A posteriori error estimates and stopping criteria for a two-phase flow with nonlinear complementarity constraints

Ibtihel Ben Gharbia, Jad Dabaghi, Vincent Martin, Martin Vohralík

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Outline

Introduction

System of PDEs with nonlinear complementarity constraints:
Find $\boldsymbol{U} \in \mathbb{R}^n$ such that

$$\mathcal{A}(\boldsymbol{U}) = 0$$
$$\mathcal{K}(\boldsymbol{U}) \geq 0, \quad \mathcal{G}(\boldsymbol{U}) \geq 0, \quad \mathcal{K}(\boldsymbol{U})^T \mathcal{G}(\boldsymbol{U}) = 0.$$

Motivation

- Treat nonlinearities on the constraints with the semi-smoothness theory
- Derive a posteriori error estimates at each semismooth step
- Formulate adaptive stopping criteria **to save computational time**

Application

►►► Compositional two-phase flow with phase transition in porous media.

Outline

Compositional two-phase flow with phase transition

$$\begin{cases} \partial_t l_w + \nabla \cdot (\rho_w^l \mathbf{q}_l + \mathbf{J}_w^l) = Q_w, \\ \partial_t l_h + \nabla \cdot (\rho_h^l \mathbf{q}_l + \rho_h^g \mathbf{q}_g + \mathbf{J}_h^l) = Q_h, \\ 1 - S_l \geq 0, \; HP_g - \beta_l \chi_h^l \geq 0, \; (1 - S_l)^T (HP_g - \beta_l \chi_h^l) = 0 \end{cases}$$

Unknowns: S_l, P_l, χ_h^l

Darcy's law:

$$\mathbf{q}_l = -\underline{\mathbf{K}} \frac{k_{rl}(S_l)}{\mu_l} \left[\nabla P_l - \left[\rho_w^l + \rho_h^l\right] g \nabla z \right]$$

$$\mathbf{q}_g = -\underline{\mathbf{K}} \frac{k_{rg}(S_g)}{\mu_g} \left[\nabla P_g - \left[\rho_h^l + \rho_h^g\right] g \nabla z \right]$$

Amount of components:

$$l_w = \phi \rho_w^l S_l + \phi \rho_w^g S_g$$

$$l_h = \phi \rho_h^l S_l + \phi \rho_h^g S_g$$

Fick flux:

$$\mathbf{J}_h^l = -\phi M^h S_l C_l D_h^l \nabla \chi_h^l$$

Algebraic closure:

$$S_l + S_g = 1, \quad \chi_h^l + \chi_w^l = 1, \quad \chi_h^g = 1$$

Capillary pressure: $P_g = P_l + P_c(S_l)$

Assumption

Water incompressible only present in liquid phase and gas slightly compressible

$$\rho_w^l = \text{cst}, \quad \rho_w^g = 0, \quad \rho_g = \beta_g P_g, \quad \rho_h^l = \beta_l \chi_h^l, \quad \chi_h^g = 1, \quad \chi_w^g = 0$$

Compositional two-phase flow with phase transition

$$\begin{cases} \partial_t l_w + \nabla \cdot (\rho_w^l \mathbf{q}_l + \mathbf{J}_w^l) = Q_w, \\ \partial_t l_h + \nabla \cdot (\rho_h^l \mathbf{q}_l + \rho_h^g \mathbf{q}_g + \mathbf{J}_h^l) = Q_h, \\ 1 - S_l \geq 0, \ HP_g - \beta_l \chi_h^l \geq 0, \ (1 - S_l)^T (HP_g - \beta_l \chi_h^l) = 0 \end{cases}$$

Unknowns: S_l, P_l, χ_h^l

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$$\mathbf{q}_l = -\underline{\mathbf{K}} \frac{k_{rl}(S_l)}{\mu_l} \left[\nabla P_l - \left[\rho_w^l + \rho_h^l \right] g \nabla z \right]$$

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Compositional two-phase flow with phase transition

$$\begin{cases} \partial_t l_{\rm w} + \nabla\cdot(\rho_{\rm w}^{\rm l}\mathbf{q}_{\rm l} + \mathbf{J}_{\rm w}^{\rm l}) = Q_{\rm w}, \\ \partial_t l_{\rm h} + \nabla\cdot(\rho_{\rm h}^{\rm l}\mathbf{q}_{\rm l} + \rho_{\rm h}^{\rm g}\mathbf{q}_{\rm g} + \mathbf{J}_{\rm h}^{\rm l}) = Q_{\rm h}, \\ 1 - S_{\rm l} \geq 0,\ HP_{\rm g} - \beta_{\rm l}\chi_{\rm h}^{\rm l} \geq 0,\ (1 - S_{\rm l})^T \left(HP_{\rm g} - \beta_{\rm l}\chi_{\rm h}^{\rm l}\right) = 0 \end{cases}$$

Unknowns: $S_{\rm l}, P_{\rm l}, \chi_{\rm h}^{\rm l}$

Amount of components:

$$l_{\rm w} = \phi\rho_{\rm w}^{\rm l}S_{\rm l} + \phi\rho_{\rm w}^{\rm g}S_{\rm g}$$
$$l_{\rm h} = \phi\rho_{\rm h}^{\rm l}S_{\rm l} + \phi\rho_{\rm h}^{\rm g}S_{\rm g}$$

