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

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We develop an a-posteriori-steered algorithm for the compositional liquid-gas flow with gas appearance/disappearance in porous media. The discretization of our model is based on the backward Euler scheme in time and the finite volume scheme in space. The resulting nonlinear system is solved via an inexact semismooth Newton method. The key ingredient for the a posteriori analysis are the discretization, linearization, and algebraic flux reconstructions allowing to devise estimators for each error component. These enable to formulate criteria for stopping the algebraic and linearization solver whenever the corresponding error do not affect significantly the overall error. Numerical experiments are performed using the semismooth Newton-min algorithm and the GMRES solver.

Model problem

We consider the compositional two-phase liquid-gas flow in $(0,L)\times(0,t_{\rm F})$

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

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:

$$\mathbf{q}^{\rm l} = -\underline{\mathbf{K}}\frac{k_{\rm rl}(S^{\rm l})}{\mu_{\rm l}}\left[\nabla P^{\rm l} - \left[\rho_{\rm w}^{\rm l}+\rho_{\rm h}^{\rm l}\right]g\nabla z\right]$$
$$\mathbf{q}^{\rm g} = -\underline{\mathbf{K}}\frac{k_{\rm rg}(S^{\rm g})}{\mu_{\rm g}}\left[\nabla P^{\rm g} - \rho_{\rm h}^{\rm g}g\nabla z\right]$$

Capillary pressure:

$$P_c(S^{\rm l}) = P^{\rm g} - P^{\rm l}$$

Initial conditions: $l_c(\cdot,t^0) = l_c^0$

Unknowns: $S^{\rm l},\quad P^{\rm l},\quad \chi_{\rm h}^{\rm l}$

Closure: $S^{\rm l}+S^{\rm g} = 1$

Assumption 1. *Water incompressible only present in liquid phase and gas slightly compressible.*

Discretization and discrete complementarity constraints

Numerical solution: $U^n := (U_K^n)_{K\in\mathcal{T}_h}$, $\quad U_K^n := (S_K^n, P_K^n, \chi_K^n)$ **one value per cell**
Time discretization: $t_0 = 0 < t_1 < \cdots < t_{N_t} = t_{\rm F} = N_t\Delta t$, with constant time step Δt.
Space discretization: intervals of size h. Number of cells: $N_{\rm sp}$.
Discretization of the component equations by finite volumes:

$$\frac{l_{c,K}(U^n) - l_{c,K}(U^{n-1})}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K^{\rm int}} F_{c,K,\sigma}(U^n) - |K|Q_{c,K}^n = 0.$$

Reformulation of complementarity constraints for the two-phase model

$$1-S_K^n\geq 0,\ H(P_K^n+P_c(S_K^n))-\beta_{\rm l}\chi_K^n\geq 0,\ (1-S_K^n)^T(H(P_K^n+P_c(S_K^n))-\beta_{\rm l}\chi_K^n) = 0$$
$$\Updownarrow$$
$$\min\left(1-S_K^n, H(P_K^n+P_c(S_K^n))-\beta_{\rm l}\chi_K^n\right) = 0$$

Linearization by semismooth Newton method and algebraic solver

Linearization at semismooth step k and at step i of any algebraic solver of component equations

