



Coupled porous media and free flow

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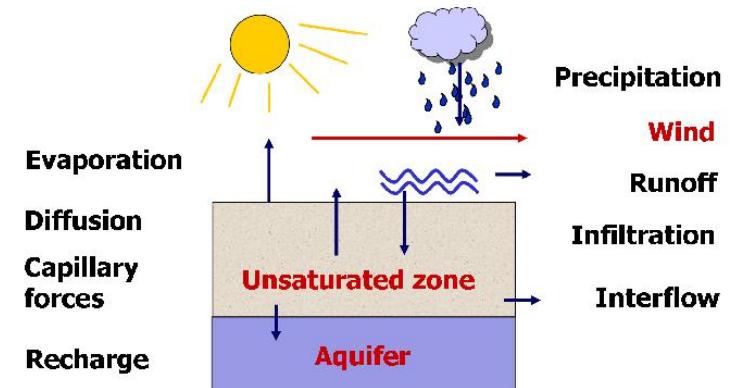
Outline

- **Motivation**
- **Two-domain approach**
 - Porous media model
 - Free flow model
 - Interface conditions
 - DG approach
- **Phase transition**
 - Multi-phase PDE model
 - Physical constraints
 - Inequality system
 - Newton solver
- **Conclusions & Outlook**

Motivation

- Transport phenomena in **multi-structures** appear in many applications

- filtration processes in fuel cells
- flow of nutrients in biological tissues
- environmental evaporation processes



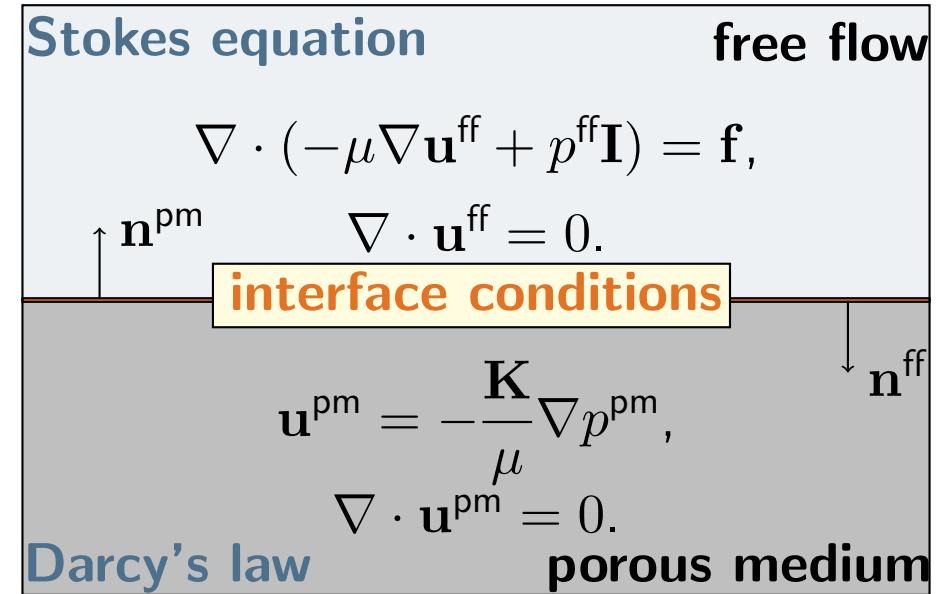
- **One-domain** approaches
 - do only exist in simplified situations, e.g., Brinkmann
 - can be extremely complex
- **Multi-physics** models on subdomains allow for
 - mathematical models on different scales
 - models of different dimensions, e.g., 2D fractures in 3D

Motivation

- **State-of-the-art:** Finite element methods (FEM) are standard for the solution of 2nd order elliptic partial differential equations (PDEs)
- **Observation:** The mathematical modeling for more complex systems gives rise to PDEs with different structure
- **Coupling concepts for subdomains:** Two alternatives exist
 - **Single domain approach:** One PDE system is globally used
but the parameters vary drastically
 - **Two domain approach:** Different PDE systems are used subdomain-wise
and interface condition are required
- **Modelling concept:** PDE system has to be closed by constitutive relations, e.g. flow rule in plasticity

Single- versus two-domain approach

Brinkman/Stokes	free flow $K \gg 1$
$-\nabla \cdot (\tilde{\mu} \nabla \mathbf{u}) + \mu \mathbf{K}^{-1} \mathbf{u} + \nabla p = \mathbf{f}$	
$\nabla \cdot \mathbf{u} = 0$	
transition zone	
Brinkman/Darcy	porous medium $K \ll 1$
$-\nabla \cdot (\tilde{\mu} \nabla \mathbf{u}) + \mu \mathbf{K}^{-1} \mathbf{u} + \nabla p = \mathbf{0}$	
$\nabla \cdot \mathbf{u} = 0 \quad \left(\mathbf{u} = -\frac{\mathbf{K}}{\mu} \nabla p \right)$	



Brinkmann: microscopic
Second order in \mathbf{u} , first order in p

Limit “ $K = \infty$ ”: Stokes

Limit “ $K = 0$ ”: Darcy

Transition zone?

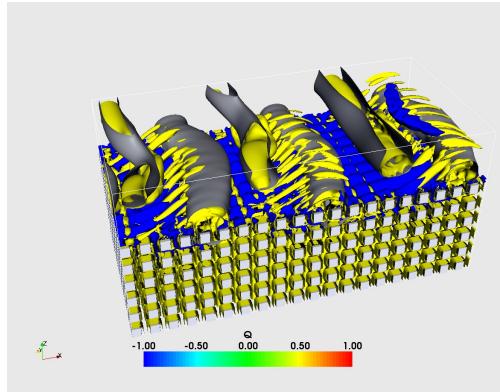
Stokes: microscopic
Second order in \mathbf{u} , first order in p

Darcy: macroscopic
Second order in p

Interface conditions?

Coupled flow problems

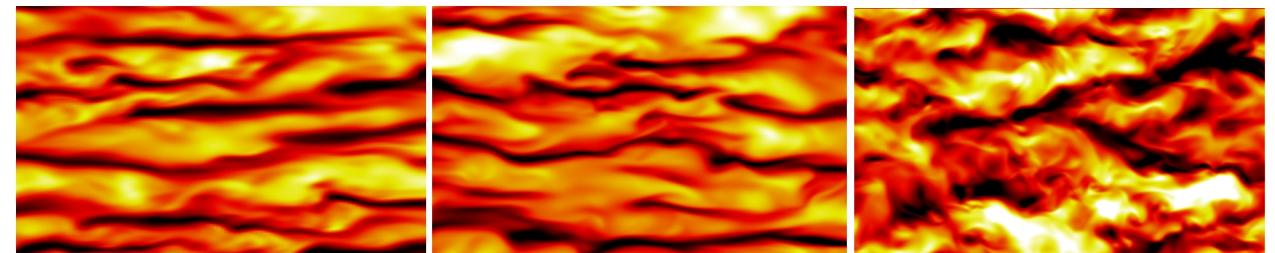
- Navier-Stokes and permeable wall coupling



smooth

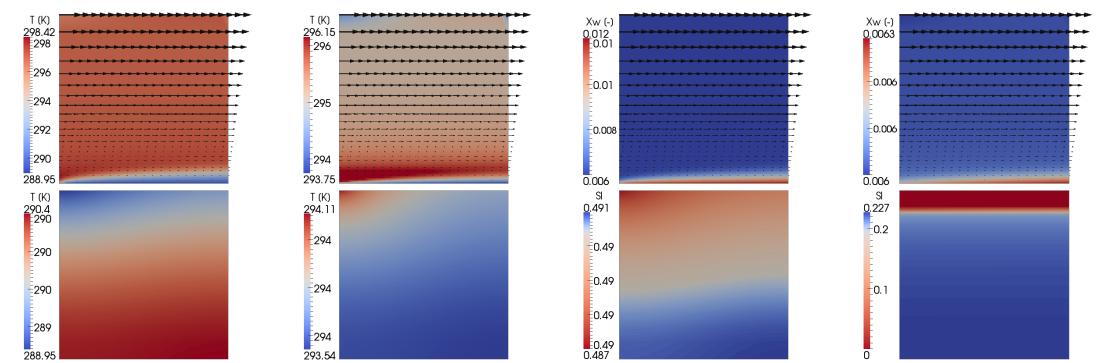
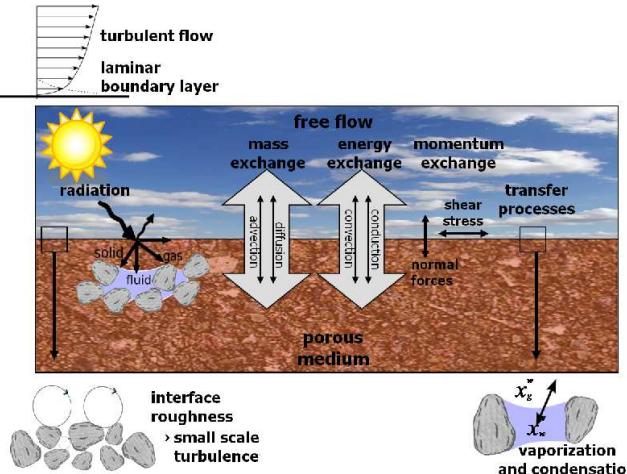
rough

porous



permeability influences turbulence structure and dissipation
jww M. Manhart (TUM) and A. Hokpunna