Darcy's law:

$$\mathbf{q}_{\rm l} = -\underline{\mathbf{K}}\frac{k_{r{\rm l}}(S_{\rm l})}{\mu_{\rm l}}\left[\nabla P_{\rm l} - \left[\rho_{\rm w}^{\rm l} + \rho_{\rm h}^{\rm l}\right]g\nabla z\right]$$
$$\mathbf{q}_{\rm g} = -\underline{\mathbf{K}}\frac{k_{r{\rm g}}(S_{\rm g})}{\mu_{\rm g}}\left[\nabla P_{\rm g} - \left[\rho_{\rm h}^{\rm l} + \rho_{\rm h}^{\rm g}\right]g\nabla z\right]$$

Fick flux:

$$\mathbf{J}_{\rm h}^{\rm l} = -\phi M^{\rm h}S_{\rm l}C_{\rm l}D_{\rm h}^{\rm l}\nabla\chi_{\rm h}^{\rm l}$$

Algebraic closure:

$$S_{\rm l} + S_{\rm g} = 1, \quad \chi_{\rm h}^{\rm l} + \chi_{\rm w}^{\rm l} = 1, \quad \chi_{\rm h}^{\rm g} = 1$$

Capillary pressure: $P_{\rm g} = P_{\rm l} + P_c(S_{\rm l})$

Assumption

Water incompressible only present in liquid phase and gas slightly compressible

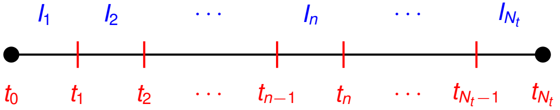
$$\rho_{\rm w}^{\rm l} = \mathrm{cst}, \quad \rho_{\rm w}^{\rm g} = 0, \quad \rho_{\rm g} = \beta_{\rm g}P_{\rm g}, \quad \rho_{\rm h}^{\rm l} = \beta_{\rm l}\chi_{\rm h}^{\rm l}, \quad \chi_{\rm h}^{\rm g} = 1, \quad \chi_{\rm w}^{\rm g} = 0$$

Discretization by the finite volume method

Numerical solution:

$$\boldsymbol{U}^n := (\boldsymbol{U}_K^n)_{K \in \mathcal{T}_h}, \qquad \boldsymbol{U}_K^n := (S_K^n, P_K^n, \chi_K^n) \quad \textbf{one value per cell}$$

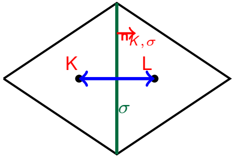
Time discretization: Consider: $t_0 = 0 < t_1 < \cdots < t_{N_t} = t_{\mathrm{F}} = N_t \Delta t$ with constant time step Δt.



$$\partial_t^n v_K := \frac{v_K^n - v_K^{n-1}}{\Delta t}.$$

Space discretization: $\mathcal{T}_h$ a superadmissible family of conforming simplicial meshes (Ciarlet) of the space domain Ω.

$$(\boldsymbol{\nabla} v \cdot \boldsymbol{n}_{K,\sigma}, 1)_\sigma := |\sigma| \frac{v_L - v_K}{d_{KL}} \quad \sigma \in \mathcal{E}_K^{\mathrm{int}},$$



Discretization of water equation

$$\boldsymbol{S}^n_{\mathrm{w},K}(\boldsymbol{U}^n) = \partial^n_t l_{\mathrm{w},K} + \sum_{\sigma \in \mathcal{E}^{\mathrm{int}}_K} F_{\mathrm{w},K,\sigma}(\boldsymbol{U}^n) - Q^n_{\mathrm{w,K}} = 0,$$

Total flux

$$F_{\mathrm{w},K,\sigma}(\boldsymbol{U}^n) = (\mathfrak{M}^{\mathrm{l}})^n_\sigma (\psi^{\mathrm{l}})^n_\sigma + (\mathrm{j}^{\mathrm{l}}_{\mathrm{w}})^n_\sigma \quad \sigma \in \mathcal{E}^{\mathrm{int}}_K$$

Discretization of hydrogen equation

$$\boldsymbol{S}^n_{\mathrm{h},K}(\boldsymbol{U}^n) = |K| \partial^n_t l_{\mathrm{h},K} + \sum_{\sigma \in \mathcal{E}^{\mathrm{int}}_K} F_{\mathrm{h},K,\sigma}(\boldsymbol{U}^n) - Q^n_{\mathrm{h,K}} = 0,$$

Total flux

$$F_{\mathrm{h},K,\sigma}(\boldsymbol{U}^n) = \chi^n_K (\mathfrak{M}^{\mathrm{l}})^n_\sigma (\psi^{\mathrm{l}})^n_\sigma + (\psi^{\mathrm{g}})^n_\sigma (\mathfrak{M}^{\mathrm{g}})^n_\sigma (\rho^*_{\mathrm{g}})^n_\sigma + (\mathrm{j}^{\mathrm{l}}_{\mathrm{h}})^n_\sigma, \quad \sigma \in \mathcal{E}^{\mathrm{int}}_K$$

