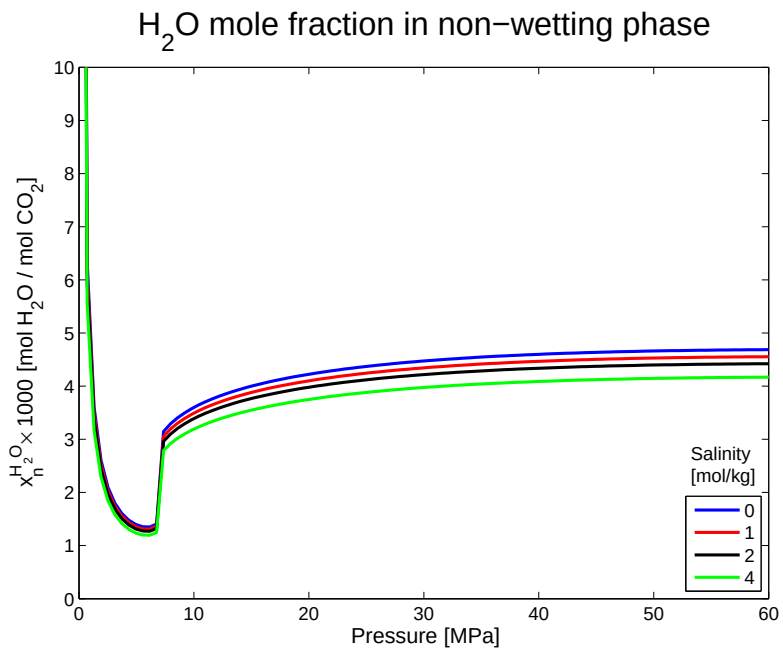


Solubility

Solubility of CO_2 in brine:
$x_w^{CO_2} = x_w^{CO_2}(p_n, T, \text{sal})$
(Spycher et al., 2005)

Solubility of H_2O in gas:
$x_n^{H_2O} = x_n^{H_2O}(p_n, T, \text{sal})$
(Spycher et al., 2005)





Temperature: $T = 30\ ^\circ\text{C}$, Salinity: Different molalities of NaCl.

Numerical simulation of CO_2 injection.

Summary and conclusion

Summary:

- Test of preconditioners and iterative solvers
- CO_2 injection into highly heterogeneous porous media
- Convergence study
- Comparison of automatic differentiation (AD) and finite differences (FD)

Conclusion:

- Difficulties with algebraic multigrid due to hyperbolic character of equations
- Geometric multigrid performs favorable
- Linear increase of computation time
- AD outperforms FD in terms of precision and speed

Thank you for your attention!

Vector Form

Assuming constant density and porosity

$$S\frac{\partial u}{\partial t} - \operatorname{div}(c\nabla u - G) = f$$

with

$$S = \begin{pmatrix} 0 & -\phi\rho_w \\ 0 & \phi\rho_n \end{pmatrix}, \quad c = \begin{pmatrix} \rho_w\lambda_w(S_n)K & 0 \\ \rho_n\lambda_n(S_n)K & \rho_n\lambda_n(S_n)K\frac{dp_c(S_n)}{dS_n} \end{pmatrix}$$

$$f = \begin{pmatrix} \rho_w q_w \\ \rho_n q_n \end{pmatrix}, \quad G = \begin{pmatrix} \rho_w\lambda_w(S_n)K\rho_w\boldsymbol{g} \\ \rho_n\lambda_n(S_n)K\rho_n\boldsymbol{g} \end{pmatrix} \text{ and } u = \begin{pmatrix} p_w \\ S_n \end{pmatrix}.$$

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