- Free flow and porous media



jww R. Helmig and K. Mosthaf (University Stuttgart)

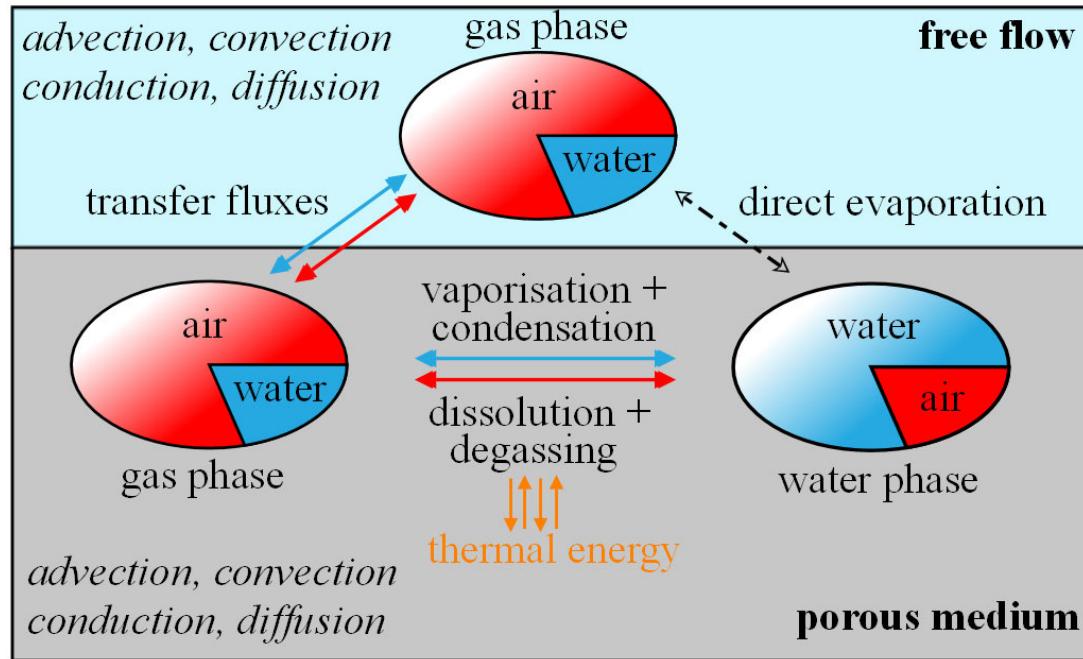


Two domain approach:

the porous medium model and

the free flow model

Model concept



Porous medium:

- two-phases: water phase w , gas phase g ,
- two components: water w , air a ,
- multiphase Darcy's law for velocity,
- component transfer between phases,
- fully-coupled non-isothermal model,
- thermodynamic equilibrium.

Free flow:

- single-phase: gas phase g ,
- two components: water w , air a ,
- momentum balance equation,
- transport eq. for each component (mass balance),
- energy balance equation,
- thermodynamic equilibrium.



Porous medium model

Transport equation one for each component $\kappa \in \{w, a\}$:

$$\sum_{\alpha \in \{w, g\}} \phi \frac{\partial (\varrho_\alpha X_\alpha^\kappa S_\alpha)}{\partial t} + \nabla \cdot \mathbf{F}^\kappa - \sum_{\alpha \in \{w, g\}} q_\alpha^\kappa = 0. \quad (1)$$

Energy balance equation (thermal equilibrium):

$$\sum_{\alpha \in \{w, g\}} \phi \frac{\partial (\varrho_\alpha u_\alpha S_\alpha)}{\partial t} + (1 - \phi) \frac{\partial (\varrho_s c_s T)}{\partial t} + \nabla \cdot \mathbf{F}_T - q_T = 0. \quad (2)$$

Component flux and heat flux:

$$\mathbf{F}^\kappa = \sum_{\alpha \in \{w, g\}} (\varrho_\alpha X_\alpha^\kappa \mathbf{v}_\alpha - D_{\alpha, pm} \varrho_\alpha \nabla X_\alpha^\kappa), \quad \mathbf{F}_T = \sum_{\alpha \in \{w, g\}} \varrho_\alpha h_\alpha \mathbf{v}_\alpha - \lambda_{pm} \nabla T.$$

Multiphase Darcy's law: $\mathbf{v}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha} \mathbf{K} (\nabla p_\alpha - \varrho_\alpha \mathbf{g}).$ **PV:** p_g, S_w, T



Primary variables:

p_g - pressure of the gas phase,

S_w - water saturation (X_g^w - mass fraction of water in the gas phase),

T - temperature.

Constitutive relationships:

- Saturations: $S_w + S_g = 1$,
- Capillary pressure: $p_c(S_w) = p_g - p_w$,
- Mass fractions: $X_\alpha^w + X_\alpha^g = 1$, $\alpha \in \{w, g\}$,
- Mole fractions: $x_\alpha^w + x_\alpha^g = 1$, $\alpha \in \{w, g\}$,
- Dalton's law: $p_g = p_g^w + p_g^a$,
- $x_g^w = \frac{p_{sat}^w}{p_g}$ (computation of mole fractions in gas phase),
- Henry's law: $x_w^a = p_g^a / H_{gw}^a$ (computation of mole fractions in water phase),
- Specific enthalpies: $h_\alpha = u_\alpha + p_\alpha / \rho_\alpha$.



Free flow model

Transport equation one for each component $\kappa \in \{w, a\}$:

PV: $\mathbf{v}_g, p_g, X_g^w, T$

$$\frac{\partial (\rho_g X_g^\kappa)}{\partial t} + \nabla \cdot \mathbf{F}^\kappa - q_g^\kappa = 0, \quad \kappa \in \{w, a\}. \quad (3)$$

Momentum balance equation:

$$\frac{\partial (\rho_g \mathbf{v}_g)}{\partial t} + \nabla \cdot \mathbf{F}_u - \rho_g \mathbf{g} = 0. \quad (4)$$

Energy balance equation:

$$\frac{\partial (\rho_g u_g)}{\partial t} + \nabla \cdot \mathbf{F}_T - q_T = 0. \quad (5)$$

Component fluxes, momentum flux and heat flux:

$$\mathbf{F}^\kappa = \rho_g \mathbf{v}_g X_g^\kappa - \mathbf{D}_g \rho_g \nabla X_g^\kappa, \quad \mathbf{F}_u = (p_g \mathbf{I} - \boldsymbol{\tau}), \quad \mathbf{F}_T = \rho_g h_g \mathbf{v}_g - \lambda_g \nabla T.$$

Primary variables:

\mathbf{v}_g - velocity of the gas phase,

p_g - pressure of the gas phase,

X_g^w - mass fraction of water in the gas phase,

T - temperature.

Constitutive relationships:

- Mass fractions: $X_g^w + X_g^a = 1$,
- Specific enthalpies: $h_g = u_g + p_g/\rho_g$,
- Shear stress: $\boldsymbol{\tau} = 2\mu_g(\frac{1}{2}(\nabla \mathbf{v}_g + \nabla \mathbf{v}_g^\top) - \frac{1}{3}\operatorname{div} \mathbf{v}_g \mathbf{I})$.

Note: Under the assumption of binary system (diffusion coefficients $D_g^w = D_g^a = D_g$), the sum of two transport equations (3) gives us the **mass balance equation**

$$\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{v}_g) - q_g = 0.$$

The constitutive relation for mass fractions ($X_g^w + X_g^a = 1$) is used.



From one subdomain...

