

Numerical simulation of flow and contaminant transport in porous media

Martin Vohralík

INRIA Paris-Rocquencourt

Pardubice, December 17, 2013

Outline

- 1 Introduction and motivation
- 2 Basic mathematical model
- 3 Numerical difficulties
- 4 A posteriori error estimates
- 5 Extension to multiphase compositional flows

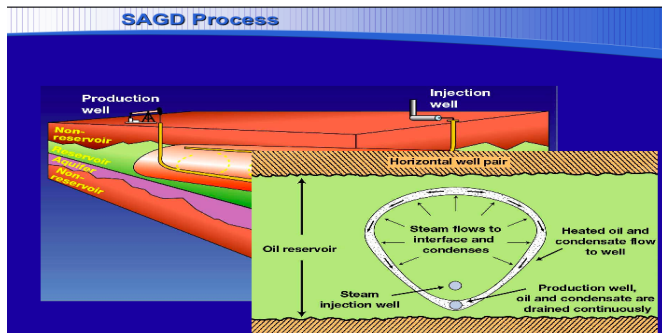
Outline

- 1 Introduction and motivation
- 2 Basic mathematical model
- 3 Numerical difficulties
- 4 A posteriori error estimates
- 5 Extension to multiphase compositional flows

Oil production

Oil production

- oil – one of the major **energy supply** of today's world
- need for **efficient production**
- high prices – question of **rentability**



Reservoir

Changing the viscosity by heating

Changing the viscosity by heating

- inject steam into the reservoir
- increase the pressure
- heat the oil
- objective: **viscosity reduction** of the oil

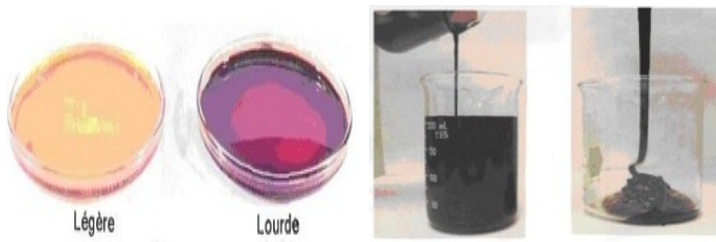


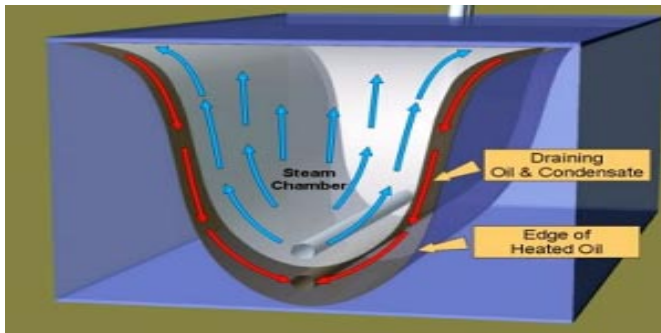
FIG. 1.3 – Huiles lourdes

Heated and cold oil

Efficient oil production

Efficient oil production

- capture the heated oil
- **increase** the production **efficiency**



Steam-assisted gravity drainage

Outline

- 1 Introduction and motivation
- 2 Basic mathematical model**
- 3 Numerical difficulties
- 4 A posteriori error estimates
- 5 Extension to multiphase compositional flows

Basic mathematical model: two-phase flow

Mathematical model

$$\partial_t(\phi \mathbf{s}_\alpha) + \nabla \cdot \left(\overbrace{-\frac{k_{r,\alpha}(\mathbf{s}_w)}{\mu_\alpha} \underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha \mathbf{g} \nabla z)}^{\text{Darcy velocity } \mathbf{u}_\alpha} \right) = q_\alpha, \quad \alpha \in \{\mathbf{n}, \mathbf{w}\},$$

$$\mathbf{s}_n + \mathbf{s}_w = 1,$$

$$p_n - p_w = p_c(\mathbf{s}_w)$$

- two immiscible, incompressible fluids
- space–time domain $\Omega \times (0, T)$
- + initial & boundary conditions
- p_n, p_w : unknown nonwetting and wetting phase pressures
- $\mathbf{s}_n, \mathbf{s}_w$: unknown nonwetting and wetting phase saturations
- $p_c(\cdot)$: the nonlinear capillary pressure
- $k_{r,\alpha}(\cdot)$: the nonlinear relative permeability
- ϕ porosity; $\underline{\mathbf{K}}$ permeability tensor; $\mu_\alpha, \rho_\alpha, q_\alpha$: viscosities, densities, sources; z vertical coordinate; g gravity