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

linear perturbation in the accumulation

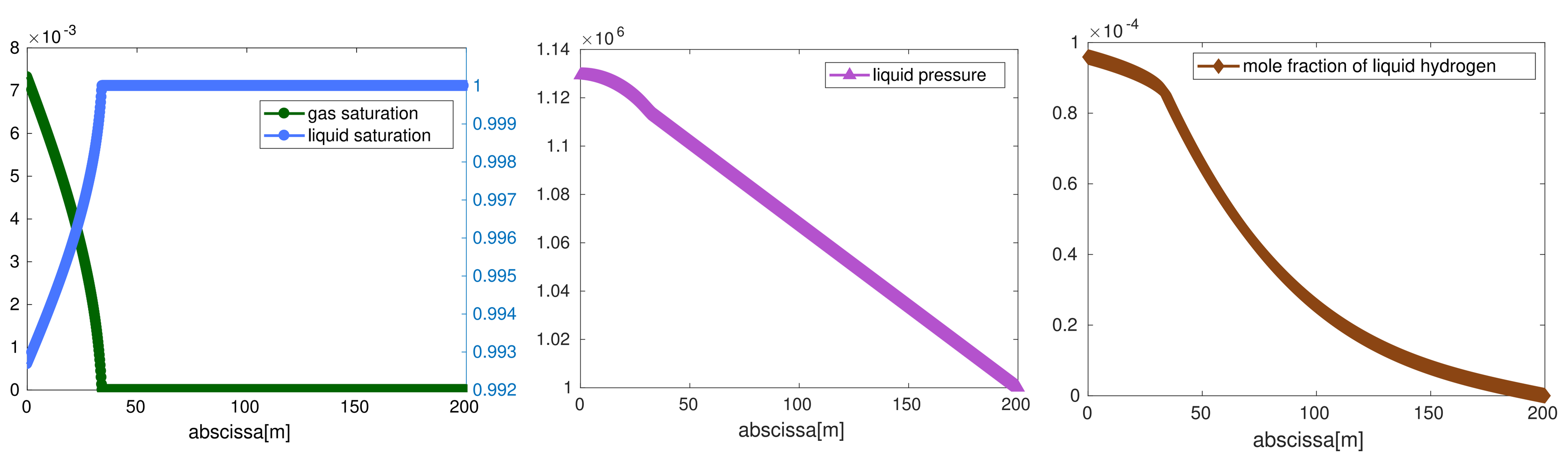
$$\mathscr{L}_{c,K}^{n,k,i} = \sum_{K'\in\mathcal{T}_h}\frac{|K|}{\Delta t}\frac{\partial l_{c,K}^n}{\partial U_{K'}^n}(U_{K'}^{n,k-1})\left[U_{K'}^{n,k,i} - U_{K'}^{n,k-1}\right]$$

linearized component flux

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

Numerical illustration

$N_{\rm sp} = 1000 \qquad t = 4.5\times 10^4$year.



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I. Ben Gharbia, J. Dabaghi, V. Martin, and M. Vohralík, *A posteriori error estimates and stopping criteria for a two-phase flow with nonlinear complementarity constraints.* In preparation, 2018.

Weak solution

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

Assumption 2 (Weak formulation)**.**

$P^{\rm l}, P^{\rm g}, \chi_{\rm h}^{\rm l}\in X,\quad S^{\rm l}, S^{\rm g}, l_{\rm w}, l_{\rm h}\in Y\quad (\Phi_{\rm w} = \rho_{\rm w}^{\rm l}\mathbf{q}^{\rm l} - \mathbf{J}_{\rm w}^{\rm l}, \Phi_{\rm h} = \rho_{\rm h}^{\rm l}\mathbf{q}^{\rm l} + \rho_{\rm h}^{\rm g}\mathbf{q}^{\rm g} - \mathbf{J}_{\rm h}^{\rm l}) \in [L^2((0,t_{\rm F});\mathbf{H}(\mathrm{div},\Omega)]^d,$

$$\int_0^{t_{\rm F}}(\partial_t l_c,\varphi)_\Omega(t)\,\mathrm{d}t - (\Phi_c,\nabla\varphi)_\Omega(t)\,\mathrm{d}t - (Q_c,\varphi)_\Omega(t)\,\mathrm{d}t = 0\quad\forall\varphi\in X,\ c = \mathrm{w},\mathrm{h},$$
$$\int_0^{t_{\rm F}}\left(\lambda - (1-S^{\rm l}), HP^{\rm g} - \beta_{\rm l}\chi_{\rm h}^{\rm l}\right)_\Omega(t)\,\mathrm{d}t\geq 0\quad\forall\lambda\in Z,\quad 1-S^{\rm l}\in Z,\ c = \mathrm{w},\mathrm{h},$$

The initial condition, the algebraic closure relation, and Darcy's law hold.

$\|\varphi\|_X = \left\{\sum_{n=1}^{N_t}\int_{I_n}\sum_{K\in\mathcal{T}_h}\left(\varepsilon h_K^{-2}\|\varphi\|_K^2 + \|\nabla\varphi\|_K^2\right)\mathrm{d}t\right\}^{\frac12}$. *Define $\mathscr{C}^0$ and piecewise $\mathbb{P}_1$ in time and discontinuous in space functions:* $\underbrace{l_{c,h\tau}^{n,k,i}(\cdot,t^n) = l_{c,h}^{n,k,i}}_{\in\mathbb{P}_0(\mathcal{T}_h)}$, $\underbrace{S_{h\tau}^{n,k,i}(\cdot,t^n) = S_h^{n,k,i}}_{\in\mathbb{P}_0(\mathcal{T}_h)}$, $\underbrace{P_{h\tau}^{n,k,i}(\cdot,t^n) = P_h^{n,k,i}}_{\in\mathbb{P}_2(\mathcal{T}_h)}$, $\underbrace{\chi_{h\tau}^{n,k,i}(\cdot,t^n) = \chi_h^{n,k,i}}_{\in\mathbb{P}_2(\mathcal{T}_h)}$