... via the interface ...

to the adjacent subdomain

Interface conditions

Free flow model

\mathbf{v}_g, X_g^w, T

Interface conditions

Porous medium model

p_g, S_w, T

Mechanical equilibrium

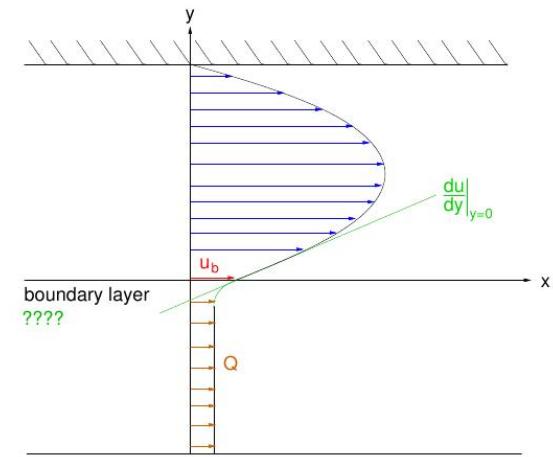
Continuity of normal stresses for each component $\kappa \in \{w, a\}$ in the gas phase

$$[x_g^\kappa ((p_g \mathbf{I} - \boldsymbol{\tau}) \cdot \mathbf{n}) \cdot \mathbf{n}]^{\text{ff}} = [x_g^\kappa p_g]^{\text{pm}}. \quad (6)$$

Condition on tangential component of free flow velocity

[Beavers, Joseph 67], [Saffman 71], [Jäger, Mikelić 00, 09]

$$\left[\mathbf{v}_g \cdot \mathbf{t} + \frac{\sqrt{k}}{\alpha \mu_g} \boldsymbol{\tau} \mathbf{n} \cdot \mathbf{t} \right]^{\text{ff}} = 0. \quad (7)$$





Thermal equilibrium

Continuity of temperature

$$[T]^{\text{ff}} = [T]^{\text{pm}}. \quad (8)$$

Continuity of heat fluxes

$$[(\rho_g h_g \mathbf{v}_g - \lambda_g \nabla T) \cdot \mathbf{n}]^{\text{ff}} = - [(\rho_g h_g \mathbf{v}_g + \rho_w h_w \mathbf{v}_w - \lambda_{pm} \nabla T) \cdot \mathbf{n}]^{\text{pm}}. \quad (9)$$

Chemical equilibrium

Continuity of the mole fractions for each component $\kappa \in \{w, a\}$:

$$[x_g^\kappa]^{\text{ff}} = - [x_g^\kappa]^{\text{pm}} \quad (10)$$

Continuity of mass fluxes for each component $\kappa \in \{w, a\}$:

$$\begin{aligned} [(\rho_g \mathbf{v}_g X_g^\kappa - D_g \rho_g \nabla X_g^\kappa) \cdot \mathbf{n}]^{\text{ff}} &= - [(\rho_g \mathbf{v}_g X_g^\kappa - D_{g,pm} \rho_g \nabla X_g^\kappa) \cdot \mathbf{n}]^{\text{pm}} \\ &\quad - [(\rho_w \mathbf{v}_w X_w^\kappa - D_{w,pm} \rho_w \nabla X_w^\kappa) \cdot \mathbf{n}]^{\text{pm}}. \end{aligned} \quad (11)$$

Overview of the applied interface conditions

Equilibrium	Property	Porous medium	Free flow
Mechanical:	normal stress $a+w$ (6) tangential velocity (7)	—	Neumann for $\mathbf{v}_g \cdot \mathbf{n}$ Cauchy for $\mathbf{v}_g \cdot \mathbf{t}$
Thermal:	temperature (8) heat flux (9)	Cauchy for T	Dirichlet for T
Chemical:	mole fraction (10) component flux w (11) component flux $a+w$ (11)	non-linear Cauchy for S_w non-linear Neumann for p_g	Dirichlet for X_g^w

Note: IC (11) ($a+w$) guarantees also the continuity of the mechanical fluxes

$$[\rho_g \mathbf{v}_g \cdot \mathbf{n}]^{\text{ff}} = -[(\rho_g \mathbf{v}_g + \rho_w \mathbf{v}_w) \cdot \mathbf{n}]^{\text{pm}}.$$

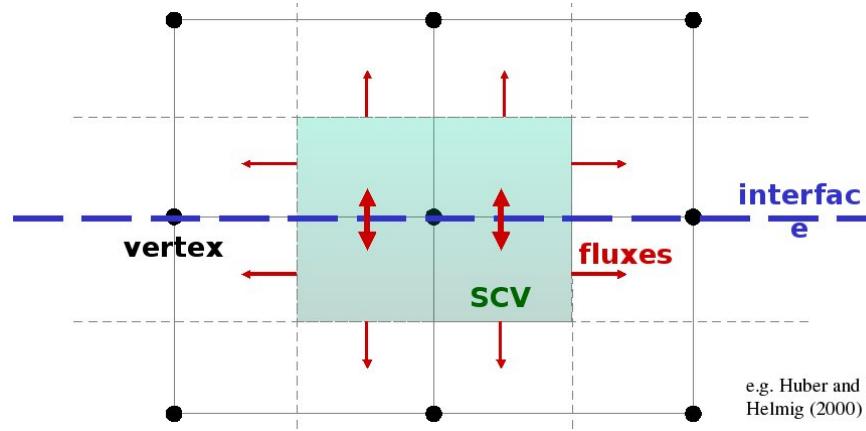
IC (6) ($a+w$) guarantees also the continuity of mole fractions (10).

Computational algorithm

- **Non-linear** system in space and time: $\chi = (p_g^{\text{ff}}, X_g^{w,\text{ff}}, \mathbf{v}_g^{\text{ff}}, T^{\text{ff}}, p_g^{\text{pm}}, X_g^{w,\text{pm}}, T^{\text{pm}})^T$

$$\frac{\partial \mathbf{M}(\chi)}{\partial t} - \nabla \cdot \mathbf{A}(\chi) = \mathbf{F}(\chi), \quad \mathbf{M}(\cdot) \text{ storage, } \mathbf{A}(\cdot) \text{ flux, } \mathbf{F}(\cdot) \text{ source}$$

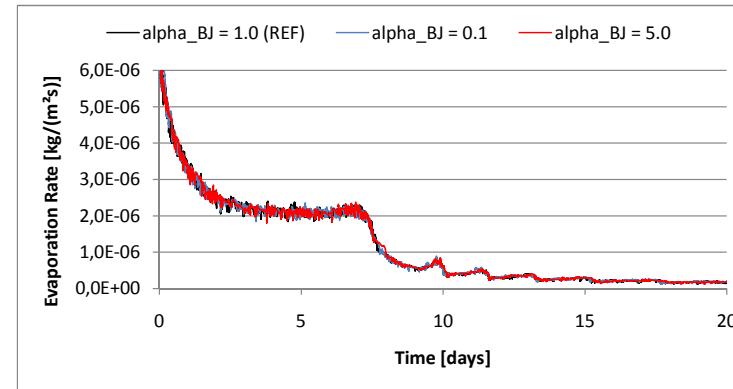
- **Conservative box scheme** guarantees consistent flux transport at the interface



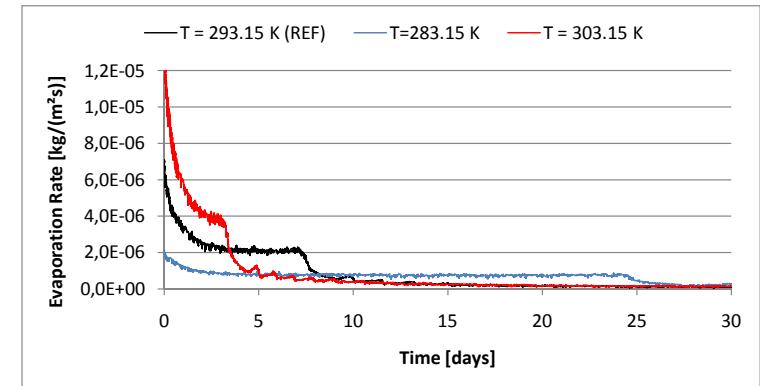
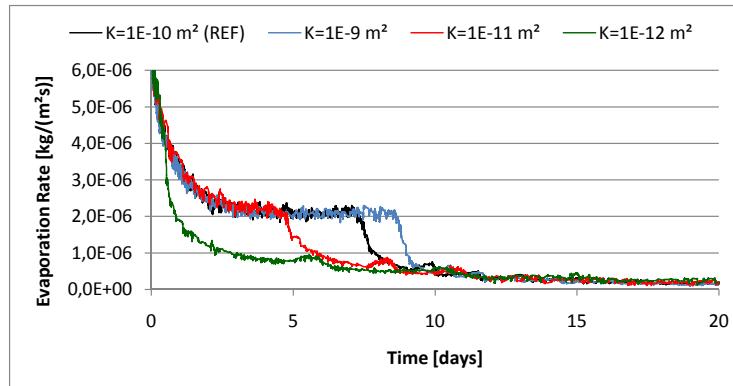
- **Stabilization** based on pressure [Franca, Hughes, Stenberg 93]
- **Implementation** based on DUNE [Bastian et.al.], DuMuX [Flemisch et.al]