- $\mathfrak{M}^{\mathrm{l}}$: mobility of liquid phase
- $\mathfrak{M}^{\mathrm{g}}$: mobility of gas phase
- ψ^{l}: potential of liquid phase
- ψ^{g}: potential of gas phase
- $\mathrm{j}^{\mathrm{l}}_{\mathrm{h}}$: discrete Fick term
- $Q^n_{\mathrm{w,K}}$, $Q^n_{\mathrm{h,K}}$: source term constant in space and time

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Total flux

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$$F_{\mathrm{h},K,\sigma}(\boldsymbol{U}^n) = \chi^n_K(\mathfrak{M}^{\mathrm{l}})^n_\sigma(\psi^{\mathrm{l}})^n_\sigma + (\psi^{\mathrm{g}})^n_\sigma(\mathfrak{M}^{\mathrm{g}})^n_\sigma(\rho^*_{\mathrm{g}})^n_\sigma + (\mathrm{j}^{\mathrm{l}}_{\mathrm{h}})^n_\sigma, \quad \sigma\in\mathcal{E}^{\mathrm{int}}_K$$

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Discrete complementarity problem

To reformulate the discrete constraints:

Definition (C-function)

$$\forall (\boldsymbol{a}, \boldsymbol{b}) \in \mathbb{R}^n \times \mathbb{R}^n, \; f(\boldsymbol{a}, \boldsymbol{b}) = 0 \iff \boldsymbol{a} \geq 0, \; \boldsymbol{b} \geq 0, \; \boldsymbol{a}^T \boldsymbol{b} = 0$$

min-function: $\min(\boldsymbol{a}, \boldsymbol{b}) = 0 \iff \boldsymbol{a} \geq 0, \; \boldsymbol{b} \geq 0, \; \boldsymbol{a}^T \boldsymbol{b} = 0.$

Application: complementarity constraints for the two-phase model

$$1 - S_K^n \geq 0, \; H(P_K^n + P_c(S_K^n)) - \beta_1 \chi_K^n \geq 0, \; (1 - S_K^n)^T (H(P_K^n + P_c(S_K^n)) - \beta_1 \chi_K^n) = 0$$

$$\Updownarrow$$

$$\min\left(1 - S_K^n, H(P_K^n + P_c(S_K^n)) - \beta_1 \chi_K^n\right) = 0$$

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Outline

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Global overview

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Weak solution

$$X = L^2((0,t_\mathrm{F}); H^1(\Omega)),\ Y = H^1((0,t_\mathrm{F}); L^2(\Omega)), Z = \left\{v \in L^2((0,t_\mathrm{F}); L^2(\Omega)),\ v \geq 0\right\}$$

Assumption (Weak formulation)

$$P_\mathrm{l}, P_\mathrm{g}, \chi_\mathrm{h}^\mathrm{l} \in X, \qquad S_\mathrm{l}, S_\mathrm{g}, l_\mathrm{w}, l_\mathrm{h}, \in Y \qquad \mathbf{\Phi}_\mathrm{w}, \mathbf{\Phi}_\mathrm{h} \in [L^2((0,t_\mathrm{F}); \mathbf{H}(\mathrm{div},\Omega)]^d$$

$$\int_0^{t_\mathrm{F}} (\partial_t l_c, \varphi)_\Omega(t)\,\mathrm{d}t - (\mathbf{\Phi}_c, \nabla\varphi)_\Omega(t)\,\mathrm{d}t - (Q_c, \varphi)_\Omega(t)\,\mathrm{d}t = 0 \quad \forall \varphi \in X,\ c = \mathrm{w}, \mathrm{h}$$

$$\int_0^{t_\mathrm{F}} (\lambda - (1 - S_\mathrm{l}), HP_\mathrm{g} - \beta_\mathrm{l}\chi_\mathrm{h}^\mathrm{l})_\Omega(t)\,\mathrm{d}t \geq 0 \quad \forall \lambda \in Z, \quad 1 - S_\mathrm{l} \in Z,\ c = \mathrm{w}, \mathrm{h}$$

The initial condition, as well as the algebraic closure hold.

$$\|\varphi\|_X = \left\{\sum_{n=1}^{N_t} \int_{I_n} \sum_{K\in\mathcal{T}_h} \|\varphi\|_{X,K}^2\,\mathrm{d}t\right\}^{\frac{1}{2}}, \quad \|\varphi\|_{X,K}^2 = \varepsilon h_K^{-2}\|\varphi\|_K^2 + \|\nabla\varphi\|_K^2.$$

Define continious and piecewise $\mathbb{P}_1$ in time and discontinous in space functions:

$$\underbrace{l_{c,h\tau}(\cdot,t^n) = l_{c,h}^n}_{\in\mathbb{P}_0}, \quad \underbrace{S_{h\tau}(\cdot,t^n) = S_h^n}_{\in\mathbb{P}_0}, \quad \underbrace{P_{h\tau}(\cdot,t^n) = P_h^n}_{\in\mathbb{P}_2}, \quad \underbrace{\chi_{h\tau}(\cdot,t^n) = \chi_h^n}_{\in\mathbb{P}_2}$$