Error measure

Dual norm of the residual for the components

$$\left\|\mathscr{R}_c(S_{h\tau}^{n,k,i},P_{h\tau}^{n,k,i},\chi_{h\tau}^{n,k,i})\right\|_{X'} = \sup_{\varphi\in X,\|\varphi\|_X=1}\left|\int_0^{t_{\rm F}}\left(Q_c - \partial_t l_{c,h\tau}^{n,k,i},\varphi\right)_\Omega(t) + \left(\Phi_{c,h\tau}^{n,k,i},\nabla\varphi\right)_\Omega(t)\,\mathrm{d}t\right|.$$

Residual for the constraints

$$\mathscr{R}_{\rm e}(S_{h\tau}^{n,k,i},P_{h\tau}^{n,k,i},\chi_{h\tau}^{n,k,i}) = \int_0^{t_{\rm F}}\left(1-S_{h\tau}^{n,k,i}, H\left[P_{h\tau}^{n,k,i}+P_c(S_{h\tau}^{n,k,i})\right] - \beta_{\rm l}\chi_{h\tau}^{n,k,i}\right)_\Omega(t)\,\mathrm{d}t.$$

Distance of the pressure $P_{h\tau}^{n,k,i}$ to the space X (nonconformity of the pressure)

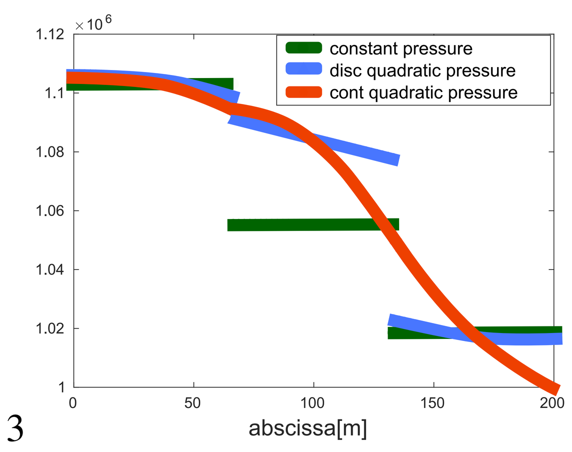
$$\mathcal{N}_p^{n,k,i} = \inf_{\delta_p^{n,k,i}\in X}\left\{\sum_{c\in\mathscr{C}_p}\int_0^{t_{\rm F}}\left\|\mu_p^{-1}k_{rp}(S^p)\rho_c^p\underline{\mathbf{K}}\nabla\left(P_{h\tau}^{n,k,i} - \delta_p^{n,k,i}\right)(t)\right\|^2\mathrm{d}t\right\}^{\frac12},$$

Distance of the mole fraction $\chi_{h\tau}^{n,k,i}$ to the space X (nonconformity of the mole fraction)

$$\mathcal{N}_\chi^{n,k,i} := \inf_{\theta^{n,k,i}\in X}\left\{\int_0^{t_{\rm F}}\left\|-M^{\rm h}S_{h\tau}^{n,k,i}\left(\rho_{\rm w}^{\rm l}/M^{\rm w} + \beta_{\rm l}/M^{\rm h}\chi_h^{n,k,i}\right)D_{\rm h}^{\rm l}\nabla(\chi_{h\tau}^{n,k,i} - \theta^{n,k,i})(t)\right\|^2\mathrm{d}t\right\}^{\frac12},$$

Error measure $\mathcal{N}^{n,k,i} := \left\{\sum_{c\in\mathscr{C}}\left\|\mathscr{R}_c(S_{h\tau}^{n,k,i},P_{h\tau}^{n,k,i},\chi_{h\tau}^{n,k,i})\right\|_{X'}^2\right\}^{\frac12} + \left\{\sum_{p\in\mathscr{P}}(\mathcal{N}_p^{n,k,i})^2 + (\mathcal{N}_\chi^{n,k,i})^2\right\}^{\frac12} + \mathscr{R}_{\rm e}(S_{h\tau}^{n,k,i},P_{h\tau}^{n,k,i},\chi_{h\tau}^{n,k,i}).$