Influence on the evaporation rate

- Influence of the **coefficient** in the Beavers–Joseph–Saffman coefficient



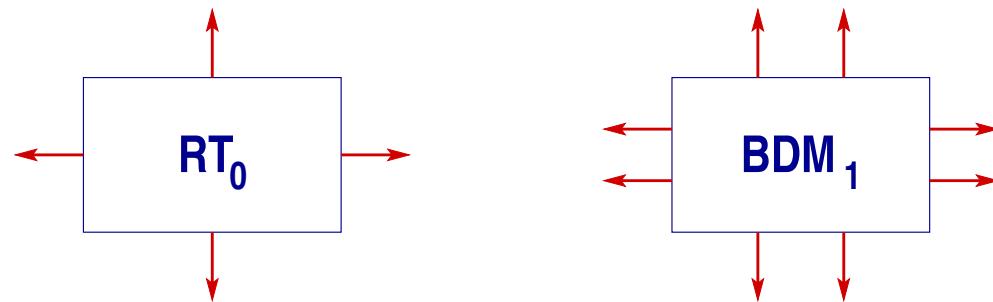
- Influence of the **permeability** (left) and **temperature** (right)



Hybrid DG discretization

Idea: Use $H(\text{div})$ -conforming fe [Rivière et.al. 05,09,10], [Lipnikov, Vassilev, Yotov 10] stabilize by interior penalty terms the velocity jump in tangential direction

- Use $RT_{k-1} \times BDM_k$ for the velocities (PM: first order, FF: second order)



- Convergence rates for the $RT_0(\Omega_{\text{PM}}) \times BDM_1(\Omega_{\text{FF}})$ coupling

	$\ u - u_h\ _{H_1(\Omega_{\text{FF}})}$	$\ u - u_h\ _{L_2(\Omega_{\text{PM}})}$	$\ p - p_h\ _{L_2(\Omega_{\text{FF}})}$	$\ p - p_h\ _{L_2(\Omega_{\text{PM}})}$
rate	0.99	1.00	1.00	0.99

- Convergence rates for the $RT_1(\Omega_{\text{PM}}) \times BDM_2(\Omega_{\text{FF}})$ coupling

	$\ u - u_h\ _{H_1(\Omega_{\text{FF}})}$	$\ u - u_h\ _{L_2(\Omega_{\text{PM}})}$	$\ p - p_h\ _{L_2(\Omega_{\text{FF}})}$	$\ p - p_h\ _{L_2(\Omega_{\text{PM}})}$
rate	1.98	1.98	1.97	1.99



From inequality...

... via the non-linear complementarity ...

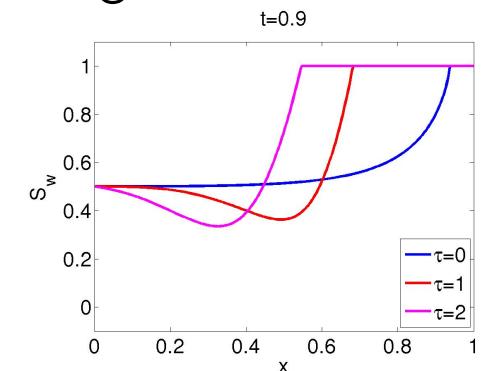
to equality

Variational inequalities in porous media

- **Signorini type:** PDE + **algebraic constraints on interfaces**

Application: Brooks–Corey type capillary pressure for heterogeneous media

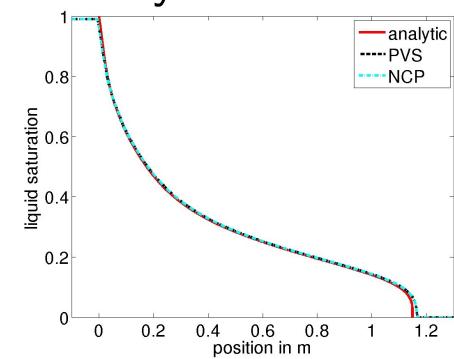
$$p_n - p_w = p_c = \underbrace{p_c^{\text{BC}}(S_w)}_{\text{[Brooks, Corey 71]}} - \tau \quad \underbrace{\frac{dS_w}{dt}}_{\text{[Hassanzadeh, Gray 90]}}$$



- **Obstacle type:** PDE + **algebraic constraints on domain**

Application: phase transition in multi-phase multi-component systems

$$\sum_{\kappa=1}^N x_{\alpha}^{\kappa} \leq 1, \quad \sum_{\kappa=1}^N x_{\alpha}^{\kappa} = 1 \text{ if phase } \alpha \text{ is present.}$$



How to discretize and how to solve?



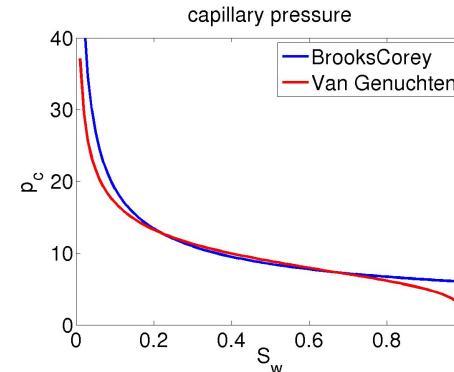
From bi-directional coupled...

... via fractional flow ...

to one-directional coupled equalities

Extension: Heterogeneous media

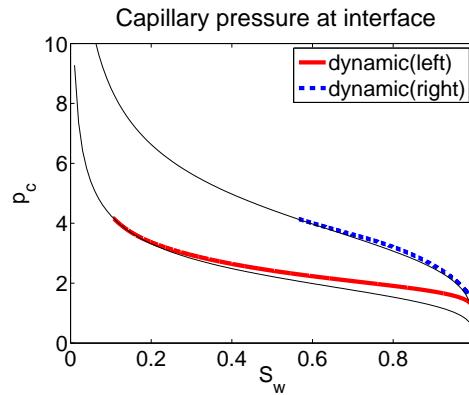
- **Van-Genuchten [80]:** Regularization at $S_w = 1$ of Brooks–Corey [64]



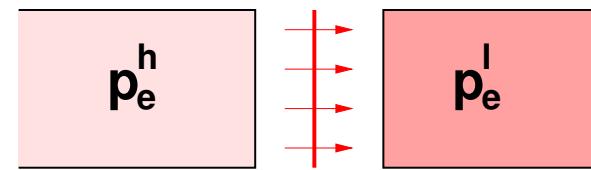
⇒ Regularized model numerically easier but introduces artificial diffusion

- **Heterogeneous** media possibly results in jumps in $[p_e]$ [DeNeef 00]