Basic mathematical model: two-phase flow

Mathematical model

$$\partial_t(\phi \mathbf{s}_\alpha) + \nabla \cdot \left(\overbrace{-\frac{k_{r,\alpha}(\mathbf{s}_w)}{\mu_\alpha} \underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha \mathbf{g} \nabla z)}^{\text{Darcy velocity } \mathbf{u}_\alpha} \right) = q_\alpha, \quad \alpha \in \{\mathbf{n}, \mathbf{w}\},$$

$$\mathbf{s}_n + \mathbf{s}_w = 1,$$

$$p_n - p_w = p_c(\mathbf{s}_w)$$

- two immiscible, incompressible fluids
- space–time domain $\Omega \times (0, T)$
- + initial & boundary conditions
- p_n, p_w : unknown nonwetting and wetting phase pressures
- $\mathbf{s}_n, \mathbf{s}_w$: unknown nonwetting and wetting phase saturations
- $p_c(\cdot)$: the nonlinear capillary pressure
- $k_{r,\alpha}(\cdot)$: the nonlinear relative permeability
- ϕ porosity; $\underline{\mathbf{K}}$ permeability tensor; $\mu_\alpha, \rho_\alpha, q_\alpha$: viscosities, densities, sources; z vertical coordinate; g gravity

Basic mathematical model: two-phase flow

Mathematical model

$$\partial_t(\phi \mathbf{s}_\alpha) + \nabla \cdot \left(\overbrace{-\frac{k_{r,\alpha}(\mathbf{s}_w)}{\mu_\alpha} \underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha \mathbf{g} \nabla z)}^{\text{Darcy velocity } \mathbf{u}_\alpha} \right) = q_\alpha, \quad \alpha \in \{\mathbf{n}, \mathbf{w}\},$$

$$\mathbf{s}_n + \mathbf{s}_w = 1,$$

$$p_n - p_w = p_c(\mathbf{s}_w)$$

- two immiscible, incompressible fluids
- space–time domain $\Omega \times (0, T)$
- + initial & boundary conditions
- p_n, p_w : unknown nonwetting and wetting **phase pressures**
- $\mathbf{s}_n, \mathbf{s}_w$: unknown nonwetting and wetting **phase saturations**
- $p_c(\cdot)$: the nonlinear **capillary pressure**
- $k_{r,\alpha}(\cdot)$: the nonlinear **relative permeability**
- ϕ porosity; $\underline{\mathbf{K}}$ permeability tensor; $\mu_\alpha, \rho_\alpha, q_\alpha$: viscosities, densities, sources; z vertical coordinate; g gravity

Basic mathematical model: two-phase flow

Mathematical model

$$\partial_t(\phi \mathbf{s}_\alpha) + \nabla \cdot \left(\overbrace{-\frac{k_{r,\alpha}(\mathbf{s}_w)}{\mu_\alpha} \underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha \mathbf{g} \nabla z)}^{\text{Darcy velocity } \mathbf{u}_\alpha} \right) = q_\alpha, \quad \alpha \in \{\mathbf{n}, \mathbf{w}\},$$

$$\mathbf{s}_n + \mathbf{s}_w = 1,$$

$$p_n - p_w = p_c(\mathbf{s}_w)$$

- two immiscible, incompressible fluids
- space–time domain $\Omega \times (0, T)$
- + initial & boundary conditions
- p_n, p_w : unknown nonwetting and wetting **phase pressures**
- $\mathbf{s}_n, \mathbf{s}_w$: unknown nonwetting and wetting **phase saturations**
- $p_c(\cdot)$: the nonlinear **capillary pressure**
- $k_{r,\alpha}(\cdot)$: the nonlinear **relative permeability**
- ϕ porosity; $\underline{\mathbf{K}}$ permeability tensor; $\mu_\alpha, \rho_\alpha, q_\alpha$: viscosities, densities, sources; z vertical coordinate; g gravity

Basic mathematical model: two-phase flow

Mathematical model

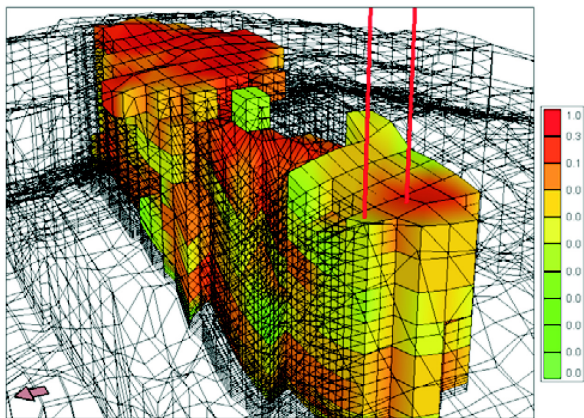
$$\partial_t(\phi \mathbf{s}_\alpha) + \nabla \cdot \left(\overbrace{-\frac{k_{r,\alpha}(\mathbf{s}_w)}{\mu_\alpha} \mathbf{K}(\nabla p_\alpha + \rho_\alpha \mathbf{g} \nabla z)}^{\text{Darcy velocity } \mathbf{u}_\alpha} \right) = q_\alpha, \quad \alpha \in \{\mathbf{n}, \mathbf{w}\},$$