Reconstruction



$N_{\rm sp} = 3$

Component flux reconstruction

Discretization flux: $\left(\Theta_{c,h,\mathrm{disc}}^{n,k,i}\cdot n_K,1\right)_\sigma = F_{c,K,\sigma}(U^{n,k,i})$,

Linearization flux: $\left(\Theta_{c,h,\mathrm{lin}}^{n,k,i}\cdot n_K,1\right)_\sigma = F_{c,K,\sigma}^{n,k,i} - F_{c,K,\sigma}(U^{n,k,i})$,

Algebraic flux: $\left(\Theta_{c,h,\mathrm{alg}}^{n,k,i}\cdot n_K,1\right)_{\partial K} = -R_{c,K}^{n,k,i}$,

Total flux: $\Theta_{c,h}^{n,k,i} = \Theta_{c,h,\mathrm{disc}}^{n,k,i} + \Theta_{c,h,\mathrm{lin}}^{n,k,i} + \Theta_{c,h,\mathrm{alg}}^{n,k,i}$.

Error estimators

Discretization estimators

$$\eta_{\mathrm{F},K,c}^{n,k,i}(t) = \left\|\Theta_{c,h}^{n,k,i} - \Phi_{c,h\tau}^{n,k,i}(t)\right\|_K,\quad \eta_{\mathrm{P},K,\mathrm{pos}}^{n,k,i}(t) = \left(\left\{1-S_{h\tau}^{n,k,i}\right\}^+(t), \left\{H\left[P_{h\tau}^{n,k,i}+P_c\left(S_{h\tau}^{n,k,i}\right)\right] - \beta_{\rm l}\chi_{h\tau}^{n,k,i}\right\}^+(t)\right)_K,$$

$$\eta_{\mathrm{R},K,c}^{n,k,i} = \min\left\{C_{\rm PW},\varepsilon^{-\frac12}\right\}h_K\left\|Q_{c,h}^n - \frac{l_{c,K}(U^{n,k-1}) - l_{c,K}^{n-1} + \mathscr{L}_{c,K}^{n,k,i}}{\tau_n} - \nabla\cdot\Theta_{c,h}^{n,k,i}\right\|_K,$$

$$\eta_{\mathrm{NC},K,p,c}^{n,k,i}(t) = \left\|\frac{k_{rl}(S^{\rm l})}{\mu_{\rm l}}\rho_c^p\underline{\mathbf{K}}\nabla(P_{h\tau,p}^{n,k,i} - I_{\rm os}(P_{h,p}^{n,k,i}))(t)\right\|_K,$$

Linearization estimators

$$\eta_{\mathrm{NA},K,c}^{n,k,i} = \varepsilon^{-\frac12}h_K(\tau_n)^{-1}\left\|l_{c,K}(U^{n,k,i}) - l_{c,K}(U^{n,k-1}) - \mathscr{L}_{c,K}^{n,k,i}\right\|_K,$$

$$\eta_{\mathrm{P},K,\mathrm{neg}}^{n,k,i}(t) = \left(\left\{1-S_{h\tau}^{n,k,i}\right\}^-(t), \left\{H\left[P_{h\tau}^{n,k,i}+P_c\left(S_{h\tau}^{n,k,i}\right)\right] - \beta_{\rm l}\chi_{h\tau}^{n,k,i}\right\}^-(t)\right)_K,$$

Algebraic estimator

$$\eta_{\mathrm{alg},K,c}^{n,k,i} = \left\|\Theta_{c,h,\mathrm{alg}}^{n,k,i}\right\|_K,\qquad \mathcal{N}^{n,k,i}\leq\eta_{\rm disc}^{n,k,i} + \eta_{\rm lin}^{n,k,i} + \eta_{\rm alg}^{n,k,i}$$

Adaptivity

Stopping criterion algebraic solver: $\eta_{\rm alg}^{n,k,i}\leq\gamma_{\rm alg}\max\left\{\eta_{\rm disc}^{n,k,i},\eta_{\rm lin}^{n,k,i}\right\}$

Stopping criterion linear solver: $\eta_{\rm lin}^{n,k,i}\leq\gamma_{\rm lin}\eta_{\rm disc}^{n,k,i}$