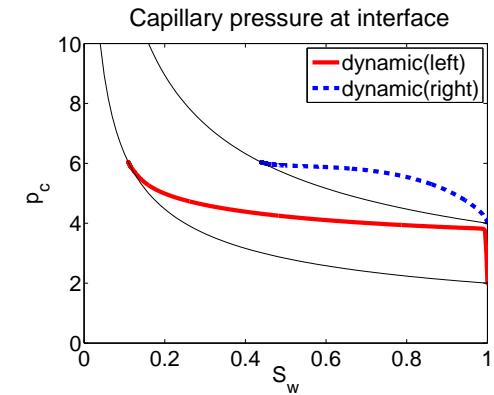
$[p_e] = 0$: v. Genuchten



high permeability low permeability



$[p_e] > 0$: Brooks–Corey

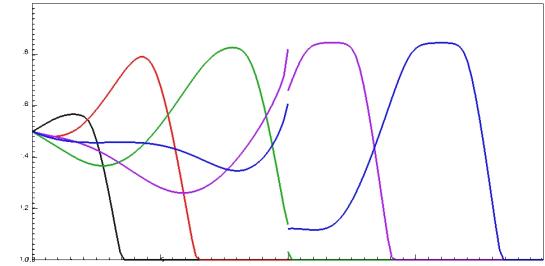
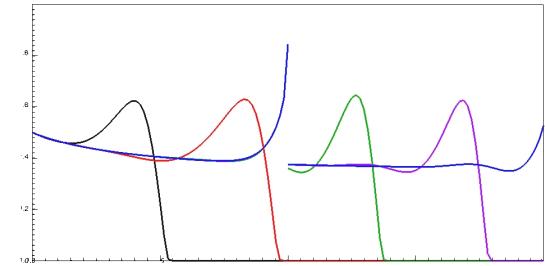
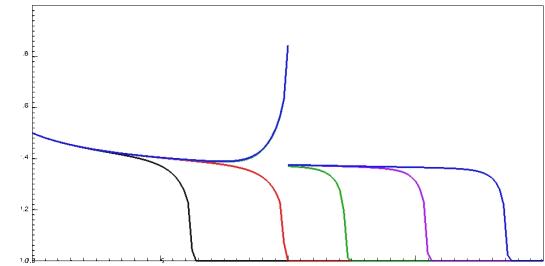


$$[p_e] \geq [p_c] \geq 0, S_n^l \geq 0, [p_c]S_n^l = 0$$

Inequality constraint

Two domains - Influence of τ and $[p_e]$

cuts at $t = 0.2, \dots, 1.0$



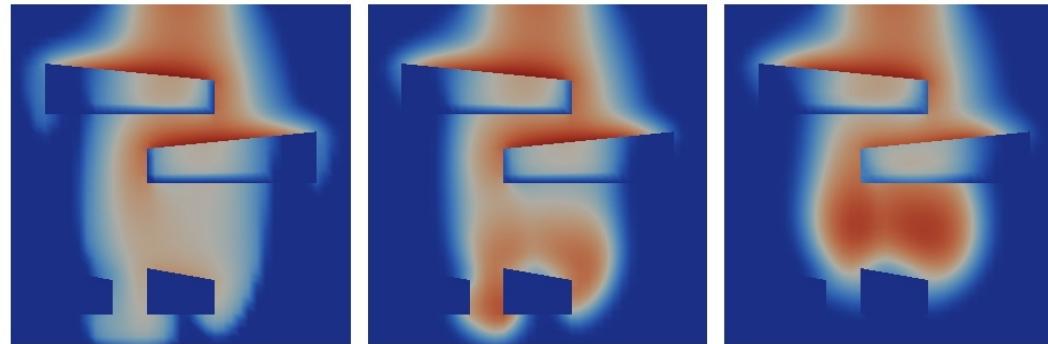
Brooks–Corey model: $k_{rw} = s^{3+\frac{2}{\theta}}$, $k_{rn} = (1-s)^2(1-s^{1+\frac{2}{\theta}})$, $p_c^{\text{stat}} = p_e s^{-\frac{1}{\theta}}$, $\theta = 2$

⇒ Results in **sharper** wave fronts

Influence of τ at different time-points t_i , $i = 1, 2, 3$

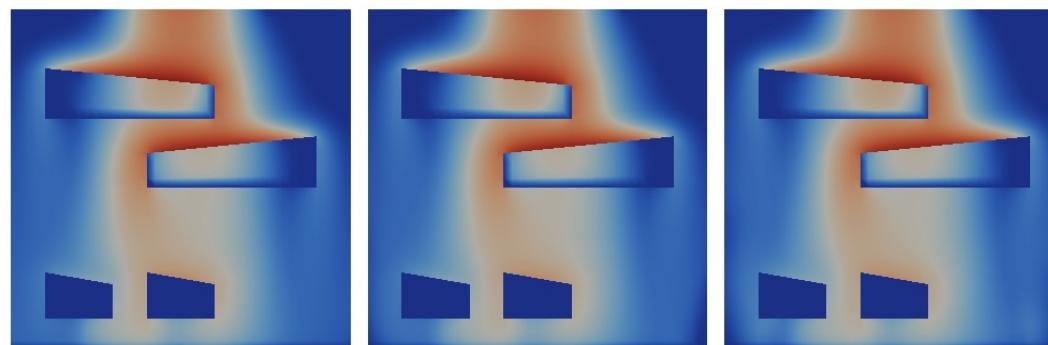
$t_1 = 0$:

⇒ more diffusive



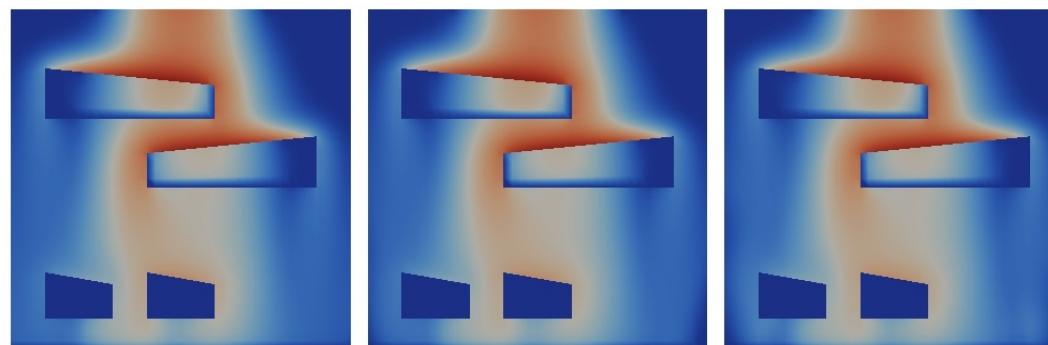
$t_2 = 60$:

⇒ different wave fronts



$t_3 = 200$:

⇒ no difference
in the long-range



How to solve the coupled porous media system?

Popular approach for standard model: Fractional flow formulation (FFF)

Advantages:

- 1D-case can be analyzed
- Natural decoupling for time integration
- Computation of v_t based on elliptic equation for global pressure

Disadvantages:

- Physical interpretation of global pressure?
- **Dynamic capillary** pressure does not yield decoupling
- **Inequality interface conditions** for global pressure are difficult to formulate

Longrightarrow Numerical scheme for extended model should not be based on standard FFF

Fractional flow formulation

Approach: Decoupling of the system in terms of total velocity and global pressure
[Helmig 97, Chavent and Jaffre 86, Morel–Seytoux 73]

$$\mathbf{v}_t := \mathbf{v}_n + \mathbf{v}_w, \quad \operatorname{div} \mathbf{v}_t = q_n + q_w, \quad \operatorname{div} ((\lambda_n + \lambda_w) K \nabla p) = q_p$$

⇒ solve **elliptic** “pressure equation” in each time-step as pre-process

Evolution equation for the saturation:

$$\Phi \frac{dS_w}{dt} + \operatorname{div} (f_w(S_w) \mathbf{v}_t + \bar{\lambda}(S_w) K (\nabla p_c - \varrho_\Delta \mathbf{g})) = 0,$$

with fractional flow functions $f_w := \frac{\lambda_w}{\lambda_n + \lambda_w}$, $\bar{\lambda} := \frac{\lambda_n \lambda_w}{\lambda_n + \lambda_w}$, $\lambda_\alpha := \frac{k_{r\alpha}}{\mu_\alpha}$, $\varrho_\Delta := \varrho_w - \varrho_n$.