$$\mathbf{s}_n + \mathbf{s}_w = 1,$$

$$p_n - p_w = p_c(\mathbf{s}_w)$$

- two immiscible, incompressible fluids
- space–time domain $\Omega \times (0, T)$
- + initial & boundary conditions
- p_n, p_w : unknown nonwetting and wetting **phase pressures**
- $\mathbf{s}_n, \mathbf{s}_w$: unknown nonwetting and wetting **phase saturations**
- $p_c(\cdot)$: the nonlinear **capillary pressure**
- $k_{r,\alpha}(\cdot)$: the nonlinear **relative permeability**
- ϕ porosity; \mathbf{K} permeability tensor; $\mu_\alpha, \rho_\alpha, q_\alpha$: viscosities, densities, sources; z vertical coordinate; g gravity

Geometry and meshes



Geometry and meshes example

Outline

- 1 Introduction and motivation
- 2 Basic mathematical model
- 3 Numerical difficulties**
- 4 A posteriori error estimates
- 5 Extension to multiphase compositional flows

Numerical difficulties

Numerical difficulties

- highly nonlinear (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects

Numerical difficulties

Numerical difficulties

- highly nonlinear (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects

Numerical difficulties

Numerical difficulties

- highly nonlinear (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects

Numerical difficulties

Numerical difficulties

- highly nonlinear (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects

Numerical difficulties

Numerical difficulties

- highly nonlinear (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects

Numerical difficulties

Numerical difficulties

- highly nonlinear (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects

Numerical difficulties

Numerical difficulties

- highly nonlinear (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects

Numerical difficulties

Numerical difficulties

- highly nonlinear (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects

Numerical difficulties

Numerical difficulties

- highly nonlinear (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects

Outline

- 1 Introduction and motivation
- 2 Basic mathematical model
- 3 Numerical difficulties
- 4 A posteriori error estimates**
- 5 Extension to multiphase compositional flows

Tools and goals

Tools

- **a posteriori error estimators** for determining the parts of the spatio-temporal domain with **increased error** (material discontinuities, sources and sinks, moving sharp fronts)
- **adaptive stopping criteria**
- **adaptive mesh refinement**

Goals

- **increase the precision** while simultaneously **decreasing the cost** (**increase efficiency**)
- **guarantee** a user-given **precision** of the calculation

Tools and goals

Tools

- **a posteriori error estimators** for determining the parts of the spatio-temporal domain with **increased error** (material discontinuities, sources and sinks, moving sharp fronts)
- **adaptive stopping criteria**
- **adaptive mesh refinement**

Goals

- **increase** the **precision** while simultaneously **decreasing** the **cost** (**increase efficiency**)
- **guarantee** a user-given **precision** of the calculation

Tools and goals

Tools

- **a posteriori error estimators** for determining the parts of the spatio-temporal domain with **increased error** (material discontinuities, sources and sinks, moving sharp fronts)
- **adaptive stopping criteria**
- **adaptive mesh refinement**

Goals

- **increase** the **precision** while simultaneously **decreasing** the **cost** (**increase efficiency**)
- **guarantee** a user-given **precision** of the calculation

Estimate distinguishing different error components

Theorem (Distinguishing different error components)

Consider

- *time step* n ,
- *linearization step* k ,
- *iterative algebraic solver step* i ,

and the corresponding approximations $s_{w,h\tau}^{n,k,i}$ and $p_{w,h\tau}^{n,k,i}$. Then

$$\| (s_w - s_{w,h\tau}^{n,k,i}, p_w - p_{w,h\tau}^{n,k,i}) \|_{l_n} \leq \eta_{sp}^{n,k,i} + \eta_{tm}^{n,k,i} + \eta_{lin}^{n,k,i} + \eta_{alg}^{n,k,i}.$$

Error components

- $\eta_{sp}^{n,k,i}$: spatial discretization
- $\eta_{tm}^{n,k,i}$: temporal discretization
- $\eta_{lin}^{n,k,i}$: linearization
- $\eta_{alg}^{n,k,i}$: algebraic solver

Estimate distinguishing different error components

Theorem (Distinguishing different error components)