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$$\int_0^{t_{\mathrm{F}}} (\partial_t l_c, \varphi)_\Omega(t)\,\mathrm{dt} - (\mathbf{\Phi}_c, \nabla\varphi)_\Omega(t)\,\mathrm{dt} - (Q_{\mathrm{c}}, \varphi)_\Omega(t)\,\mathrm{dt} = 0 \quad \forall \varphi \in X,\ c = \mathrm{w},\mathrm{h}$$

$$\int_0^{t_{\mathrm{F}}} (\lambda - (1 - S_{\mathrm{l}}), HP_{\mathrm{g}} - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}})_\Omega(t)\,\mathrm{dt} \geq 0 \quad \forall \lambda \in Z, \quad 1 - S_{\mathrm{l}} \in Z,\ c = \mathrm{w},\mathrm{h}$$

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Error measure

Dual norm of the residual for the components

$$\|\mathcal{R}_c(S_{h\tau}, P_{h\tau}, \chi_{h\tau})\|_{X'} = \sup_{\varphi \in X, \|\varphi\|_X = 1} \left| \int_0^{t_F} (Q_c - \partial_t l_{c,h\tau}, \varphi)_\Omega (t) + (\mathbf{\Phi}_{c,h\tau}, \nabla\varphi)_\Omega (t)\, \mathrm{dt} \right| .$$

Residual for the constraints

$$\mathcal{R}_e(S_{h\tau}, P_{h\tau}, \chi_{h\tau}) = \int_0^{t_F} (1 - S_{h\tau}, H\left[P_{h\tau} + P_c(S_{h\tau})\right] - \beta_l \chi_{h\tau})_\Omega (t)\, \mathrm{dt}.$$

Error measure for the nonconformity of the pressure

$$\mathcal{N}_p = \inf_{\delta_p \in X} \left\{ \sum_{c \in \mathcal{C}_p} \int_0^{t_F} \left\| \mu_p^{-1} k_{rp}(S_p) \rho_c^p \underline{\mathbf{K}} \nabla \left(P_{h\tau} - \delta_p\right)(t) \right\|^2 \mathrm{dt} \right\}^{\frac{1}{2}},$$

Error measure for nonconformity of the mole fraction

$$\mathcal{N}_\chi := \inf_{\theta \in X} \left\{ \int_0^{t_F} \left\| -M^{\mathrm{h}} S_{h\tau} \left(\rho_{\mathrm{w}}^{\mathrm{l}}/M^{\mathrm{w}} + \beta_l/M^{\mathrm{h}} \chi_{h\tau}\right) D_{\mathrm{h}}^{\mathrm{l}} \nabla(\chi_{h\tau} - \theta)(t) \right\|^2 \mathrm{dt} \right\}^{\frac{1}{2}},$$

Definition (Error measure)

$$\mathcal{N} = \left\{ \sum_{c \in \mathcal{C}} \|\mathcal{R}_c(S_{h\tau}, P_{h\tau}, \chi_{h\tau})\|_{X'}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{p \in \mathcal{P}} \mathcal{N}_p^2 + \mathcal{N}_\chi^2 \right\}^{\frac{1}{2}} + \mathcal{R}_e(S_{h\tau}, P_{h\tau}, \chi_{h\tau})$$

Raviart Thomas spaces

Definition

The lowest-order Raviart–Thomas space is defined by

$$\mathbf{RT}_0(\Omega) = \{\boldsymbol{w}_h \in \mathbf{H}(\mathrm{div},\Omega), \boldsymbol{w}_h|_K \in \mathbf{RT}_0(K)\ \forall K \in \mathcal{T}_h\}$$

$$\mathbf{RT}_0(K) = [\mathbb{P}_0(K)]^2 + \vec{\boldsymbol{x}} \cdot \mathbb{P}_0(K)$$

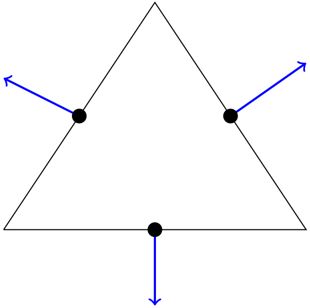


Figure: $\mathbf{RT}_0$ space.