⇒ possibly degenerated **parabolic** equation ($s = S_w$):

$$\Phi \frac{ds}{dt} + \operatorname{div} \left(f_w(s) \mathbf{v}_t + \bar{\lambda}(s) K \left(\underbrace{\frac{dp_c^{\text{stat}}(s)}{ds}}_{\text{[v. Genuchten 80]}} \nabla s - \varrho_\Delta \mathbf{g} \right) - \bar{\lambda}(s) K \tau \nabla \frac{ds}{dt} \right) = 0.$$

[v. Genuchten 80]
[Brooks–Corey 64]



Alternative flow formulation

Assumption: Water saturation higher than residual saturation $\Rightarrow \lambda_w > 0$

non-wetting velocity:

$$\begin{aligned}\mathbf{v}_n &= -\lambda_n K (\nabla p_n - \varrho_n \mathbf{g}) \\ &= -\lambda_n K (\nabla p_w + \nabla p_c - \varrho_n \mathbf{g}) \\ &= \frac{\lambda_n}{\lambda_w} \mathbf{v}_w - \lambda_n K (\nabla p_c + \varrho_\Delta \mathbf{g})\end{aligned}$$

Pressure equation from mass balance:

$$-\operatorname{div} (\lambda_w K (\nabla p_w - \varrho_w \mathbf{g})) = q_w - \Phi \frac{dS_w}{dt}$$

Evolution equation for the saturation:

$$-\Phi \frac{dS_w}{dt} + \operatorname{div} \left(\frac{\lambda_n}{\lambda_w} \mathbf{v}_w - \lambda_n K \left(\frac{\partial p_c^{\text{stat}}}{\partial S_w} \nabla S_w + \varrho_\Delta \mathbf{g} - \tau \frac{dS_w}{dt} \right) \right) = q_n$$

⇒ **Interface** conditions only needed in S_w and p_c

⇒ **Dynamic** capillary effect does not enter into pressure equation



Decoupled time integration

Step 1:

Compute pressure p_w^{n+1} /velocity \mathbf{v}_w^{n+1} using saturation s^n, s^{n-1} :

$$-\operatorname{div}(\lambda_w(s^n)K(\nabla p_w^{n+1} - \varrho_w \mathbf{g})) = q_w^{n+1} - \Phi \frac{s^n - s^{n-1}}{\Delta t}$$

⇒ static **linear elliptic** equation for pressure p_w

Step 2:

Compute saturation s^{n+1} time-implicit using \mathbf{v}_w^{n+1} : $\lambda_\alpha^{n+1} := \lambda_\alpha(s^{n+1}), \tau^{n+1} := \tau(s^{n+1})$

$$\begin{aligned} -\Phi \frac{s^{n+1}}{\Delta t} + \operatorname{div} \left(\frac{\lambda_n^{n+1}}{\lambda_w^{n+1}} \mathbf{v}_w^{n+1} - \lambda_n^{n+1} K \left(\frac{dp_c^{\text{stat}}(s^{n+1})}{ds} \nabla s^{n+1} + \varrho_\Delta \mathbf{g} - \tau^{n+1} \frac{s^{n+1} - s^n}{\Delta t} \right) \right) \\ = q_n^{n+1} - \Phi \frac{s^n}{\Delta t} \end{aligned}$$

⇒ (degenerated) **non-linear parabolic** equation for saturation $S_w = s$, FV, upwinding

Comparison of v_w update

left: no update (initial pressure), **middle:** fully coupled, **right:** decoupling in time

⇒ Decoupling in time is **efficient** and **stable**

Semi-smooth Newton for two-phase flow problems

Step 3: Inequality constraint for Brooks–Corey at interface:

$$[p_c] \geq 0, \quad S_n^l \geq 0, \quad [p_c]S_n^l = 0$$

NCP-function:

$$C([p_c], S_n^l) := [p_c] - \max(0, [p_c] - cS_n^l), \quad c > 0$$

Active set strategy:

Active node $p \in \mathcal{A}$: $[p_c]_p = 0$, Dirichlet condition in pressure

Inactive node $p \in \mathcal{I}$: $s_p = 1$, Dirichlet condition in saturation, ($s = 1 - S_n^l$)

Iteration to find correct active set: Start with $\mathcal{A}_0 = \mathcal{A}^{\text{old}}$, $\mathcal{I}_0 = \mathcal{I}^{\text{old}}$

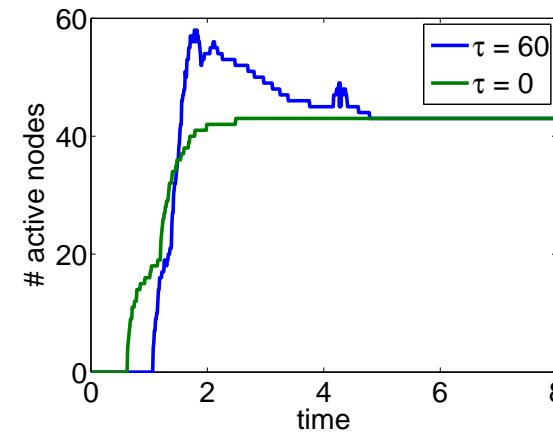
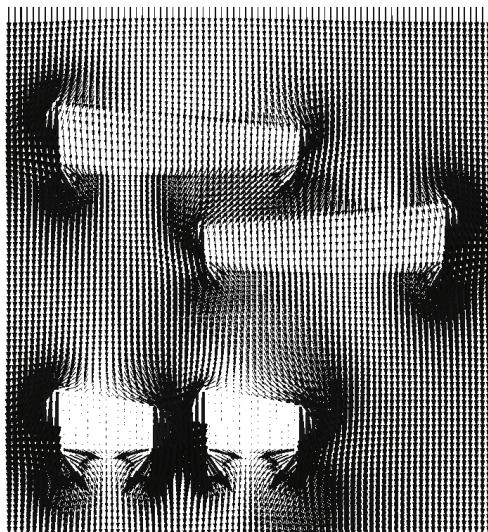
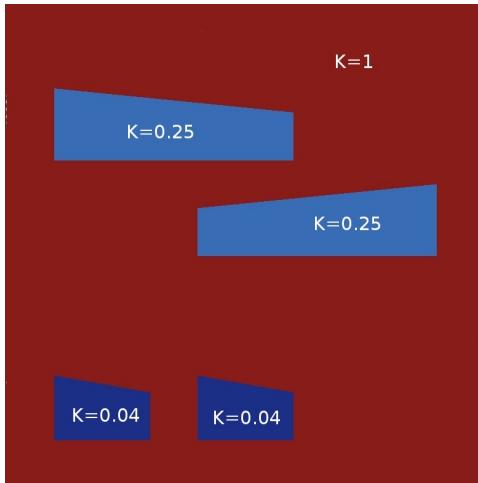
If $p \in \mathcal{A}$ and $s_p > 1$ → set p inactive in next iteration step

If $p \in \mathcal{I}$ and $[p_c]_p < 0$ → set p active in next iteration step

Similar approach to include condition $[p_e] \geq [p_c]$ in model and discretization

Domain with lenses - active sets

Setting:





From multi-phase multi-component...

... constitutive relations ...

to coupled equalities

MpNc system

- Considering a system with N different components and with M different phases, we have $MN + 2M + N + 1$ unknowns

T	temperature
p_α	pressure in phase $\alpha \in \{1, \dots, M\}$
S_α	saturation of phase $\alpha \in \{1, \dots, M\}$
f^κ	fugacity of comp. $\kappa \in \{1, \dots, N\}$
x_α^κ	mole fraction of comp. $\kappa \in \{1, \dots, N\}$ in phase $\alpha \in \{1, \dots, M\}$

- Non-linear constitutive relations

$\mu_\alpha(T)$	viscosity of phase α
$\rho_{\text{mol},\alpha}(p_\alpha, x_\alpha^\kappa, T)$	molar density of phase α
$\rho_{\text{mass},\alpha}(p_\alpha, x_\alpha^\kappa, T)$	mass density of phase α
$u_\alpha(p_\alpha, x_\alpha^\kappa, T)$	specific internal energy of phase α
$h_\alpha(p_\alpha, x_\alpha^\kappa, T)$	specific enthalpy of phase α
$k_{r\alpha}(S_\alpha)$	relative permeability of phase α
$\lambda_{\text{pm}}(p_\alpha, x_\alpha^\kappa, S_\alpha, T)$	heat conduction coefficient

- $N + 1$ balance equations of the form $\frac{\partial \xi}{\partial t} + \nabla \cdot \Psi - q = 0$

Balance equations

- N mass conservation of the components $\kappa \in \{1, \dots, N\}$

$$\xi = \phi \sum_{\alpha=1}^M \rho_{\text{mol},\alpha} x_{\alpha}^{\kappa} S_{\alpha}, \quad \rho_{\text{mass},\alpha} = \rho_{\text{mol},\alpha} \sum_{\kappa=1}^N x_{\alpha}^{\kappa} M^{\kappa}.$$

$$\Psi = - \sum_{\alpha=1}^M \left(\frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\text{mol},\alpha} x_{\alpha}^{\kappa} \mathbf{K} (\nabla p_{\alpha} - \rho_{\text{mass},\alpha} \mathbf{g}) + D_{\text{pm}}^{\kappa} \rho_{\text{mol},\alpha} \nabla x_{\alpha}^{\kappa} \right),$$