Consider

- *time step* n ,
- *linearization step* k ,
- *iterative algebraic solver step* i ,

and the corresponding approximations $s_{w,h\tau}^{n,k,i}$ and $p_{w,h\tau}^{n,k,i}$. Then

$$\| (s_w - s_{w,h\tau}^{n,k,i}, p_w - p_{w,h\tau}^{n,k,i}) \|_I \leq \eta_{sp}^{n,k,i} + \eta_{tm}^{n,k,i} + \eta_{lin}^{n,k,i} + \eta_{alg}^{n,k,i}.$$

Error components

- $\eta_{sp}^{n,k,i}$: **spatial discretization**
- $\eta_{tm}^{n,k,i}$: **temporal discretization**
- $\eta_{lin}^{n,k,i}$: **linearization**
- $\eta_{alg}^{n,k,i}$: **algebraic solver**

Local estimators

- spatial estimators*

$$\eta_{\text{sp},K}^{n,k,i}(t) := \left\{ \begin{aligned} & \sum_{\alpha \in \{\mathbf{n}, \mathbf{w}\}} (\|\mathbf{d}_{\alpha,h}^{n,k,i} - \mathbf{v}_{\alpha}(p_{\mathbf{w},h}^{n,k,i}, \mathbf{s}_{\mathbf{w},h}^{n,k,i})\|_K \\ & + h_K/\pi \|q_{\alpha}^n - \partial_t^n(\phi \mathbf{s}_{\alpha,h\tau}^{n,k,i}) - \nabla \cdot \mathbf{u}_{\alpha,h}^{n,k,i}\|_K)^2 \\ & + (\|\underline{\mathbf{K}}(\lambda_{\mathbf{w}}(\mathbf{s}_{\mathbf{w},h\tau}^{n,k,i}) + \lambda_{\mathbf{n}}(\mathbf{s}_{\mathbf{w},h\tau}^{n,k,i}))\nabla(p(p_{\mathbf{w},h\tau}^{n,k,i}, \mathbf{s}_{\mathbf{w},h\tau}^{n,k,i}) - \bar{p}_{h\tau}^{n,k,i})\|_K(t))^2 \\ & + (\|\underline{\mathbf{K}}\nabla(q(\mathbf{s}_{\mathbf{w},h\tau}^{n,k,i}) - \bar{q}_{h\tau}^{n,k,i})\|_K(t))^2 \end{aligned} \right\}^{\frac{1}{2}}$$

- temporal estimators*

$$\eta_{\text{tm},K,\alpha}^{n,k,i}(t) := \|\mathbf{v}_{\alpha}(p_{\mathbf{w},h\tau}^{n,k,i}, \mathbf{s}_{\mathbf{w},h\tau}^{n,k,i})(t) - \mathbf{v}_{\alpha}(p_{\mathbf{w},h\tau}^{n,k,i}, \mathbf{s}_{\mathbf{w},h\tau}^{n,k,i})(t^n)\|_K \quad \alpha \in \{\mathbf{n}, \mathbf{w}\}$$

- linearization estimators*

$$\eta_{\text{lin},K,\alpha}^{n,k,i} := \|\mathbf{l}_{\alpha,h}^{n,k,i}\|_K \quad \alpha \in \{\mathbf{n}, \mathbf{w}\}$$

- algebraic estimators*

$$\eta_{\text{alg},K,\alpha}^{n,k,i} := \|\mathbf{a}_{\alpha,h}^{n,k,i}\|_K \quad \alpha \in \{\mathbf{n}, \mathbf{w}\}$$

Model problem

Horizontal flow

$$\partial_t(\phi \mathbf{s}_\alpha) - \nabla \cdot \left(\frac{k_{r,\alpha}(\mathbf{s}_w)}{\mu_\alpha} \underline{\mathbf{K}} \nabla p_\alpha \right) = 0,$$

$$\mathbf{s}_n + \mathbf{s}_w = 1,$$

$$p_n - p_w = p_c(\mathbf{s}_w)$$

Brooks–Corey model

- relative permeabilities

$$k_{r,w}(\mathbf{s}_w) = s_e^4, \quad k_{r,n}(\mathbf{s}_w) = (1 - s_e)^2(1 - s_e^2)$$

- capillary pressure

$$p_c(\mathbf{s}_w) = p_d s_e^{-\frac{1}{2}}$$

-

$$s_e := \frac{s_w - s_{rw}}{1 - s_{rw} - s_{rn}}$$

Model problem

Horizontal flow

$$\partial_t(\phi s_\alpha) - \nabla \cdot \left(\frac{k_{r,\alpha}(s_w)}{\mu_\alpha} \underline{\mathbf{K}} \nabla p_\alpha \right) = 0,$$