Degrees of freedom:

$$v_j = (\boldsymbol{v}\cdot\boldsymbol{n}_{e_j}, 1)_{e_j}, \quad e_j \in \partial K, \quad j = \{1,2,3\}.$$

Phase pressure reconstruction

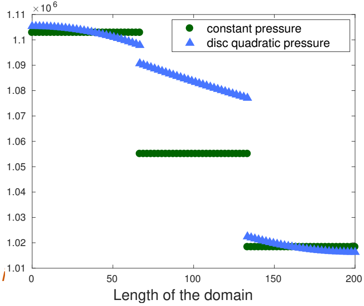
$P_K^{n,k,i}$ **constant** $\Rightarrow \nabla P_K^{n,k,i} = 0.$

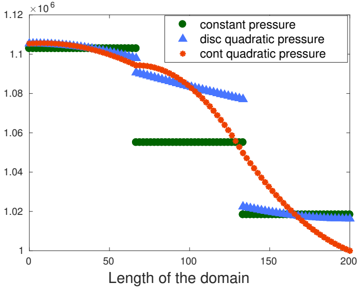
Define $\xi_{1,h}^{n,k,i} \in \mathbf{RT}_0(K)$

$$\left(\xi_{1,h}^{n,k,i} \cdot \boldsymbol{n}_K, 1\right)_\sigma = -|\sigma| \frac{P_L^{n,k,i} - P_K^{n,k,i}}{d_{KL}}$$

The **discontinuous** $\mathbb{P}_2$ liquid phase pressure $P_h^{n,k,i}$ satisfy

$$\left(-\nabla P_h^{n,k,i}\right)|_K = \left(\xi_{1,h}^n\right)_K, \quad \left(P_h^{n,k,i}, 1\right)_K = |K| P_K^{n,k,i}$$





The Oswald interpolation operator defines continous $\mathbb{P}_2$ functions:

- $I_{\rm os}(P_h^{n,k,i}) \in \mathbb{P}_2 \cap H_0^1(\Omega)$
- $I_{\rm os}(\widehat{P}_h^{n,k,i}) \in \mathbb{P}_2 \cap H_0^1(\Omega)$

Inexact semismooth Newton method

The finite volume scheme provides

$$|K|\partial_t^n l_{c,K} + \sum_{\sigma\in\mathcal{E}_K} F_{c,K,\sigma}(\boldsymbol{U}^n) = |K| Q^n_{\mathrm{h,K}},$$

Inexact semismooth linearization

$$\frac{|K|}{\Delta t}\left[l_{c,K}\left(\boldsymbol{U}^{n,k-1}\right) - l_{c,K}^{n-1} + \mathcal{L}_{c,K}^{n,k,i}\right] + \sum_{\sigma\in\mathcal{E}_K^{\mathrm{int}}} F_{c,K,\sigma}^{n,k,i} - |K| Q^n_{\mathrm{c,K}} + \boldsymbol{R}_{c,K}^{n,k,i} = 0$$

Linear perturbation in the accumulation

$$\mathcal{L}_{c,K}^{n,k,i} = \sum_{K'\in\mathcal{T}_h} \frac{|K|}{\Delta t}\frac{\partial l_{c,K}^n}{\partial \boldsymbol{U}_{K'}^n}(\boldsymbol{U}_{K'}^{n,k-1})\left[\boldsymbol{U}_{K'}^{n,k,i} - \boldsymbol{U}_{K'}^{n,k-1}\right],$$

Linearized component flux

$$F_{c,K,\sigma}^{n,k,i} = \sum_{K'\in\mathcal{T}_h} \frac{\partial F_{c,K,\sigma}}{\partial \boldsymbol{U}_{K'}^n}\left(\boldsymbol{U}^{n,k-1}\right)\left[\boldsymbol{U}_{K'}^{n,k,i} - \boldsymbol{U}_{K'}^{n,k-1}\right] + F_{c,K,\sigma}\left(\boldsymbol{U}^{n,k-1}\right).$$

Component flux reconstructions

Discretization flux reconstruction:

$$\left(\boldsymbol{\Theta}_{c,\mathrm{h,disc}}^{n,k,i} \cdot \boldsymbol{n}_K, 1\right)_\sigma = F_{c,K,\sigma}\left(\boldsymbol{U}^{n,k,i}\right) \quad \forall K \in \mathcal{T}_h$$

Linearization flux reconstruction:

$$\left(\boldsymbol{\Theta}_{c,\mathrm{h,lin}}^{n,k,i} \cdot \boldsymbol{n}_K, 1\right)_\sigma = F_{c,K,\sigma}^{n,k,i} - F_{c,K,\sigma}\left(\boldsymbol{U}^{n,k,i}\right) \quad \forall K \in \mathcal{T}_h,$$

Agebraic flux reconstruction:

$$\left(\boldsymbol{\Theta}_{c,\mathrm{h,alg}}^{n,k,i} \cdot \boldsymbol{n}_K, 1\right)_{\partial K} = -\boldsymbol{R}_{c,K}^{n,k,i} \quad \forall K \in \mathcal{T}_h$$

Total flux reconstruction:

$$\boldsymbol{\Theta}_{c,\mathrm{h}}^{n,k,i} = \boldsymbol{\Theta}_{c,\mathrm{h,disc}}^{n,k,i} + \boldsymbol{\Theta}_{c,\mathrm{h,lin}}^{n,k,i} + \boldsymbol{\Theta}_{c,\mathrm{h,alg}}^{n,k,i}$$

Proposition (Equilibration property)

$$\left(Q_{\mathrm{c,K}}^n - \frac{l_{c,K}(\boldsymbol{U}^{n,k-1}) - l_{c,K}^{n-1} + \mathcal{L}_{c,K}^{n,k,i}}{\tau_n} - \boldsymbol{\nabla} \cdot \boldsymbol{\Theta}_{c,\mathrm{h}}^{n,k,i}, 1\right)_K = 0$$