- One energy conservation

$$\xi = \phi \sum_{\alpha=1}^M \rho_{\text{mass},\alpha} u_{\alpha} S_{\alpha} + (1 - \phi) \rho_s c_s \mathbf{T},$$

$$\Psi = - \sum_{\alpha=1}^M \left(\frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\text{mass},\alpha} h_{\alpha} \mathbf{K} (\nabla p_{\alpha} - \rho_{\text{mass},\alpha} \mathbf{g}) \right)$$

$$- \sum_{\kappa=1}^N \sum_{\alpha=1}^M \left(D_{\text{pm}}^{\kappa} \rho_{\text{mol},\alpha} h_{\alpha}^{\kappa} M^{\kappa} \nabla x_{\alpha}^{\kappa} \right) - \lambda_{\text{pm}} \nabla \mathbf{T}$$



Constitutive relations

- One saturation scaling:

$$\sum_{\alpha=1}^M S_\alpha = 1$$

- $M-1$ capillary pressure relations: $\alpha \in \{2, \dots, M\}$

$$p_{\alpha-1} - p_\alpha = p_{c,(\alpha-1)\alpha}(S_\alpha)$$

- MN fugacity relations: $\kappa \in \{1, \dots, N\}$, $\alpha \in \{1, \dots, M\}$

$$f^\kappa = \Phi_\alpha^\kappa(p_\alpha, x_\alpha^1, \dots, x_\alpha^N, T) x_\alpha^\kappa p_\alpha, \quad x_\alpha^\kappa = x_\alpha^\kappa(p_1, f^1, \dots, f^N, T)$$

⇒ $N + 1$ PDES and $1 + (M - 1) + MN$ constitutive relations

⇒ $MN + 2M + N + 1 - (N + 1 + M + NM) = M$ missing conditions

Phase transition

- **Sum** of mole fractions per phase is **bounded**:

$$\sum_{\kappa=1}^N x_{\alpha}^{\kappa} \leq 1, \quad \sum_{\kappa=1}^N x_{\alpha}^{\kappa} = 1 \text{ if phase } \alpha \text{ is present.}$$

- **Saturation** S_{α} for face α is **non-negative**:

$$1 - \sum_{\kappa=1}^N x_{\alpha}^{\kappa} \geq 0, \quad S_{\alpha} \geq 0, \quad S_{\alpha} \left(1 - \sum_{\kappa=1}^N x_{\alpha}^{\kappa} \right) = 0.$$

- **Elimination** of the MN mole fractions, S_1 and p_{α} , $\alpha \in \{2, \dots, M\}$ results in a complex system with $N + 1 + M$ unknowns

$$(p_1, f^1, \dots, f^N, S_2, \dots, S_M, T)$$

$N + 1$ PDEs plus M Karush–Kuhn–Tucker triplets



Semi-smooth Newton for two-phase flow problems

Inequality constraint for phase transition in domain:

$$S_\alpha \geq 0, \quad 1 - \sum_{\kappa=1}^N x_\alpha^\kappa \geq 0, \quad (1 - \sum_{\kappa=1}^N x_\alpha^\kappa) S_\alpha = 0, \quad \alpha = 1, \dots, M,$$

where S_α phase saturation, x_α^κ mole fraction of component κ

NCP-functions: $C_\alpha := S_\alpha - \max(0, S_\alpha - c_\alpha(1 - \sum_{\kappa=1}^N x_\alpha^\kappa))$, $c_\alpha > 0$

But: S_α , x_α^κ are not the primary variables

Primary variables: $p_1, T, S_2, \dots, S_M, x_1^1, \dots, x_1^N$

Rewrite: $S_1 = 1 - \sum_{\alpha=2}^M S_\alpha$, $x_\alpha^\kappa = \gamma_\alpha^\kappa(T, p_1)x_1^\kappa$, $\alpha = 2, \dots, M$, $\kappa = 1, \dots, N$,

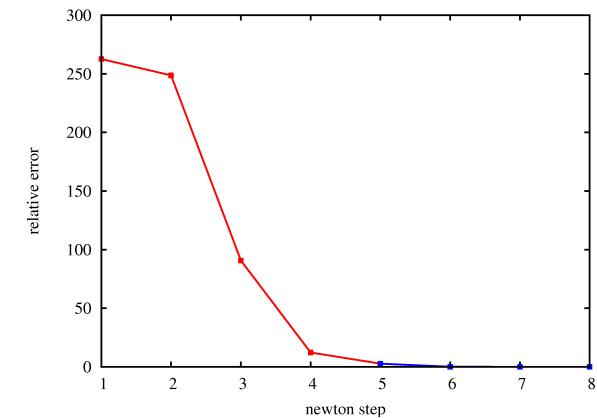
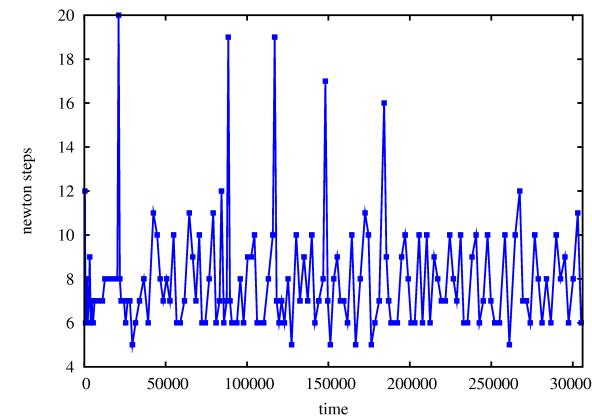
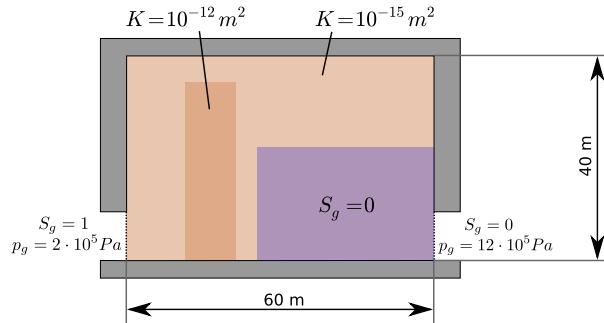
where the factor γ_α^κ depends on Dalton's, Henry's, Raoult's law

⇒ **New NCP** functions in terms of **primary** variables

⇒ Semismooth Newton can be applied to the coupled non-linear system

Semismooth Newton for a two phase system

- Setting and Newton iteration



- Saturation and active sets

Comparison between a PVS and a NCP approach

PVS: primary variable switch

[Class, Helmig, Bastian 02], [Falta, Pruess, Javandel, Witherspoon 92]

NCP: Non-linear complementarity

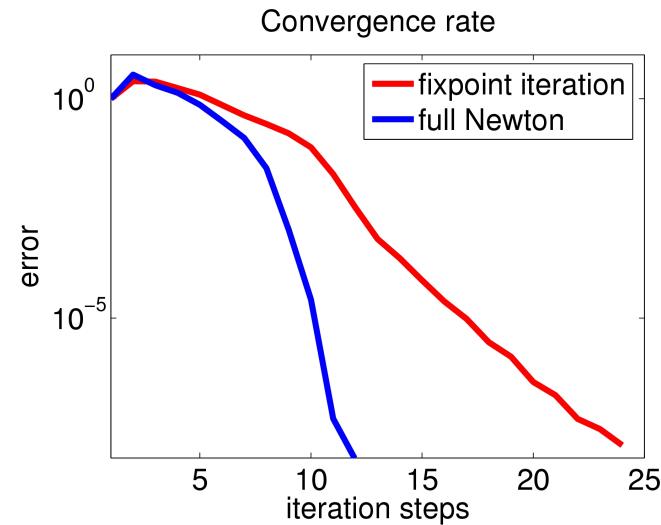
Feature	PVS	NCP
size of linearized system	$(N + 1) \cdot \mathcal{N} $	$(N + M + 1) \cdot \mathcal{N} $
size of solved linear systems	$(N + 1) \cdot \mathcal{N} $	$(N + 1) \cdot \mathcal{N} $
local linearization cost	$O((N + 1)^2)$	$O((N + M + 1)^2)$
no. of update procedures	$2^M - 1$	1
phase-change robustness	bad	good
extension to large M, N	demanding	straightforward

Comparison of the PVS method and the new NCP formulation

M and N represent the number of phases and components, $|\mathcal{N}|$ is the number of degrees of freedom (DOF) of the spatial discretization