$$s_n + s_w = 1,$$

$$p_n - p_w = p_c(s_w)$$

Brooks–Corey model

- relative permeabilities

$$k_{r,w}(s_w) = s_e^4, \quad k_{r,n}(s_w) = (1 - s_e)^2(1 - s_e^2)$$

- capillary pressure

$$p_c(s_w) = p_d s_e^{-\frac{1}{2}}$$

-

$$s_e := \frac{s_w - s_{rw}}{1 - s_{rw} - s_{rn}}$$

Fully implicit cell-centered finite volume scheme

Fully implicit cell-centered two-point finite volumes

For all $1 \leq n \leq N$, look for $s_{w,h}^n, \bar{p}_{w,h}^n$ such that

$$\phi \frac{s_{w,K}^n - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KL} \in \mathcal{E}_K^{\text{int}}} F_{w,e_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

$$-\phi \frac{s_{w,K}^n - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KL} \in \mathcal{E}_K^{\text{int}}} F_{n,e_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

where the normal fluxes are given by

$$F_{w,e_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) := - \frac{\lambda_{r,w}(s_{w,K}^n) + \lambda_{r,w}(s_{w,L}^n)}{2} |\underline{\mathbf{K}}| \frac{\bar{p}_{w,L}^n - \bar{p}_{w,K}^n}{|\mathbf{x}_K - \mathbf{x}_L|} |e_{KL}|,$$

$$F_{n,e_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) := - \frac{\lambda_{r,n}(s_{w,K}^n) + \lambda_{r,n}(s_{w,L}^n)}{2} |\underline{\mathbf{K}}| \times \frac{\bar{p}_{w,L}^n + p_c(s_{w,L}^n) - (\bar{p}_{w,K}^n + p_c(s_{w,K}^n))}{|\mathbf{x}_K - \mathbf{x}_L|}$$

Fully implicit cell-centered finite volume scheme

Fully implicit cell-centered two-point finite volumes

For all $1 \leq n \leq N$, look for $s_{w,h}^n, \bar{p}_{w,h}^n$ such that

$$\phi \frac{s_{w,K}^n - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KL} \in \mathcal{E}_K^{\text{int}}} F_{w,e_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

$$-\phi \frac{s_{w,K}^n - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KL} \in \mathcal{E}_K^{\text{int}}} F_{n,e_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

where the normal fluxes are given by

$$F_{w,e_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) := - \frac{\lambda_{r,w}(s_{w,K}^n) + \lambda_{r,w}(s_{w,L}^n)}{2} |\underline{\mathbf{K}}| \frac{\bar{p}_{w,L}^n - \bar{p}_{w,K}^n}{|\mathbf{x}_K - \mathbf{x}_L|} |e_{KL}|,$$

$$F_{n,e_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) := - \frac{\lambda_{r,n}(s_{w,K}^n) + \lambda_{r,n}(s_{w,L}^n)}{2} |\underline{\mathbf{K}}| \times \frac{\bar{p}_{w,L}^n + p_c(s_{w,L}^n) - (\bar{p}_{w,K}^n + p_c(s_{w,K}^n))}{|\mathbf{x}_K - \mathbf{x}_L|}$$

Linearization and algebraic solution

Linearization step k and algebraic step i

Couple $s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}$ such that

$$\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KL} \in \mathcal{E}_K^{\text{int}}} F_{w,e_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{w,K}^{n,k,i},$$

$$-\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KL} \in \mathcal{E}_K^{\text{int}}} F_{n,e_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{n,K}^{n,k,i},$$

where the linearized normal fluxes are given by

$$\begin{aligned} F_{\alpha,e_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) &:= F_{\alpha,e_{KL}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,e_{KL}}}{\partial s_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (s_{w,M}^{n,k,i} - s_{w,M}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,e_{KL}}}{\partial \bar{p}_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k,i} - \bar{p}_{w,M}^{n,k-1}). \end{aligned}$$

Linearization and algebraic solution

Linearization step k and algebraic step i

Couple $s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}$ such that

$$\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KL} \in \mathcal{E}_K^{\text{int}}} F_{w,e_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{w,K}^{n,k,i},$$

$$-\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KL} \in \mathcal{E}_K^{\text{int}}} F_{n,e_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{n,K}^{n,k,i},$$

where the linearized normal fluxes are given by

$$F_{\alpha,e_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) := F_{\alpha,e_{KL}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1})$$

$$+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,e_{KL}}}{\partial s_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (s_{w,M}^{n,k,i} - s_{w,M}^{n,k-1})$$

$$+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,e_{KL}}}{\partial \bar{p}_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k,i} - \bar{p}_{w,M}^{n,k-1}).$$

Velocities reconstructions

Velocities reconstructions

$$\begin{aligned}
 (\mathbf{d}_{\alpha,h}^{n,k,i} \cdot \mathbf{n}_K, 1)_{e_{KL}} &:= F_{\alpha, e_{KL}}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 ((\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i}) \cdot \mathbf{n}_K, 1)_{e_{KL}} &:= F_{\alpha, e_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 \mathbf{a}_{\alpha,h}^{n,k,i} &:= \mathbf{d}_{\alpha,h}^{n,k,i+\nu} + \mathbf{l}_{\alpha,h}^{n,k,i+\nu} - (\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i})
 \end{aligned}$$