Error estimators

$$\left.\begin{aligned}
\eta_{\mathrm{R},K,c}^{n,k,i} &= \min\left\{C_{\mathrm{PW}}, \varepsilon^{-\frac{1}{2}}\right\} h_K \left\| Q_{c,h}^{n} - \frac{l_{c,K}(\boldsymbol{U}^{n,k-1}) - l_{c,K}^{n-1} + \mathcal{L}_{c,K}^{n,k,i}}{\tau_n} - \nabla\cdot\boldsymbol{\Theta}_{c,\mathrm{h}}^{n,k,i}\right\|_K \\
\eta_{\mathrm{F},K,c}^{n,k,i}(t) &= \left\|\boldsymbol{\Theta}_{c,\mathrm{h}}^{n,k,i} - \boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t)\right\|_K \\
\eta_{\mathrm{NC},K,p,c}^{n,k,i}(t) &= \left\|\frac{k_{r1}(S_1)}{\mu_1}\rho_c^p \underline{\mathbf{K}}\nabla(P_{h\tau,p}^{n,k,i} - I_{\mathrm{os}}(P_{h,p}^{n,k,i}))(t)\right\|_K \qquad t\in I_n, \\
\eta_{\mathrm{P},K,\mathrm{pos}}^{n,k,i}(t) &= \left(\left\{1 - S_{h\tau}^{n,k,i}\right\}^{+}(t), \left\{H\left[P_{h\tau}^{n,k,i} + P_c\left(S_{h\tau}^{n,k,i}\right)\right] - \beta_1\chi_{h\tau}^{n,k,i}\right\}^{+}(t)\right)_K
\end{aligned}\right\}\ \eta_{\mathrm{disc}}^{n,k,i}$$

$$\left.\begin{aligned}
\eta_{\mathrm{NA},K,c}^{n,k,i} &= \varepsilon^{-\frac{1}{2}} h_K (\tau_n)^{-1}\left\| l_{c,K}(\boldsymbol{U}^{n,k,i}) - l_{c,K}(\boldsymbol{U}^{n,k-1}) - \mathcal{L}_{c,K}^{n,k,i}\right\|_K \\
\eta_{\mathrm{P},K,\mathrm{neg}}^{n,k,i}(t) &= \left(\left\{1 - S_{h\tau}^{n,k,i}\right\}^{-}(t), \left\{H\left[P_{h\tau}^{n,k,i} + P_c\left(S_{h\tau}^{n,k,i}\right)\right] - \beta_1\chi_{h\tau}^{n,k,i}\right\}^{-}(t)\right)_K
\end{aligned}\right\}\ \eta_{\mathrm{lin}}^{n,k,i}$$

$$\eta_{\mathrm{alg,K,c}}^{n,k,i} = \left\|\boldsymbol{\Theta}_{c,\mathrm{h,alg}}^{n,k,i}\right\|_K \to \eta_{\mathrm{alg}}^{n,k,i}$$

Theorem

$$\mathcal{N}^n \le \eta_{\mathrm{disc}}^{n,k,i} + \eta_{\mathrm{lin}}^{n,k,i} + \eta_{\mathrm{alg}}^{n,k,i}$$

Error estimators

$$\left.\begin{aligned}
\eta^{n,k,i}_{\mathrm{R},K,c} &= \min\left\{C_{\mathrm{PW}}, \varepsilon^{-\frac{1}{2}}\right\} h_K \left\| Q^n_{c,h} - \frac{l_{c,K}(\boldsymbol{U}^{n,k-1}) - l^{n-1}_{c,K} + \mathcal{L}^{n,k,i}_{c,K}}{\tau_n} - \boldsymbol{\nabla}\cdot\boldsymbol{\Theta}^{n,k,i}_{c,\mathrm{h}} \right\|_K \\
\eta^{n,k,i}_{\mathrm{F},K,c}(t) &= \left\| \boldsymbol{\Theta}^{n,k,i}_{c,\mathrm{h}} - \boldsymbol{\Phi}^{n,k,i}_{c,h\tau}(t) \right\|_K \\
\eta^{n,k,i}_{\mathrm{NC},K,p,c}(t) &= \left\| \frac{k_{r\mathrm{l}}(S_\mathrm{l})}{\mu_\mathrm{l}} \rho^p_c \underline{\mathbf{K}} \boldsymbol{\nabla}(P^{n,k,i}_{h\tau,p} - I_{\mathrm{os}}(P^{n,k,i}_{h,p}))(t) \right\|_K \quad t \in I_n, \\
\eta^{n,k,i}_{\mathrm{P},K,\mathrm{pos}}(t) &= \left(\left\{1 - S^{n,k,i}_{h\tau}\right\}^+(t), \left\{ H\left[P^{n,k,i}_{h\tau} + P_c\left(S^{n,k,i}_{h\tau}\right)\right] - \beta_\mathrm{l}\chi^{n,k,i}_{h\tau}\right\}^+(t) \right)_K
\end{aligned}\right\} \eta^{n,k,i}_{\mathrm{disc}}$$