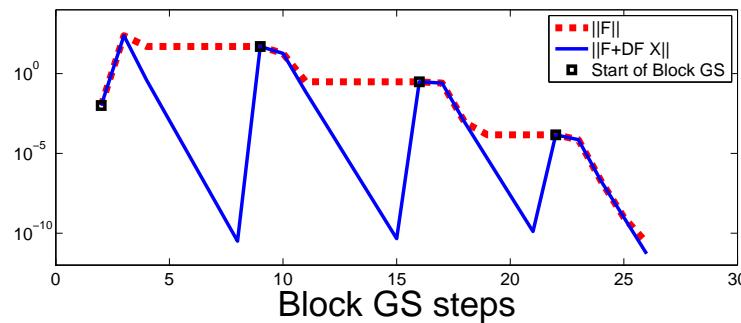
Nested non-linear solvers (structural mechanics)

- Comparison between inner/outer iteration and full Newton

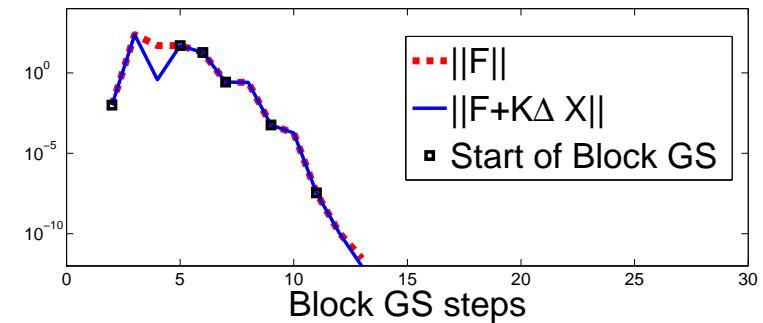


- Comparison between fully resolved and adapted linear accuracy [Eisenstat, Walker 96]

Exact Newton, 4 Newton steps

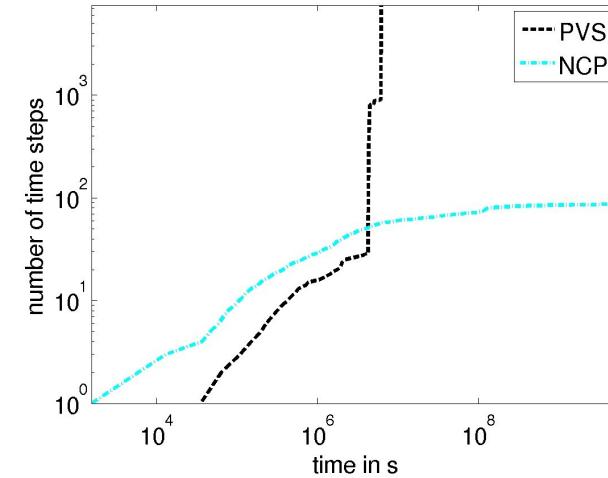
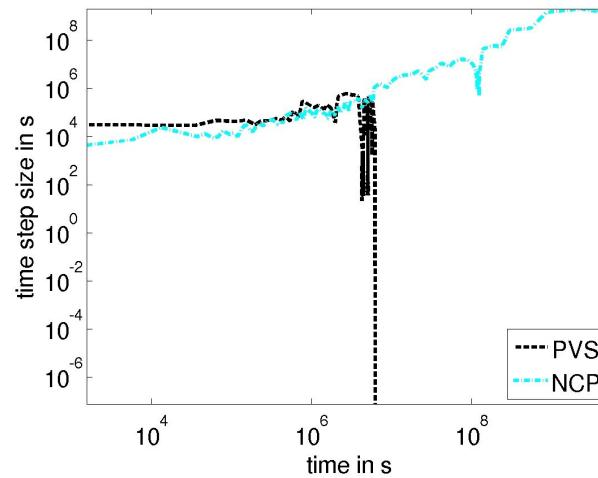


Inexact Newton, 6 Newton steps

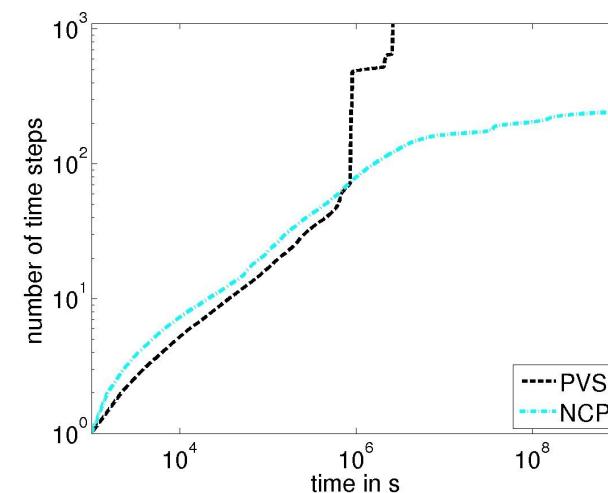
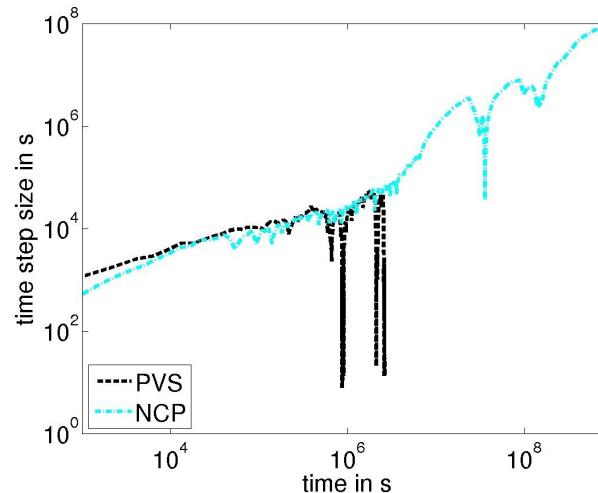


Time step-size control

- Heuristic strategy to balance number of Newton and time steps



- Heuristic strategy to maximize time step while Newton converges

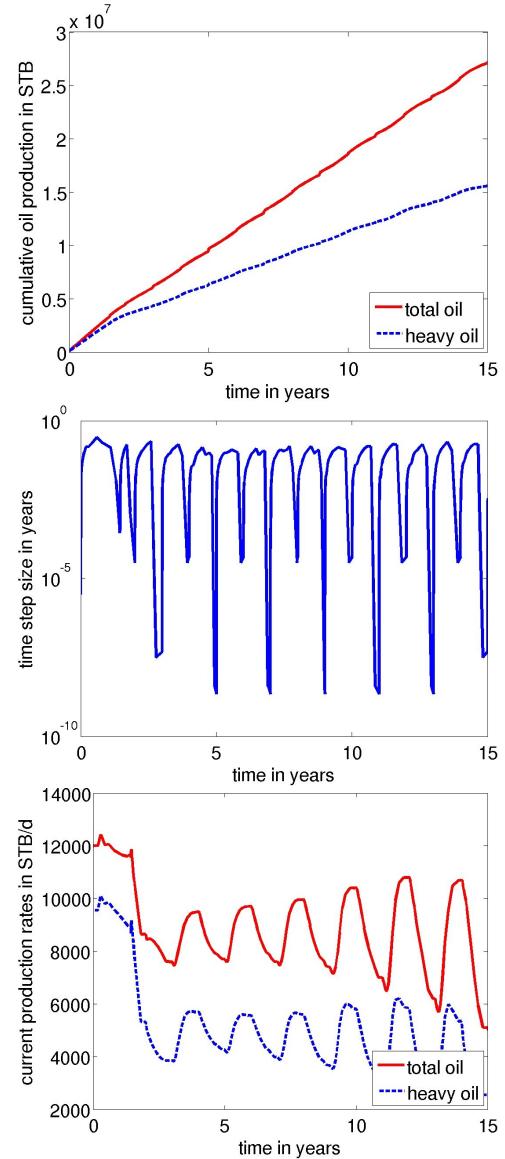


3 phases 7 component system

- **3D oil extraction problem**

5th benchmark of the Society of Petroleum Engineers
[Killough, Kossack 87]

- production well is located in one lower corner
- water alternating gas is placed in the opposite corner
- $N = 7$ components: H_2O , C_1 , C_3 , C_6 , C_{10} , C_{15} , C_{20}
- $M = 3$ phases: gas, oil, water



Conclusions

- Multi-physics model for two-component non-isothermal flow
- New coupling conditions at the interface based on thermodynamic equilibrium
- Formulation of a multi-component, multi-phase system as variational inequality
- New solver strategy based on NCP functions

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