Comments

- phase velocities reconstructions:

$$\mathbf{u}_{\alpha,h}^{n,k,i} := \mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i} + \mathbf{a}_{\alpha,h}^{n,k,i}$$

- $\mathbf{d}_{\alpha,h}^{n,k,i}$, $\mathbf{l}_{\alpha,h}^{n,k,i}$, $\mathbf{a}_{\alpha,h}^{n,k,i}$ used to identify error components

Velocities reconstructions

Velocities reconstructions

$$\begin{aligned}
 (\mathbf{d}_{\alpha,h}^{n,k,i} \cdot \mathbf{n}_K, 1)_{e_{KL}} &:= F_{\alpha, e_{KL}}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 ((\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i}) \cdot \mathbf{n}_K, 1)_{e_{KL}} &:= F_{\alpha, e_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 \mathbf{a}_{\alpha,h}^{n,k,i} &:= \mathbf{d}_{\alpha,h}^{n,k,i+\nu} + \mathbf{l}_{\alpha,h}^{n,k,i+\nu} - (\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i})
 \end{aligned}$$

Comments

- **phase velocities reconstructions:**

$$\mathbf{u}_{\alpha,h}^{n,k,i} := \mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i} + \mathbf{a}_{\alpha,h}^{n,k,i}$$

- $\mathbf{d}_{\alpha,h}^{n,k,i}$, $\mathbf{l}_{\alpha,h}^{n,k,i}$, $\mathbf{a}_{\alpha,h}^{n,k,i}$ used to identify **error components**

Data from Klieber & Rivière (2006)

Data

$$\Omega = (0, 300)\text{m} \times (0, 300)\text{m}, \quad T = 4 \cdot 10^6 \text{s},$$

$$\phi = 0.2, \quad \underline{\mathbf{K}} = 10^{-11} \underline{\mathbf{I}} \text{m}^2,$$

$$\mu_w = 5 \cdot 10^{-4} \text{kg m}^{-1} \text{s}^{-1}, \quad \mu_n = 2 \cdot 10^{-3} \text{kg m}^{-1} \text{s}^{-1},$$

$$s_{rw} = s_{rn} = 0, \quad \rho_d = 5 \cdot 10^3 \text{kg m}^{-1} \text{s}^{-2}$$

Initial condition (\tilde{K} 18m \times 18m lower left corner block)

$$s_w^0 = 0.2 \text{ on } K \in \mathcal{T}_h, K \notin \tilde{K},$$

$$s_w^0 = 0.95 \text{ on } K \in \mathcal{T}_h, K \in \tilde{K}$$

Boundary conditions (\hat{K} 18m \times 18m upper right corner block)

- no flow Neumann boundary conditions everywhere except of $\partial\tilde{K} \cap \partial\Omega$ and $\partial\hat{K} \cap \partial\Omega$

- \tilde{K} – injection well: $s_w = 0.95$, $\rho_w = 3.45 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$

- \hat{K} – production well: $s_w = 0.2$, $\rho_w = 2.41 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$

Data from Klieber & Rivière (2006)

Data

$$\Omega = (0, 300)\text{m} \times (0, 300)\text{m}, \quad T = 4 \cdot 10^6 \text{s},$$

$$\phi = 0.2, \quad \mathbf{K} = 10^{-11} \mathbf{I} \text{m}^2,$$

$$\mu_w = 5 \cdot 10^{-4} \text{kg m}^{-1} \text{s}^{-1}, \quad \mu_n = 2 \cdot 10^{-3} \text{kg m}^{-1} \text{s}^{-1},$$

$$s_{rw} = s_{rn} = 0, \quad \rho_d = 5 \cdot 10^3 \text{kg m}^{-1} \text{s}^{-2}$$

Initial condition (\tilde{K} 18m \times 18m lower left corner block)

$$s_w^0 = 0.2 \text{ on } K \in \mathcal{T}_h, K \notin \tilde{K},$$

$$s_w^0 = 0.95 \text{ on } K \in \mathcal{T}_h, K \in \tilde{K}$$

Boundary conditions (\hat{K} 18m \times 18m upper right corner block)

- no flow Neumann boundary conditions everywhere except of $\partial\tilde{K} \cap \partial\Omega$ and $\partial\hat{K} \cap \partial\Omega$
- \tilde{K} – injection well: $s_w = 0.95$, $\rho_w = 3.45 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$
- \hat{K} – production well: $s_w = 0.2$, $\rho_w = 2.41 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$