$$\left.\begin{aligned}
\eta^{n,k,i}_{\mathrm{NA},K,c} &= \varepsilon^{-\frac{1}{2}} h_K (\tau_n)^{-1} \left\| l_{c,K}(\boldsymbol{U}^{n,k,i}) - l_{c,K}(\boldsymbol{U}^{n,k-1}) - \mathcal{L}^{n,k,i}_{c,K} \right\|_K \\
\eta^{n,k,i}_{\mathrm{P},K,\mathrm{neg}}(t) &= \left(\left\{1 - S^{n,k,i}_{h\tau}\right\}^-(t), \left\{ H\left[P^{n,k,i}_{h\tau} + P_c\left(S^{n,k,i}_{h\tau}\right)\right] - \beta_\mathrm{l}\chi^{n,k,i}_{h\tau}\right\}^-(t) \right)_K
\end{aligned}\right\} \eta^{n,k,i}_{\mathrm{lin}}$$

$$\eta^{n,k,i}_{\mathrm{alg,K,c}} = \left\| \boldsymbol{\Theta}^{n,k,i}_{c,\mathrm{h,alg}} \right\|_K \to \eta^{n,k,i}_{\mathrm{alg}}$$

Theorem

$$\mathcal{N}^n \leq \eta^{n,k,i}_{\mathrm{disc}} + \eta^{n,k,i}_{\mathrm{lin}} + \eta^{n,k,i}_{\mathrm{alg}}$$

Error estimators

$$\left.\begin{aligned}
\eta_{\mathrm{R},K,c}^{n,k,i} &= \min\left\{C_{\mathrm{PW}},\varepsilon^{-\frac{1}{2}}\right\} h_K \left\| Q_{c,h}^n - \frac{l_{c,K}(\boldsymbol{U}^{n,k-1}) - l_{c,K}^{n-1} + \mathcal{L}_{c,K}^{n,k,i}}{\tau_n} - \boldsymbol{\nabla}\cdot\boldsymbol{\Theta}_{c,\mathrm{h}}^{n,k,i}\right\|_K \\
\eta_{\mathrm{F},K,c}^{n,k,i}(t) &= \left\|\boldsymbol{\Theta}_{c,\mathrm{h}}^{n,k,i} - \boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t)\right\|_K \\
\eta_{\mathrm{NC},K,p,c}^{n,k,i}(t) &= \left\|\frac{k_{r\mathrm{l}}(S_{\mathrm{l}})}{\mu_{\mathrm{l}}}\rho_c^p \underline{\mathbf{K}}\boldsymbol{\nabla}(P_{h\tau,p}^{n,k,i} - I_{\mathrm{os}}(P_{h,p}^{n,k,i}))(t)\right\|_K \qquad t\in I_n, \\
\eta_{\mathrm{P},K,\mathrm{pos}}^{n,k,i}(t) &= \left(\left\{1-S_{h\tau}^{n,k,i}\right\}^+(t), \left\{H\left[P_{h\tau}^{n,k,i}+P_c\left(S_{h\tau}^{n,k,i}\right)\right] - \beta_{\mathrm{l}}\chi_{h\tau}^{n,k,i}\right\}^+(t)\right)_K
\end{aligned}\right\}\ \eta_{\mathrm{disc}}^{n,k,i}$$

$$\left.\begin{aligned}
\eta_{\mathrm{NA},K,c}^{n,k,i} &= \varepsilon^{-\frac{1}{2}} h_K (\tau_n)^{-1}\left\| l_{c,K}(\boldsymbol{U}^{n,k,i}) - l_{c,K}(\boldsymbol{U}^{n,k-1}) - \mathcal{L}_{c,K}^{n,k,i}\right\|_K \\
\eta_{\mathrm{P},K,\mathrm{neg}}^{n,k,i}(t) &= \left(\left\{1-S_{h\tau}^{n,k,i}\right\}^-(t), \left\{H\left[P_{h\tau}^{n,k,i}+P_c\left(S_{h\tau}^{n,k,i}\right)\right] - \beta_{\mathrm{l}}\chi_{h\tau}^{n,k,i}\right\}^-(t)\right)_K
\end{aligned}\right\}\ \eta_{\mathrm{lin}}^{n,k,i}$$

$$\eta_{\mathrm{alg,K,c}}^{n,k,i} = \left\|\boldsymbol{\Theta}_{c,\mathrm{h,alg}}^{n,k,i}\right\|_K \to \eta_{\mathrm{alg}}^{n,k,i}$$

Theorem

$$\mathcal{N}^n \le \eta_{\mathrm{disc}}^{n,k,i} + \eta_{\mathrm{lin}}^{n,k,i} + \eta_{\mathrm{alg}}^{n,k,i}$$

Adaptivity

Algorithm 1 Adaptive inexact semismooth Newton algorithm

Initialization: Choose an initial vector $\boldsymbol{U}^{n,0} \in \mathcal{M}_{3N_h,1}(\mathbb{R})$, $(k=0)$