Data from Klieber & Rivière (2006)

Data

$$\Omega = (0, 300)\text{m} \times (0, 300)\text{m}, \quad T = 4 \cdot 10^6 \text{s},$$

$$\phi = 0.2, \quad \mathbf{K} = 10^{-11} \mathbf{I} \text{m}^2,$$

$$\mu_w = 5 \cdot 10^{-4} \text{kg m}^{-1} \text{s}^{-1}, \quad \mu_n = 2 \cdot 10^{-3} \text{kg m}^{-1} \text{s}^{-1},$$

$$s_{rw} = s_{rn} = 0, \quad \rho_d = 5 \cdot 10^3 \text{kg m}^{-1} \text{s}^{-2}$$

Initial condition (\tilde{K} 18m \times 18m lower left corner block)

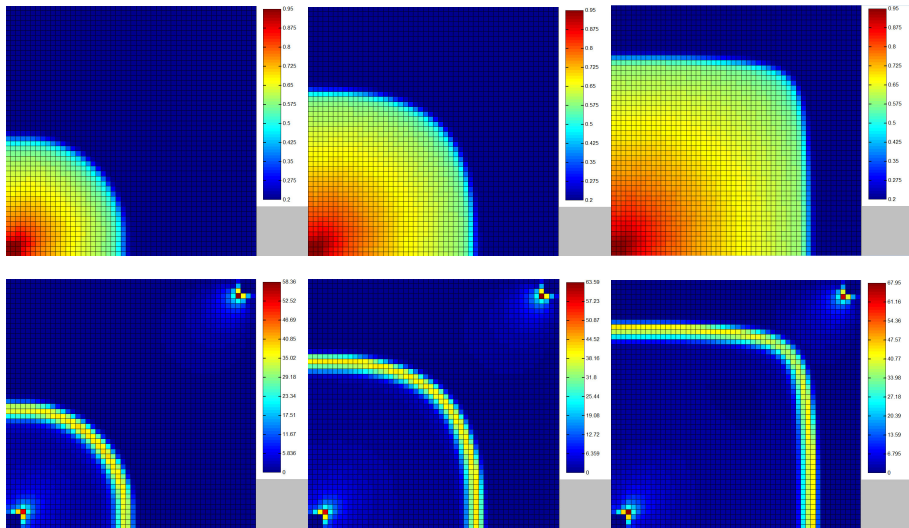
$$s_w^0 = 0.2 \text{ on } K \in \mathcal{T}_h, K \notin \tilde{K},$$

$$s_w^0 = 0.95 \text{ on } K \in \mathcal{T}_h, K \in \tilde{K}$$

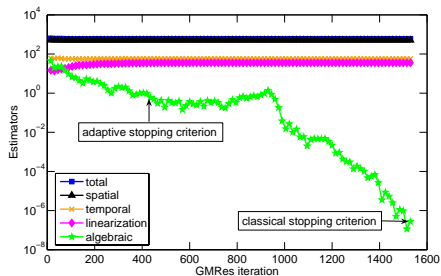
Boundary conditions (\hat{K} 18m \times 18m upper right corner block)

- no flow Neumann boundary conditions everywhere except of $\partial\tilde{K} \cap \partial\Omega$ and $\partial\hat{K} \cap \partial\Omega$
- \tilde{K} – injection well: $s_w = 0.95$, $p_w = 3.45 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$
- \hat{K} – production well: $s_w = 0.2$, $p_w = 2.41 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$

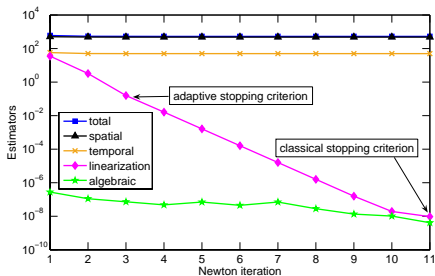
Water saturation/estimators evolution



Estimators and stopping criteria

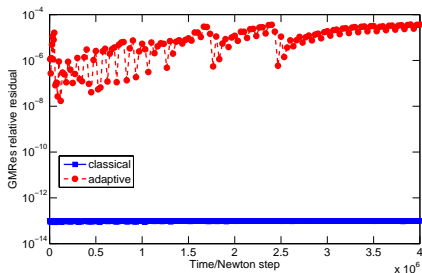


Estimators in function of
GMRes iterations

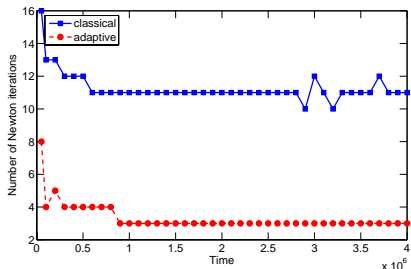


Estimators in function of
Newton iterations

GMRes relative residual/Newton iterations

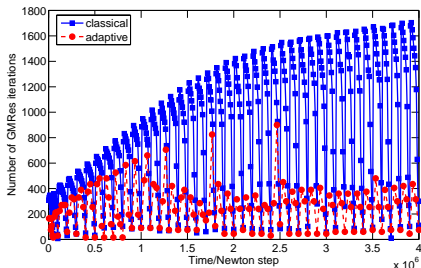


GMRes relative residual

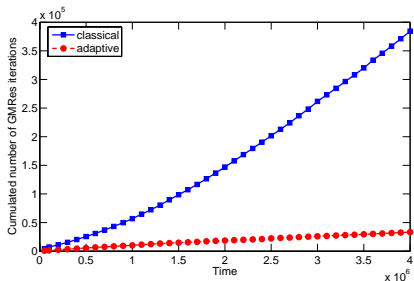


Newton iterations

GMRes iterations



Per time and Newton step



Cumulated

Outline

- 1 Introduction and motivation
- 2 Basic mathematical model
- 3 Numerical difficulties
- 4 A posteriori error estimates
- 5 Extension to multiphase compositional flows

Extension to multiphase compositional flows

Multiphase compositional flows

- N_P phases, N_C components
- miscible, compressible
- isothermal/thermal
- Ph.D. theses of Carole Henry and Soleiman Yousef (Paris 6/IFPEN)

Multiphase compositional flows

Unknowns

- phase saturations S_p
- component molar fractions $C_{p,c}$
- reference pressure P

Constitutive laws

- phase pressures – reference pressure – capillary pressure

$$P_p := P + P_{c_p}(\mathbf{S})$$

- Darcy's law

$$\mathbf{v}_p(P_p, \mathbf{C}_p) := -\Lambda (\nabla P_p - \rho_p(P_p, \mathbf{C}_p)\mathbf{g})$$

- component fluxes

$$\Phi_c := \sum_{p \in \mathcal{P}_c} \Phi_{p,c}, \quad \Phi_{p,c} := \nu_p(P_p, \mathbf{S}, \mathbf{C}_p) C_{p,c} \mathbf{v}_p(P_p, \mathbf{C}_p)$$

- amount of moles of component c per unit volume

$$I_c := \phi \sum_{p \in \mathcal{P}_c} \zeta_p(P_p, \mathbf{C}_p) S_p C_{p,c}$$

Multiphase compositional flows

Unknowns

- phase saturations S_p
- component molar fractions $C_{p,c}$
- reference pressure P

Constitutive laws

- phase pressures – reference pressure – capillary pressure

$$P_p := P + P_{c_p}(\mathbf{S})$$

- Darcy's law

$$\mathbf{v}_p(P_p, \mathbf{C}_p) := -\Lambda (\nabla P_p - \rho_p(P_p, \mathbf{C}_p)\mathbf{g})$$

- component fluxes

$$\Phi_c := \sum_{p \in \mathcal{P}_c} \Phi_{p,c}, \quad \Phi_{p,c} := \nu_p(P_p, \mathbf{S}, \mathbf{C}_p) C_{p,c} \mathbf{v}_p(P_p, \mathbf{C}_p)$$

- amount of moles of component c per unit volume

$$I_c := \phi \sum_{p \in \mathcal{P}_c} \zeta_p(P_p, \mathbf{C}_p) S_p C_{p,c}$$

Multiphase compositional flows

Governing partial differential equations

- conservation of mass

$$\partial_t l_c + \nabla \cdot \Phi_c = q_c, \quad \forall c \in \mathcal{C}$$

- + boundary & initial conditions

Closure algebraic equations

- conservation of pore volume

$$\sum_{p \in \mathcal{P}} S_p = 1$$

- conservation of the quantity of the matter

$$\sum_{c \in \mathcal{C}_p} C_{p,c} = 1 \quad \forall p \in \mathcal{P}$$

- thermodynamic equilibrium

$$\sum_{c \in \mathcal{C}} (N_{\mathcal{P}_c} - 1) \text{ equations}$$

Multiphase compositional flows

Governing partial differential equations

- conservation of mass

$$\partial_t l_c + \nabla \cdot \Phi_c = q_c, \quad \forall c \in \mathcal{C}$$

- + boundary & initial conditions

Closure algebraic equations

- conservation of pore volume

$$\sum_{p \in \mathcal{P}} S_p = 1$$

- conservation of the quantity of the matter

$$\sum_{c \in \mathcal{C}_p} C_{p,c} = 1 \quad \forall p \in \mathcal{P}$$

- thermodynamic equilibrium

$$\sum_{c \in \mathcal{C}} (N_{\mathcal{P}_c} - 1) \text{ equations}$$