Do

$k = k+1$

Compute $\mathbb{A}^{n,k-1} \in \mathcal{M}_{3N_h,3N_h}(\mathbb{R})$, $\boldsymbol{B}^{n,k-1} \in \mathcal{M}_{3N_h,1}(\mathbb{R})$

Consider $\mathbb{A}^{n,k-1}\boldsymbol{U}^{n,k} = \boldsymbol{B}^{n,k-1}$

Initialization for the linear solver: Define $\boldsymbol{U}^{n,k,0} = \boldsymbol{U}^{n,k-1}$, $(i=0)$

Do

$i = i+1$

Compute Residual: $\boldsymbol{R}^{n,k,i} = \boldsymbol{B}^{n,k-1} - \mathbb{A}^{n,k-1}\boldsymbol{U}^{n,k,i}$

Compute estimators

While $\eta_{\text{alg}}^{n,k,i} \geq \gamma_{\text{alg}} \max\left\{\eta_{\text{disc}}^{n,k,i}, \eta_{\text{lin}}^{n,k,i}\right\}$

While $\eta_{\text{lin}}^{n,k,i} \geq \gamma_{\text{lin}}\eta_{\text{disc}}^{n,k,i}$

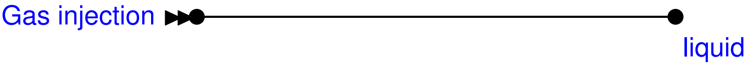
End

J. Dabaghi, V. Martin, and M. Vohralík, *Adaptive inexact semismooth Newton methods for the contact problem between two membranes.* submitted for publication, 2017.

Outline

Numerical experiments

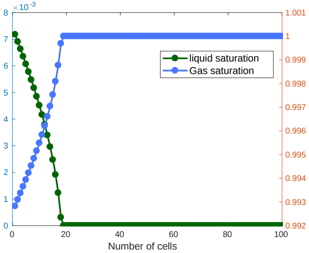
Ω: one-dimensional core with length $L = 200m$. We consider the **semismooth Newton-min solver** and assume that the algebraic solver has converged.

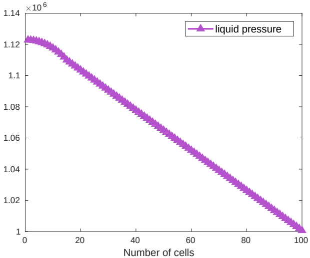


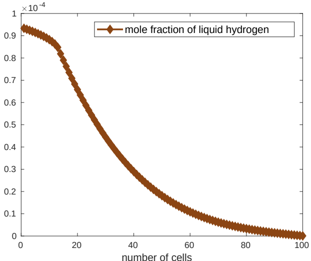
Van Genuchten–Mualem model:

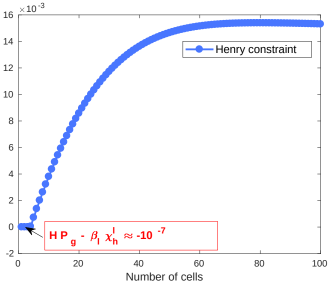
$$P_c(S_\mathrm{l}) = P_r\left(S_{le}^{-\frac{1}{m}} - 1\right)^{\frac{1}{n}}$$

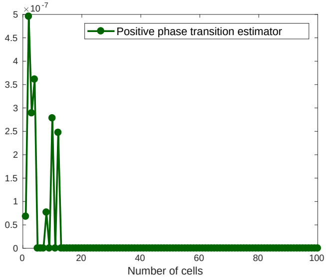
$$k_{\mathrm{rl}}(S_\mathrm{l}) = \sqrt{S_{le}}\left(1-(1-S_{le}^{\frac{1}{m}})^m\right)^2, \quad k_{\mathrm{rg}}(S_\mathrm{l}) = \sqrt{1-S_{le}}\left(1-S_{le}^{\frac{1}{m}}\right)^{2m}$$

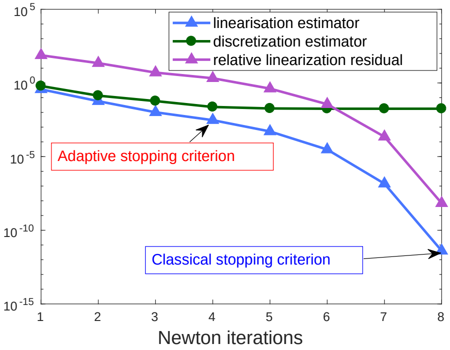







×10^-3
Henry constraint
$H P_g - \beta_l \chi_h^l \approx -10^{-7}$
Number of cells


×10^-7
Positive phase transition estimator
Number of cells


linearisation estimator
discretization estimator
relative linearization residual
Adaptive stopping criterion
Classical stopping criterion
Newton iterations

Outline

Conclusion

- We devised an a posteriori error estimate between the exact and approximate solution for a wide class of semi-smooth Newton methods.
- This estimate distinguishes the error components $\Rightarrow$ adaptive stopping criteria.
- The adaptive semismooth Newton method requires less iterations.

Ongoing work:

- Devise adaptive stopping criteria for algebraic solver
- Devise space-time adaptivity

Thank you for your attention!